GEORGIA INSTITUTE OF TECHNOLOGY **OFFICE OF CONTRACT ADMINISTRATION**

PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. ____

Project No. G-37-605 GIT DATE 1/6/84

Project Director: E M Harrell MISC School/~~Lab~~ MATH

Sponsor: Alfred P. Sloan Foundation, 650 Fifth Avenue, New York, N.Y. 10111

Type Agreement: Grant No. BR-2347

Award Period: From 9-16-83 To 9-15-87 (Performance) 11-15-85 (Reports)

Sponsor Amount:

	This Change	Total to Date
Estimated:	$	$ 25,000
Funded:	$	$ 12,500

Cost Sharing Amount: $ None Cost Sharing No: ____

Title: Research Fellowship for Dr E. M. Harrell

ADMINISTRATIVE DATA OCA Contact Don Hasty

1) Sponsor Technical Contact:

2) Sponsor Admin/Contractual Matters:

Mrs Margaret Borst
Fellowships for Basic Research
Alfred P. Sloan Foundation

Defense Priority Rating: N/A

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(or) Company/Industrial Proprietary: N/A

RESTRICTIONS

See Attached N/A Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval – Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with N/A – None authorized

COMMENTS:

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SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

88-781

Date November 4, 1987

Project No. G-37-605

School/Lab Mathematics

Includes Subproject No.(s) N/A

Project Director(s) E. M. Harrell GTRC/GIT

Sponsor Alfred P. Sloan Foundation / New York, NY

Title Research Fellowship for Dr. E. M. Harrell

Effective Completion Date: 9/15/87 (Performance) 11/15/87 (Reports)

Grant/Contract Closeout Actions Remaining:

- [ ] None
- [x] Final Invoice or Final Fiscal Report
- [ ] Closing Documents
- [ ] Final Report of Inventions
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- [ ] Classified Material Certificate
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NEW YORK, N. Y. 10111

FELLOWSHIPS FOR BASIC RESEARCH — PROGRAM ADMINISTRATOR

May 15, 1985

G-37-605

Professor Evans M. Harrell II
School of Mathematics
Georgia Institute of Technology
Atlanta, GA 30332

Dear Professor Harrell:

This is a reminder that the scheduled termination date of your Sloan Research Fellowship is September 15, 1985 If you anticipate having unexpended funds as of that date, you may request an extension by writing to me. Please note that extensions are limited to a maximum of two years. After that, unexpended funds greater than $100 must be returned to the Foundation. Unused funds amounting to $100 or less should be retained and made available for your use or for your institution's general purposes.

I also wish to remind you that the conditions of the grant state, "The Alfred P. Sloan Research Fellow will provide the Foundation with a short annual scientific progress report and a final report which briefly describes the results accomplished with the aid of the grant. Reprints or preprints of scientific papers will be accepted in lieu of ~~such~~ reports." Your reports should reach me no later than November 15 each year for as long as your fellowship remains ~~active~~.

Sincerely,

Maureen Gassman
Administrative Assistant

G-37-605

School of Mathematics
Georgia Institute of Technology
Atlanta GA 30332-0160
404 233 3381
404 894 2715

October 10, 1985

The Alfred P. Sloan Foundation
630 Fifth Ave.
New York NY 10111-0242

Dear Sir or Madam:

Please accept the enclosed papers in lieu of a formal report of my progress during the second year of my Sloan fellowship.

Allow me again to express my gratitude for your very valuable assistance, and also for your unburdensome reporting requirements.

Sincerely yours,

Evans M. Harrell II

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sent

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The $1/R$ Expansion for H_2^+: Analyticity, Summability, and Asymptotics

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Received January 14, 1985

It is proved that the $1/R$ expansion for H_2^+ is divergent and Borel summable to a complex eigenvalue of a non-self-adjoint operator, which has the same $1/R$ expansion. The Borel sum is related to the H_2^+ system as follows: its real part agrees with the eigenvalue doublet asymptotically to all orders, and its imaginary part determines the asymptotics of the $1/R$ expansion coefficients via a dispersion relation. A rigorous estimate of the leading behavior of the imaginary part is obtained, and as a consequence the approximate formula of Brézin and Zinn-Justin relating the square of the eigenvalue gap to the asymptotics of the $1/R$ expansion is put on a rigorous basis. © 1985 Academic Press, Inc.

Contents. I. Introduction. II. Separated equations and perturbation theory. III. Stability, analyticity, and summability. IV. Imaginary parts, asymptotics, and the formula of Brézin and Zinn-Justin. Appendix A. Appendix B. List of symbols

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I. INTRODUCTION

Consider the two-center problem of an electron in the field of two fixed point charges Z_A, Z_B at a distance R apart. In non-relativistic quantum mechanics its Hamiltonian is

$$H(R, Z_A, Z_B) = -\tfrac{1}{2}\Delta - Z_A|x|^{-1} - Z_B|x - R\hat{e}|^{-1} \qquad (1.1)$$

in atomic units, with $x \in \mathbb{R}^3$, $\hat{e} = (1, 0, 0)$. If $Z_A = Z_B = 1$ this describes the hydrogen molecular ion H_2^+ in the clamped nuclei approximation, which is an important double-well problem having the virtue of being separable. In the normalization of (1.1) the formal limit as $R \to \infty$ is the Hamiltonian of hydrogen.

The series in negative powers of R obtained by expanding $|x - R\hat{e}|^{-1}$ and applying Rayleigh-Schrödinger perturbation theory exists, is called the $1/R$ expansion, and is a classic textbook example [1]. However, (1.1) also furnishes a classic example of unstable perturbation: although the H_2^+ eigenvalues approach those of hydrogen as $R \to \infty$ (first proved by Aventini and Seiler [2]), and the rate of convergence is correctly described by the asymptotic $1/R$ expansion (Morgan and Simon [3]), they are doubly asymptotically degenerate as $R \to \infty$. That is, near any given bound state of H, for $1/R$ small enough there are two bound states of H_2^+ with an energy gap of order $R^{2k+1} \exp(-R/n)$, where n and k are the usual principal and parabolic quantum numbers [1].

The instability is a double-well phenomenon, (1.1) being somewhat analogous to the one-dimensional double-well anharmonic oscillator $p^2 + x^2(1 + gx)^2$. It is similarly clear that the $1/R$ expansion cannot be Borel summable to an eigenvalue. How could the series decide which eigenvalue to sum to? Numerically, the series has been found [3] to be factorially divergent with coefficients of one sign, in analogy to the double-well oscillator [4].

In addition, it has been discovered by Brézin and Zinn-Justin [5], also numerically, that the square of the gap between the eigenvalue doublet converging to the hydrogen ground state is related to the asymptotics of the $1/R$ expansion. This typical non-perturbative tunneling quantity, $O(R^2 e^{-2R})$ for the ground state, is reminiscent of the resonance width in the Lo Surdo-Stark effect, for which a one-to-one relationship with the perturbation series has been proved and exploited [6, 31]. That proof was based on the Borel summability of the perturbation series to the resonance [7]. More specifically, the imaginary part of the Borel sum determines the asymptotics of the perturbation series and, conversely, the asymptotic behavior of the series determines the leading behavior of the imaginary part of the sum. In the case of the Lo Surdo-Stark effect the Borel sum is a resonance in the standard sense of dilatation analyticity [7-10]. Although the imaginary part of the double-well oscillator eigenvalue does not seem to have a physical interpretation as a resonance, it determines the eigenvalue gap asymptotically [11].

The purpose of this paper is to show these phenomena rigorously in the case of the $1/R$ expansion of H_2^+. We will prove that the Borel sum of the $1/R$ expansion exists as the complex eigenvalue of a non-self-adjoint problem that has the same

$1/R$ expansion as H_2^+ but is stable as $R \to \infty$. The imaginary part of the Borel sum determines the asymptotics of the perturbation coefficients and conversely. (For a general overview of this kind of result for the anharmonic oscillator and the Lo Surdo-Stark effect, see Simon [12].) Furthermore, we derive rigorously the asymptotic form of the imaginary part of the Borel sum, which verifies the approximate formula of Brézin and Zinn-Justin. Notice that the $1/R$ expansion not only determines the position of the H_2^+ doublet asymptotically, but also the gap to leading order.

Although this result is closely analogous to the ones for the double-well oscillator and the Lo Surdo-Stark effect mentioned above, it requires a more subtle analysis, looking into the relationship between H_2^+ and the system of an electron in the field of a stationary proton and a stationary anti-proton,

$$H'(R, Z_A, -Z_A) = -\tfrac{1}{2}\Delta - Z_A|x|^{-1} + Z_A|x + R\hat{e}|^{-1} \qquad (1.2)$$

(in [14] H' was denoted K) the $1/R$ expansion of which is identical to that of H_2^+ but with R replaced by $-R$, so that the signs alternate. A plausible starting point of the analysis would be to prove Borel summability of eigenvalues of (1.2) and then analytically continue from $-R$ to $+R$, where they should develop a branch cut and thus an imaginary part. However, we shall see that although (1.2) is a stable, single-well problem, its alternating-sign $1/R$ expansion is not Borel summable to its eigenvalues, thus answering in the negative a question raised by Morgan and Simon [3]. Incidentically, we remark that this is, to our knowledge, the only example of this type which has a direct physical interest.

The identification of the Borel sum will involve relating (1.1) and (1.2) in a more subtle way, using the separability in elliptic coordinates to be implemented in Section II, which also contains a detailed description of the generation of the $1/R$ expansion from the separated equations. In Section III we shall describe the stability, analyticity, and implicit funtion arguments which, together with the remainder estimates, allow the Borel sum to be identified as a function holomorphic in some half-disk $|1/R| < M$, Im $R > 0$, which admits analytic continuation across the branch cut along the real axis (Theorem III.2). In Section IV we shall determine the leading exponential order of the imaginary part of the Borel sum (Theorem IV.1) and establish the dispersion relation connecting it to the asymptotics of the $1/R$ expansion. The proof of the Brézin-Zinn-Justin formula (Corollary IV.2) will then be a simple consequence of this and the known estimates of the eigenvalue gap [13]. Finally, we collect some technical lemmas on Borel summability of composed and implicit function in Appendix A and the JWKB estimates of the tunneling factors needed to estimate imaginary parts in Appendix B.

We conclude this Introduction by mentioning that this work represents the first of the two papers announced in Ref. [14], in which part of the above results are briefly described together with a semiclassical procedure for generating all exponentially small corrections to the $1/R$ expansion for the bound states of H_2^+.

II. Separated Equations and Perturbation Theory

Let us begin by collecting some well-known relevant facts about the family of Schrödinger operators describing the general two-center problem. Since, as will become evident, the natural variable is $\rho = 1/R$ rather than R, the operator (1.1) will henceforth be denoted $H(\rho, Z_A, Z_B)$. Unless otherwise specified, the operator-theoretic notation used throughout this paper is that of Reed and Simon [15].

Proposition II.1. *Let $\rho^{-1} = R > 0$, and $Z_A, Z_B \in \mathbb{R}$. Let $H(\rho, Z_A, Z_B)$ denote the family of operators on $L^2(\mathbb{R}^3)$ defined as the action of $-\frac{1}{2}\Delta - Z_A|x|^{-1} - Z_B|x - R\hat{e}|^{-1}$ on the domain of definition $H^2(\mathbb{R}^3)$ (Sobolev space), and let $H_0(Z_A)$ denote the hydrogen operator, i.e., the action of $-\frac{1}{2}\Delta - Z_A|x|^{-1}$ on the same domain. Then:*

(1) *$H(\rho, Z_A, Z_B)$ is self-adjoint and bounded below.*

(2) $\sigma_{ess}(H(\rho, Z_A, Z_B)) = \sigma_{ac}(H(\rho, Z_A, Z_B)) = [0, +\infty)$.

(3) *Let $E(\rho, Z_A, Z_B)$ be an eigenvalue of $H(\rho, Z_A, Z_B)$. Then $\rho \mapsto E(\rho, \cdot)$ is continuous, and $\lim_{\rho \to 0} E(\rho, \cdot)$ exists and is an eigenvalue of $H_0(Z_A)$ if $Z_A > 0$.*

(4) *If $Z_A > 0$, $Z_B < 0$, the eigenvalues of $H_0(Z_A)$ are stable (in the sense of Kato [16, Sect. VIII.1.4]) for $\rho > 0$ small.*

(5) *Fix $Z_A = Z_B > 0$, and recall that the eigenvalues of $H_0(Z_A)$ are $-Z_A^2/2n^2$, $n = 1, 2, \ldots$, with multiplicities n^2. For each such unperturbed eigenvalue and any open interval I containing only that unperturbed eigenvalue, there exists $M > 0$ such that for $\rho < M$ there are precisely $2n^2$ eigenvalues in I. The cluster of eigenvalues in I is organized in exponentially close pairs, and the two eigenvalues $E_\pm$ near $-Z_A^2/2$ in particular satisfy*

$$\Delta E(\rho, Z_A) \equiv E_+(\rho, Z_A) - E_-(\rho, Z_A) = O(Re^{-R}).$$

(6) *The Rayleigh–Schrödinger perturbation expansion in powers of ρ near $E_0(Z_A)$ in (5) exists and represents an asymptotic expansion for both eigenvalues $E_\pm(\rho, \cdot)$ as $\rho \to 0$.*

Remarks. (1) For the general analysis of the operator family $H(\rho, Z_A, Z_B)$ and in particular for the proof of (1)–(3), see Aventini and Seiler [2], Combes, Duclos, and Seiler [17], and Morgan and Simon [3]. The proof of (4) is briefly sketched in Proposition III.1 (2) as an easy application of the Hunziker–Vock [18] stability theorem. A proof of (5) has been given by Harrell [14] with some explicit estimates, and (6) has been proved by Morgan and Simon [3].

(2) The perturbation expansion is generated as follows (see, e.g., Morgan and Simon [3]): for $|x| < R$, we have $|x - R\hat{e}|^{-1} = \sum_{n=0}^{\infty} M_n(x) R^{-n-1}$, $M_n(x) = |x|^n P_n(\cos\theta)$, $\cos\theta = \langle x, \hat{e}\rangle/|x|$, where $P_n(\cdot)$ is the nth Legendre polynomial. Then the unperturbed operator is $H_0(Z_A)$, and the perturbation is by definition $-Z_B \sum_{n=0}^{\infty} M_n(x) \rho^{n+1}$, $|x| < \rho^{-1}$; 0, $|x| \geq \rho^{-1}$. The expansion obtained through

ordinary Rayleigh–Schrödinger perturbation theory in $\rho = 1/R$ near $E(Z_A)$ is by definition the $1/R$ expansion.

(3) The Hamiltonian for H_2^+ is completely decomposed by the magnetic and parabolic quantum numbers, conventionally denoted respectively by integers m, $n_1 = j \geq 0$ and $n_2 = k \geq 0$. The separability in elliptic coordinates detailed below implies that in any subspace of given m, j, k the eigenvalues of $H(\rho, Z_A)$ come in asymptotically degenerate doublets for ρ sufficiently small, and gap estimates and asymptotic expansions analogous to those of (5) and (6) hold. The precise statements will be formulated below.

The well-known separability of $H(\rho, Z_A, Z_B)$ in elliptic (more precisely, prolate spheroidal) coordinates goes back to Jacobi [19], who discovered its classical analogue to prove the complete integrability of the corresponding Hamilton–Jacobi equation. A thorough discussion of this problem and of its application to the Bohr–Sommerfeld quantization can be found in Born [20] (see also Strand and Reinhardt [21] for a modern analysis of the Bohr–Sommerfeld theory of H_2^+). Let us now review the formulation of the Schrödinger eigenvalue problem $H(\rho, Z_A, Z_B)\Psi = E\Psi$ in elliptic coordinates. Standard references for this are Landau and Lifshitz [1] and Komarov *et al.* [22]. Set

$$\begin{aligned} \xi &= \rho(|x| + |x - R\hat{e}|), & 1 \leq \xi \leq +\infty, \\ \eta &= \rho(|x| - |x - R\hat{e}|), & -1 \leq \eta \leq 1, \\ \phi &= \arctan(x_3/x_2), & 0 \leq \phi < 2\pi, \end{aligned} \tag{2.1}$$

inverted as

$$\begin{aligned} x_1 &= R\xi\eta, \\ x_2 &= R\sqrt{(1-\eta^2)(\xi^2-1)}\cos\phi, \\ x_3 &= R\sqrt{(1-\eta^2)(\xi^2-1)}\sin\phi. \end{aligned} \tag{2.2}$$

Since the Laplace operator in the variables (ξ, η, ϕ) has the form

$$\Delta = 4\rho^2(\xi^2 - \eta^2)^{-1}\left[\frac{\partial}{\partial\xi}(\xi^2 - 1)\frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta}(1 - \eta^2)\frac{\partial}{\partial\eta} + \frac{\xi^2 - \eta^2}{(\xi^2 - 1)(1 - \eta^2)}\frac{\partial^2}{\partial\phi^2}\right)$$

(see, e.g., Magnus Oberhettinger and Soni [23]), setting

$$\Psi(x) = e^{im\phi}\Phi_1(\xi)\,\Phi_2(\eta), \qquad \pm m = 0, 1, 2, \ldots, \tag{2.3}$$

we formally see that Ψ satisfies $H(\rho, Z_A, Z_B)\Psi = E\Psi$ iff

$$\left[-\frac{1}{2}\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi}-\frac{1}{4}R^2E(\xi^2-1)-\frac{1}{2}R(Z_A+Z_B)\xi + \frac{1}{2}m^2(\xi^2-1)^{-1}\right]\Phi_1(\xi) = -\alpha\Phi_1(\xi),$$
$$\left[-\frac{1}{2}\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta}-\frac{1}{4}R^2E(1-\eta^2)+\frac{1}{2}R(Z_A-Z_B)\eta + \frac{1}{2}m^2(1-\eta^2)^{-1}\right]\Phi_2(\eta) = \alpha\Phi_2(\eta) \tag{2.4}$$

for some separation constant $\alpha(m, R)\in\mathbb{R}$. The rest of this section is devoted to implementing this formal procedure so as to make transparent at the same time how the $1/R$ expansion is generated within the context of the separated equations. Set

$$E = \tfrac{1}{2}\gamma^{-2}, \qquad r = R\gamma^{-1}, \qquad \tau = r^{-1},$$
$$\beta_1 = \tfrac{1}{2}\gamma(Z_A+Z_B)-\alpha\tau, \qquad \beta_2 = \tfrac{1}{2}\gamma(Z_A-Z_B)+\alpha\tau \tag{2.5}$$

and note the relations

$$\beta_1+\beta_2 = \gamma Z_A; \qquad \tfrac{1}{2}\gamma(Z_A+Z_B)+\alpha\tau = \gamma(Z_A+Z_B)-\beta_1;$$
$$\tfrac{1}{2}\gamma(Z_A-Z_B)-\alpha\tau = \gamma(Z_A-Z_B)-\beta_2. \tag{2.6}$$

Then, upon first rescaling the unknown functions

$$\Phi_1(\xi)\mapsto(\xi^2-1)^{-1/2}\Phi_1(\xi), \qquad \Phi_2(\eta)\mapsto(1-\eta^2)^{-1/2}\Phi_2(\eta) \tag{2.7}$$

and then translating and rescaling the variables ξ and η,

$$u = r(\xi-1), \qquad v = r(\eta+1), \tag{2.8}$$

Eqs. (2.1) become

$$t_m(\beta_1, \beta_2, Z_A; Z_B, \tau)\, f(u) = 0,$$
$$s_m(\beta_1, \beta_2, Z_A, Z_B, \tau)\, g(v) = 0, \tag{2.9}$$

where

$$f(u) = [(\tau u+1)^2-1]^{1/2}\Phi_1(\tau u+1),$$
$$g(v) = [1-(\tau v-1)^2]^{1/2}\Phi_2(\tau v-1), \tag{2.10}$$

$$t_m(\cdot) = -\frac{d^2}{du^2}+\frac{1}{4}-\frac{\beta_1}{u}+\frac{m^2-1}{4u^2} + \left[-\frac{(\beta_1+\beta_2)Z_A^{-1}(Z_A+Z_B)-\beta_1}{u+2r}+\frac{m^2-1}{4}\left(\frac{1}{(u+2r)^2}-\frac{1}{u(u+2r)}\right)\right],$$
$$0\leqslant u< +\infty, \tag{2.11}$$

$$s_m(\cdot) = -\frac{d^2}{dv^2}+\frac{1}{4}-\frac{\beta_2}{v}-\frac{m^2-1}{4v^2} + \left[-\frac{\beta_2-Z_A^{-1}(Z_A-Z_B)(\beta_1+\beta_2)}{2r-v}+\frac{m^2-1}{4}\left(\frac{2}{v(2r-v)}+\frac{1}{(2r-v)^2}\right)\right],$$
$$0\leqslant v\leqslant 2r \tag{2.12}$$

(u and v were called x_1 and x_2 in [14]). We then have

PROPOSITION II.2. *For* $\pm m = 0, 1, 2, \ldots$, *let* $T_m(\beta_1, \beta_2, Z_A, Z_B, \tau)$, $S_m(\beta_1, \beta_2, Z_A, Z_B, \tau)$, $(\beta_1, \beta_2, Z_B)\in\mathbb{R}$, $(Z_A, \tau)\in\mathbb{R}^+$ *be the operator families in* $L^2(0, \infty)$, $L^2(0, 2r)$, *respectively, defined as the action of* $t_m(\cdot)$ *on* $D(T_m(\cdot)) = \{H^2(0, \infty)\cap H_0^1[0, \infty), |m|>0; H^2(0, +\infty)$ *with the boundary condition* $f(u) = O(u^{1/2})$ *as* $u\downarrow 0$ *for* $m=0\}$, $D(S_m(\cdot)) = \{H^2(0, 2r)\cap H_0^1[0, 2r], |m|>0; H^2(0, 2r)$ *with boundary conditions* $f(v) = O(v^{1/2})$, $v\downarrow 0$, $f(v) = O((2r-v)^{1/2})$, $v\uparrow 2r$, *for* $m=0\}$, *respectively. Then*:

(1) $T_m(\cdot)$, $S_m(\cdot)$ *are self-adjoint and bounded below.*

(2) $\sigma_{ess}(T_m(\cdot)) = \sigma_{ac}(T_M(\cdot)) = [\frac{1}{4}, +\infty)$; $\sigma_{ess}(S_M(\cdot)) = \phi$.

(3) *For any fixed* (m, j, k) *the eigenvalues* $\lambda(m, j, k;\ \beta_1, \beta_2, Z_A, Z_B, \tau)$ *of* $T_m(\cdot)$ *and* $\mu(m, k; \beta_1, \beta_2; Z_A, Z_B; \tau)$ *of* $S_m(\cdot)$ *are jointly continuously locally differentiable functions of the variables* $(\beta_1, \beta_2, Z_A, Z_B, \tau)$.

(4) *Assume that the equation* $\mu(m, k; \beta_1, \beta_2, Z_A, Z_B, \tau) = 0$ *can be solved near any given* $\bar\tau>0$ *to yield a family of locally* C^1 *implicit functions* $\tau\mapsto\beta_2(m, k; \beta_1, Z_A, Z_B, \tau)$, $(m, k; \beta_1, Z_A, Z_B)$ *fixed, and that the equation* $\lambda(m, j; \beta_1, \beta_2(m, k; \beta_1, Z_A, Z_B; \tau); Z_A, Z_B, \tau) = 0$ *can be similarly solved to yield a family of locally* C^1 *implicit functions* $\tau\mapsto\beta_1(m, j, k; Z_A, Z_B; \tau)$, (m, j, k), (Z_A, Z_B) *fixed. Set*

$$\gamma(m, j, k; Z_A, Z_B, \tau) = Z_A^{-1}[\beta_1(\cdot, \tau)+\beta_2(\cdot, \beta_1(\cdot, \tau), \cdot, \tau)] \tag{2.13}$$

and assume that $\tau\mapsto\gamma(\cdot, \tau)^{-1}\tau$ *is locally invertible near any given* $\tau>0$, (m, j, k), (Z_A, Z_B) *fixed. Let* $\rho\mapsto\Gamma(m, j, k;\ Z_A, Z_B; \rho)$ *be the inverse function of* $\tau\mapsto\gamma(\cdot, \tau)^{-1}\tau$. *Then the function*

$$E(m, j, k; Z_A, Z_B, \rho) = -\frac{Z_A^2}{2}[\gamma(m, j, k; Z_A, Z_B; \Gamma(m, j, k; Z_A, Z_B; \rho))]^{-2} \tag{2.14}$$

is an eigenvalue of $H(\rho, Z_A, Z_B)$.

(5) *Conversely, let* $\rho \mapsto E(\rho, Z_A, Z_B)$ *be an eigenvalue of* $H(\rho, Z_A, Z_B)$. *Then for one and only one triple* (m, j, k), $\pm m, j, k = 0, 1, \ldots$, *the equations* $\lambda(m, j, k; \beta_1, \beta_2, Z_A, Z_B, \tau) = 0$, $\mu(m, j, k; \beta_1, \beta_2, Z_A, Z_B; \tau) = 0$ *can be solved near any given* $\bar{\tau} > 0$ *to yield the pair of locally* C^1 *implicit functions* $\tau \mapsto \beta_2(m, k; \beta_1, Z_A, Z_B, \tau)$, $\tau \mapsto \beta_1(m, j, k; Z_A, Z_B, \tau)$ *such that* $\tau\gamma(m, j, k; Z_A, Z_B, \tau)^{-1}$, γ *defined by* (2.13), *is invertible and* $E(\rho, Z_A, Z_B)$ *admits the representation* (2.14).

Remarks. (1) Assertion (4) holds unchanged if the implicit functions are unraveled in the opposite order.

(2) The numbers (m, j, k) have the meaning of magnetic and parabolic quantum numbers, respectively. In fact, letting $R \to \infty$ in (2.1) we have

$$R\xi - R = |x| - x_1 + O(\rho), \qquad R\eta + R = |x| + x_1 + O(\rho),$$

which means that ξ and η become the usual parabolic coordinates (see, e.g., Landau and Lifshitz [1, Sect. 37]) up to rescaling and translation. Therefore, the natural number $n = |m| + j + k + 1$ has the meaning of principal quantum number.

(3) For $\tau = 0$ we recover the unperturbed operator $H_0(Z_A)$ in the following way: denote by t^0_m the differential expression obtained by setting formally $\tau = 0$ in (2.11) or, equivalently, (2.12):

$$t^0_m(\beta) \equiv t_m(\beta, 0) \equiv s_m(\beta, 0) = -\frac{d^2}{du^2} + \frac{1}{4} - \beta u^{-1} + \frac{m^2 - 1}{4u^2}, \qquad 0 \leq u < \infty. \tag{2.15}$$

Then the operator family $T^0_m(\beta) = T_m(\beta, 0)$ in $L^2(0, \infty)$ defined as the action of (2.15) on $D(T_m(\cdot))$ enjoys properties (1)-(3) above. Denote by $\lambda(m, j, \beta)$, $|m|, j = 0, 1, \ldots$ the eigenvalues of $T^0_m(\beta)$. Then it is well known that $\lambda(m, j, \beta) = 0$ iff $\beta = \beta(m, j) = j + (|m| + 1)/2$, because the confluent hypergeometric equation $-\psi'' - \beta u^{-1}\psi + \frac{1}{4}\psi + ((m^2 - 1)/4u^2)\psi = 0$ admits solutions regular at 0 and L^2 at $+\infty$ iff $\beta = \beta(m, j)$ (see, e.g., Buchholz [24]). The corresponding (normalized) eigenfunctions are

$$\left[\frac{i!}{(i + |m|)!^3(|m| + 1 + 2i)}\right]^{1/2} u^{|m| + 1/2} e^{-u/2} L^{|m|}_{|m| + i}(u),$$

where $L^\mu_\lambda(\cdot)$ are the Laguerre polynomials. Then we see at once that $\beta(m, j) + \beta(m, k) = \gamma(m, j, k) = i + k + |m| + 1$, and

$$\sigma_d(H_0(Z_A)) = \bigcup_{|m|, i, k = 0}^{\infty} -\frac{1}{2} Z_A^2 \gamma(m, i, k)^{-2}, \tag{2.16}$$

which is equivalent to assertions (4) and (5) because in this case $\gamma(\cdot, \tau)$ is τ-independent.

Proof. Assertions (1) and (2) are well known (see, e.g., Kato [16] for $m \neq 0$ or Dunford and Schwartz [25] for $m = 0$). Statement (3) follows by standard arguments of regular perturbation theory (worked out in detail for the case of the non-separated operator in Combes, Duclos and Seiler [17]). We prove (4) and (5). Denote by $f(u, m, j; \beta_1, \beta_2; Z_A, Z_B, \tau)$ and $g(v, m, k; \beta_1, \beta_2; Z_A, Z_B; \tau)$ the eigenvectors corresponding respectively to $\lambda(m, j; \cdot; \tau)$ and $\mu(m, k; \cdot; \tau)$. Then the function

$$\begin{aligned}
&(x; m, j, k; Z_A, Z_B; \rho) \mapsto \Psi(x; m, j, k; Z_A, Z_B; \rho) \\
&\quad = e^{im \arctan(x_3/x_2)}[\Gamma(m, j, k; Z_A, Z_B; \rho)[\rho(|x| + |x - R\hat{e}| - 1]]^{-1/2} \\
&\quad \cdot [\Gamma(\cdot)[\rho(|x| - |x - R\hat{e}|) + 1]]^{-1/2} f(\Gamma(\cdot)[\rho(|x| + |x - R\hat{e}|) - 1]; \\
&\quad m, j, \beta_1(\cdot, \Gamma(\cdot)), \beta_2(\cdot, \Gamma(\cdot)), \cdot, \Gamma(\cdot)) \cdot g(\Gamma(\cdot)[\rho(|x| - |x - R\hat{e}|) + 1]; \\
&\quad m, k, \beta_1(\cdot, \Gamma(\cdot)), \beta_2(\cdot, \Gamma(\cdot)), \cdot, \Gamma(\cdot))
\end{aligned} \tag{2.17}$$

belongs to $H^2(\mathbb{R}^3)$ and satisfies

$$H(\rho, Z_A, Z_B)\,\Psi = E\Psi \tag{2.18}$$

with E given by (2.14) by direct inspection by virtue of (2.1)-(2.12). Conversely, to see (5), let $(x, \rho; Z_A, Z_B) \to \Psi(x, \rho; Z_A, Z_B)$ be an eigenvector of $H(\rho, Z_A, Z_B)$; $H(\rho, Z_A, Z_B)\,\Psi = E\Psi$. The change of variables (2.1)-(2.2) induces the direct sum decomposition

$$\begin{gathered}
L^2(\mathbb{R}^3) = \bigoplus_{m = -\infty}^{+\infty} L_m, \qquad L_m = L^2(\Omega; d\omega) \otimes e^{im\phi}, \\
\Omega = \{(\xi, \eta) : 1 < \xi < \infty,\ -1 < \eta < 1\}; \\
d\omega = (\xi^2 - \eta^2)\, d\xi\, d\eta.
\end{gathered} \tag{2.19}$$

Now L_m reduces $H(\rho, Z_A, Z_B)$ for all m. Hence we can write

$$\Psi = \sum_{m = -\infty}^{+\infty} e^{im\phi} \Phi(m; \xi, \eta; E(m)) \tag{2.20}$$

with

$$\left\| (\eta^2 - \xi^2)^{-1} \left[\frac{\partial}{\partial \xi} (\xi^2 - 1) \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} + \frac{m^2(\xi^2 - \eta^2)}{(\xi^2 - 1)(1 - \eta^2)} \right] \Phi(m; \xi, \eta; E(m)) \right\|_{L^2(\Omega, d\omega)} < \infty \tag{2.21}$$

and

$$-4\rho^2(\xi^2-\eta^2)^{-1}\left[\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}-\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right.$$
$$\left.+\frac{m^2(\xi^2-\eta^2)}{(\xi^2-1)(1-\eta^2)}\right]\Phi(m;\xi,\eta;E(m))-2\rho Z_A(\xi+\eta)^{-1}\Phi(m;\xi,\eta;E(m))$$
$$-2\rho Z_B(\xi-\eta)^{-1}\Phi(m;\xi,\eta;E(m))=E(m)\,\Phi(m;\xi,\eta;E(m)) \tag{2.22}$$

for some $m \in \mathbb{Z}$, i.e., we have

$$H(\rho, Z_A, Z_B)=\bigoplus_{m=-\infty}^{+\infty} H_m(\rho, Z_A, Z_B), \tag{2.23}$$

where $H_m(\rho, Z_A, Z_B)$ is the self-adjoint operator on $L^2(\Omega, d\omega)$ defined as the action of the left side of (2.22) on all functions in $L^2(\Omega; d\omega)$ satisfying (2.21). Therefore, there is an $m \in \mathbb{Z}$ such that $E=E(m)\in\sigma_d(H_m)$. On the other hand the map $(Qf)(\xi,\eta)=(\xi^2-\eta^2)^{1/2}f(\xi,\eta)$ is unitary from $L^2(\Omega; d\omega)$ to $L^2(\Omega; d\xi\, d\eta)$ and therefore $E(m)$ is an eigenvalue of H_m if and only if 0 is eigenvalue of QH_mQ^{-1}, defined as the action of

$$-\frac{1}{2}\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}-\frac{1}{2}\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}-\frac{1}{4}R^2E[(\xi^2-1)+(1-\eta^2)]$$
$$-\frac{1}{2}R(Z_A+Z_B)\,\xi+\frac{1}{2}(Z_A+Z_B)\,\eta+\frac{1}{2}m^2[(\xi^2-1)^{-1}+(1-\eta^2)^{-1}]$$

on $QD(H_m(\cdot))$. In turn, we have

$$QH_m(\cdot)\,Q^{-1}=UT_m(\cdot)\,U^{-1}\otimes I_{L^2(0,2r)}+I_{L^2(0,\infty)}\otimes VS_m(\cdot)\,V^{-1}, \tag{2.24}$$

where $T_m(\cdot)$ and $S_m(\cdot)$ are defined above, and $(Uf)(\xi)=(\xi^2-1)^{-1/2}f(r(\xi-1))$, $(Vg)(\eta)=(1-\eta^2)^{-1/2}g(r(\eta+1))$. Therefore (2.24) and the theorem on the spectrum of tensor products (see, e.g., Reed and Simon [15, Theorem VIII.33]) precisely characterize the union of the sets of values of $E(m)$ such that $QH_m(\cdot)\,Q^{-1}$ has the eigenvalue 0, in the form (2.14). ∎

We can now formulate the $1/R$ expansion via the separated equations.

Proposition II.3. *Consider the eigenvalues* $\lambda(m, j; \beta_1, \beta_2; Z_A, Z_B; \tau)\equiv\lambda(\cdot,\tau)$ *of* $T_m(\cdot)$, *and the eigenvalues* $\mu(m, k; \beta_1, \beta_2; Z_A, Z_B; \tau)\equiv\mu(\cdot,\tau)$ *of* $S_m(\cdot)$. *Denote once again by* $\lambda(m, j, \beta)\equiv\lambda(\cdot)$ *the eigenvalues of* $T_m^0(\beta)$. *Then:*

(1) *For any fixed* m, j, $\beta_1>0$, $\beta_2>0$, $Z_A>0$, *and* $Z_B\in\mathbb{R}$, *the functions* $\lambda(\cdot,\tau)$ *and* $\mu(\cdot,\tau)$ *admit asymptotic expansions near* $\lambda(\cdot)$ *to all orders in* $\tau/2>0$ *as* $\tau\downarrow 0$:

$$\lambda(\cdot,\tau)\sim\lambda(\cdot)+\sum_{m=1}^{\infty}A_n(\cdot)(\tau/2)^n, \tag{2.25}$$

$$\mu(\cdot,\tau)\sim\lambda(\cdot)+\sum_{n=1}^{\infty}B_n(\cdot)(\tau/2)^n. \tag{2.26}$$

The coefficients $A_n(m, j, \beta_1, \beta_2, Z_A, Z_B)$, $B_n(m, k; \beta_1, \beta_2, Z_A, Z_B)$ *are given by Rayleigh–Schrödinger perturbation theory in* $L^2(0,+\infty)$ *in the following way: the unperturbed operator is* $T_m^0(\beta_1)$, $T_m^0(\beta_2)$, *respectively, and the perturbation is the maximal multiplication operator by* $F(u,\cdot,\tau)$ *in case* (2.25), $G(v,\cdot,\tau)$ *in case* (2.26), *respectively. Here*

$$F(u,\cdot,\tau)=\sum_{n=1}^{\infty}F_n(u,\cdot)(\tau/2)^n, \tag{2.27}$$

$$F_n(u,\cdot)=0,\qquad u>2r,$$
$$=[(\beta_1+\beta_2)\,Z_A^{-1}(Z_A+Z_B)-\beta_1](-1)^n u^{n-1}+\frac{m^2-1}{4}(-1)^n(n+1)\,u^{n-2},$$
$$u<2r, \tag{2.28}$$

$$G(v,\cdot,\tau)=\sum_{n=1}^{\infty}G_n(v,\cdot)(\tau/2)^n; \tag{2.29}$$

$$G_n(v,\cdot)=0,\qquad v\geqslant 2r,$$
$$=-[\beta_2-Z_A^{-1}(Z_A-Z_B)(\beta_1+\beta_2)]\,v^{n-1}+\frac{m^2-1}{4}(n+1)\,v^{n-2},$$
$$v<2r. \tag{2.30}$$

(2) *The functions* $\lambda(m, j, \beta_1, \beta_2, \cdot, \tau)$, $\mu(m, k; \beta_1, \beta_2, \cdot, \tau)$ *are* C^∞ *in* (β_1, β_2, τ) *in a neighborhood of* $\beta(m, j)\times\beta(m, k)\times\bar\tau$, $(|m|, j, k)=0, 1,\ldots,\ \bar\tau>0$. *The functions* $\tau\mapsto\beta_2(m, k, \cdot, \tau)$ *and* $\tau\mapsto\beta_1(m, j, k, \cdot, \tau)$ *are* C^∞ *near any given* $\bar\tau>0$, *and admit an asymptotic expansion to all orders as* $\tau\downarrow 0$:

$$\beta_2(m, k, \cdot, \tau)\sim\beta(m, k)+\sum_{n=1}^{\infty}L_n(m, k, \cdot)(\tau/2)^n, \tag{2.31}$$

$$\beta_1(m, j, \cdot, \tau)\sim\beta(j, k)+\sum_{n=1}^{\infty}M_n(m, j, \cdot)(\tau/2)^n. \tag{2.32}$$

The functions $\rho\mapsto\Gamma(m, j, k; \rho)$ *and* $\rho\mapsto E(m, j, k, \rho)$ *(given by* (2.14)*) are* C^∞ *near any given* $\bar\rho>0$ *and admit an asymptotic expansion to all orders as* $\rho\to 0$. *The asymptotic expansion for* $E(m, j, k; \rho)$ *coincides with the* $1/R$ *expansion near the* *eigenvalue of $H_0(Z_A)$ of magnetic quantum number m and parabolic quantum numbers (j, k) written as*

$$E(m, j, k; \rho) \sim E(m, j, k) + \sum_{n=1}^{\infty} E_n(m, j, k)\, \rho^n. \tag{2.33}$$

Remarks. (1) Remark (3) after Proposition II.1 can now be more precisely formulated as follows: for any eigenvalue $E(m, j, k) = -\frac{1}{2} Z_A^2(|m| + j + k + 1)^{-2}$ of $H_0(Z_A)$, $|m|, j, k = 0, 1, \ldots$ fixed, and any open interval I containing only $E(m, j, k)$, there is $M(m, j, k)$ such that for $\rho < M$ there are precisely two eigenvalues $E_{\pm}(m, j, k; \rho)$ of $H(\rho, Z_A)$ in I. Furthermore, we have [13]

$$\begin{aligned}\Delta E(m, j, k; \rho) &\equiv E_+(m, j, k; \rho) - E_-(m, j, k; \rho) \\ &= O(m, j, k; \rho^{-(2k+|m|+1)} \exp(-1/\rho(j+k+|m|+1))), \end{aligned} \tag{2.34}$$

where, here and elsewhere, $O(m, j, k; x)$ stands for order x with constant depending on (m, j, k).

(2) Completely analogous statements hold for $S_m(\beta_1, \beta_2, Z_A = Z_B; \tau) \equiv S_m(\beta_2, Z_A, \tau)$: given any eigenvalue $\mu(m, k; \beta_2, Z_A)$ of $S_m(\beta_2, 0)$ (defined by (2.15)) and any open interval I as above, there is a constant $M(m, k)$ such that for $\tau < M$, $S_m(\beta_2, Z_A, \tau)$ has exactly two eigenvalues $\mu_{\pm}(m, k, \beta_2, Z_A, \tau)$ in I, such that

$$\Delta\mu(m, k; \beta_2, Z_A; \tau) = \mu_+(\cdot) - \mu_-(\cdot) = O(m, k; \tau^{-(2k+|m|)} e^{-1/\tau}) \tag{2.35}$$

uniformly on compacts in $(\beta_2, Z_A) \in \mathbb{R}^4$. Hence, upon putting the implicit relation in explicit form for each fixed $\pm m, k = 0, 1, \ldots$ there are $\beta_2^{\pm}(m, k; Z_A, \tau) \to \beta(m, k; Z_A)$ as $\tau \to 0$ such that

$$\Delta\beta_2(m, k; Z_A) = \beta_2^+(\cdot) - \beta_2^-(\cdot) = O(m, k; \tau^{-(2k+|m|+1)} e^{-1/\tau}) \tag{2.36}$$

uniformly on compacts in $Z_A \in \mathbb{R}^+$. For the proof of (2.35), (2.36), see Harrell [13].

Proof. Assertion (1) can be proved by well-known arguments of singular perturbation theory (we omit the details because they have been worked out in the present case by Morgan and Simon in the more general context of the non-separated formalism). A statement stronger than (2), namely, local analyticity in (β_1, β_2, τ) can be proved by exactly the same argument as in Proposition III.3(1) for the function $\lambda(\cdot, \beta_1, \beta_2, \tau)$. If we now observe that by the unitary rescaling, $(V(r) f)(v) = r^{1/2} f(\tau v)$ mapping $L^2(0, 2r)$ onto $L^2(0, 2)$ one-to-one, $\mu(\cdot, \beta_1, \beta_2, \tau)$ is an eigenvalue of $V(r)\, S_m(\cdot)\, V(r)^{-1}$, which is the action

$$r^{-2}\left[-\frac{d^2}{dv^2} + \frac{1}{4} r^2 - \frac{r\beta_2}{v} + \frac{m^2-1}{4v^2} + r\left[-\frac{\beta_2 - Z_A^{-1}(Z_A - Z_B)(\beta_1 + \beta_2)}{2-v}\right] + \frac{m^2-1}{4}\left(\frac{2}{v(2-v)} + \frac{1}{(2-v)^2}\right)\right]$$

on $V(r)\, D(S_m(\cdot))$, we get by the same argument also the local analyticity of $(\beta_1, \beta_2, \tau) \mapsto \mu(\cdot, \beta_1, \beta_2, \tau)$ because it is immediately seen that $V(r)\, D(S_m(\cdot))$ is independent of (β_1, β_2, τ). The implicitly defined functions $\tau \mapsto \beta_1(m, j, k; \tau)$, $\tau \mapsto \beta_2(m, k; \tau)$ exist by Proposition II.2(4) and are thus locally C^∞. Hence the validity of the asymptotic expansions (2.31), (2.32) is a consequence of (1) and of the implicit-function theorem. The functions $\tau \mapsto \gamma(m, j, k; \tau)^{-1}\tau$ are invertible again by II.2(4), and $\Gamma(m, j, k; \rho)$ and $E(m, j, k; \rho)$ are locally C^∞ and admit asymptotic expansions to all orders once again by the implicit-function and local-invertibility theorems, given (2.13), (2.14), (2.31), and (2.32). Finally, we note that the expansion for $E(\cdot, \rho)$ generated via (2.31), (2.32), (2.13), and (2.14) coincides with the $1/R$ expansion because a function can have at most one asymptotic expansion. ∎

III. Stability, Analyticity, and Summability

The main purpose of this section is to identify the Borel sum of the $1/R$ expansion for H_2^+ near any eigenvalue $E(m, j, k; Z_A)$ of $H_0(Z_A)$ of magnetic quantum number m and parabolic quantum numbers (j, k).

To this end, we consider two distinct cases in the two-center operator family $H(\rho, Z_A, Z_B)$, which we now describe in order also to establish some further notation used throughout the rest of this paper.

Case A (the H_2^+ problem): $\rho > 0$, $Z_A = Z_B = 1$.

Case B: $\rho = -\rho'$, $\rho' > 0$, $Z_A = 1$, $Z_B = -1$.

We denote $H(\rho, 1, 1) \equiv H(\rho)$, $H(\rho', 1, -1) \equiv H'(\rho')$. The physical interpretation of $H'(\rho')$ was mentioned in Section I, and its relevant mathematical properties are summarized as follows:

Proposition III.1. *Let $H'(\rho')$ be the operator in $L^2(\mathbb{R}^3)$ defined as the action of $-\frac{1}{2}\Delta - |x|^{-1} + |x + \hat{e}/\rho'|^{-1}$ on $H^2(\mathbb{R}^3)$. Then $H'(\rho')$ enjoys properties* (1), (2) *of Proposition* II.1, *and, furthermore:*

(1) *Each eigenvalue E of $H_0(Z_A = 1)$ is stable (in the sense of Kato* [16, *Sect.* VIII.1.5]) *as an eigenvalue $E'(\rho')$ of $H'(\rho')$ as $\rho' \downarrow 0$.*

(2) *Let $E'(\rho')$ be the ground state of $H'(\rho')$, and $E'(\rho') \sim E + \sum_{n=1}^{\infty} E'_n\, (\rho')^n$ be its ρ' expansion near E, the ground state of $H_0(Z_A = 1)$. Then $E'_n = (-1)^n E_n$, where E_n are the coefficients of the $1/R$ expansion for H_2^+ near E.*

Remark. We will see below that actually $E'_n(m, j, k) = (-1)^n E_n(m, j, k)$ for each triple of quantum numbers $(|m|, j, k) = 0, 1, 2, \ldots$.

Proof. Assertion (1) is an immediate application of the Hunziker–Vock stability theorem [18]: in fact,

$$\| |x + \rho' \hat{e}|^{-1} \|_{L^2_{loc}(\mathbb{R}^3)} \to 0$$

as $\rho' \to 0$, and this implies (see again Ref. [8, Lemma 1.2]) that $H'(\rho')$ converges in strong-resolvent sense to $H_0(Z_A)$ as $\rho' \to 0$. Furthermore, given $x \mapsto \chi(x) \in C_0^\infty(\mathbb{R}^3)$, $\chi(x) = 1$, $|x| \leq 1$; $\chi(x) = 0$, $|x| \geq 2$, and setting $M_n(x) = 1 - \chi(x/n)$, we have $\lim_{n\to\infty} \operatorname{dist}(E, W_n(\rho')) > 0$ uniformly with respect to ρ' for all $E < 0$. Here

$$W_n(\rho') = \{z: z = \langle M_n u, H'(\rho') M_n u\rangle;\ u \in C_0^\infty(\mathbb{R}^3);\ \|u\| = 1\}.$$

In fact, $\langle -\frac{1}{2}\Delta M_n u, M_n u\rangle + \langle |x + \rho' \hat{e}|^{-1} M_n u, M_n u\rangle \geq 0$ independently of n, and $\langle -|x|^{-1} M_n u, M_n u\rangle \geq -1/n$. Since all eigenvalues of H_0 are negative, the conditions of [18, Theorem 1.1] are satisfied and (1) is proved. Assertion (2) is trivial given Remark (2) after Proposition II.1. ∎

Let us now specialize the general formalism of Propositions II.2, II.3 to the Cases A and B. We use the convention of denoting each quantity relative to $H'(\rho')$ with a prime on the corresponding quantity relative to $H(\rho)$. More specifically, considering the operators $T_m(\cdot)$ and $S_m(\cdot)$ defined in Proposition II.2, we set for Case A (the H_2^+ system $Z_A = Z_B = 1$)

$$\begin{aligned} T_m(\beta_1, \beta_2; 1, 1, \tau) &= T_m(\beta_1, \beta_2, \tau); \\ S_m(\beta_1, \beta_2, 1, 1, \tau) &= S_m(\beta_2, \tau), \end{aligned} \tag{3.1}$$

because the differential expressions $t_m(\cdot)$ and $s_m(\cdot)$ simplify to

$$\begin{aligned} t_m(\beta_1, \beta_2, \tau) = &-\frac{d^2}{du^2} + \frac{1}{4} - \frac{\beta_1}{u} + \frac{m^2-1}{4u^2} - \frac{2\beta_2 + \beta_1}{u + 2r} \\ &+ \frac{m^2-1}{4}((u+2r)^{-2} - 2u^{-1}(u+2r)^{-1}) \end{aligned} \tag{3.2}$$

and

$$\begin{aligned} s_m(\beta_2, \tau) = &-\frac{d^2}{du^2} + \frac{1}{4} - \frac{\beta_2}{v} + \frac{m^2-1}{4v^2} - \frac{\beta_2}{2r - v} \\ &+ \frac{m^2-1}{4}(2v^{-1}(2r-v)^{-1} + (2r-v)^{-2}). \end{aligned} \tag{3.3}$$

For Case B, i.e., the operator $H'(\rho')$ with $Z_A = -Z_B = 1$, $\rho' = -\rho$, the separated operators are, respectively,

$$T_m(\beta'_1, \beta'_2; 1, -1, \tau') \equiv T'_m(\beta'_1, \tau'), \tag{3.4}$$

i.e., the action on $D(T_m)$ of the differential expression

$$\begin{aligned} t'_m(\beta'_1, \tau') = &-\frac{d^2}{du^2} + \frac{1}{4} - \frac{\beta'}{u} + \frac{m^2-1}{4u^2} + \frac{\beta'_1}{2r' + u} \\ &+ \frac{m^2-1}{4}((2r'+u)^{-2} - 2u^{-1}(2r'+u)^{-1}). \end{aligned} \tag{3.5}$$

and

$$S_m(\beta'_1, \beta'_2; 1, -1, \tau') \equiv S'_m(\beta'_1, \beta'_2; \tau'), \tag{3.6}$$

i.e., the action on $D(S_m)$ of the differential expression

$$\begin{aligned} S'_m(\beta'_1, \beta'_2; \tau') = &-\frac{d^2}{dv^2} + \frac{1}{4} - \frac{\beta'_2}{v} + \frac{m^2-1}{4v^2} + \frac{2\beta'_1 + \beta'_2}{2r' - v} \\ &+ \frac{m^2-1}{4}((2r'-v)^{-2} + 2v^{-1}(2r'-v)^{-1}). \end{aligned} \tag{3.7}$$

The functions $\lambda(m, j, \beta_1, \beta_2, \tau) \equiv \lambda(m, j, \beta_1, \beta_2, 1, 1, \tau)$, $\mu(m, k, \beta_2, \tau) \equiv \mu(m, k; \beta_1, \beta_2, 1, 1, \tau)$, $\beta_2(m, k; \beta_1; \tau) \equiv \beta_2(m, k; \beta_1, 1, 1, \tau)$, $\beta_1(m, j, k; \tau) \equiv \beta_1(m, j, k; 1, 1, \tau)$, $\gamma(m, j, k; \tau) \equiv \gamma(m, j, k; 1, 1, \tau)$, $\Gamma(m, j, k; \rho) \equiv \Gamma(m, j, k; 1, 1, \rho)$, and their primed counterparts have the same meaning as in Section II. We denote again by $\lambda(m, j, \beta)$ the eigenvalues of $T_m^0(\beta)$. The functions

$$E(m, j, k; \rho) = -\tfrac{1}{2}[\gamma(m, j, k; \Gamma(m, j, k; \rho))]^{-2}, \tag{3.8}$$

$$(|m|, j, k) = 0, 1, \ldots,$$

$$E'(m, j, k; \rho') = -\tfrac{1}{2}[\gamma'(m, j, k; \Gamma'(m, j, k; \rho'))]^{-2}, \tag{3.9}$$

yield respectively the discrete spectra of $H(\rho)$ and $H'(\rho')$. Furthermore, formulae (2.27)–(2.30) together with their primed counterparts simplify to

$$\begin{aligned} F_n(u, \beta_1, \beta_2) &= 0, & u &\geq 2r, \\ &= (2\beta_2 + \beta_1)(-1)^n u^{n-1} + \frac{m^2-1}{4}(-1)^n(n+1)u^{n-2}, & u &< 2r, \end{aligned} \tag{3.10}$$

$$\begin{aligned} F'_n(u, \beta'_1) &= 0, & u &\geq 2r, \\ &= \beta'_1(-1)^{n-1}u^{n-1} + \frac{(m^2-1)}{4}(-1)^n(n+1)u^{n-2}, & u &< 2r, \end{aligned} \tag{3.11}$$

and

$$\begin{aligned} G_n(v, \beta_2) &= 0, & v &\geq 2r, \\ &= -\beta_2 v^{n-1} + \frac{m^2-1}{4}(n+1)v^{n-2}, & v &< 2r, \end{aligned} \tag{3.12}$$

$$\begin{aligned} G'_n(v, \beta'_1, \beta'_2) &= 0, \quad v \geq 2r, \\ &= (2\beta'_2 + \beta'_1)v^{n-1} + \frac{m^2-1}{4}(n+1)v^{n-2}, \end{aligned} \tag{3.13}$$

so that the expansions (2.25) and (2.26) for $\mu(m, k; \beta_2, \tau)$ and $\lambda(m, j, \beta_1, \beta_2, \tau)$ hold, together with their primed counterparts for $\mu'(m, k; \beta'_1, \beta'_2, \tau')$ and

$\lambda(m, j, \beta'_1, \tau')$. We denote their coefficients by $B_n(m, k; \beta_2)$, $A_n(m, j; \beta_1, \beta_2)$, $B'_n(m, k; \beta'_1, \beta'_2)$, and $A'_n(m, j; \beta'_1)$, respectively. Analogously, we denote by $L'_n(m, k)$ and $M'_n(m, j, k)$ the coefficients of the primed counterparts of the asymptotic expansions (2.31) and (2.32), specialized in this way. Obviously, the r-dependence implicit in Eq. (3.10)–(3.13) does not affect the computations of the perturbation coefficients; because of the exponential decay of the unperturbed eigenfunction, it introduces only exponentially small corrections.

To get the above-mentioned result on the identification of the Borel sum of the $1/R$ expansion as a complex eigenvalue obtained by interconnecting $H(\rho)$ and $H'(\rho')$, the "double-well" operator $S_m(\beta_2, \tau)$ in the finite interval $(0, 2r)$ has to be replaced by the analytic continuation up to $\tau' = e^{\pm i\pi}\tau$, $\tau > 0$, of the "single-well" operator $T_m(\beta'_1, \tau')$, $\tau' > 0$, in the infinite interval $(0, +\infty)$. This mechanism, which identifies the Borel sum for $\tau' > 0$, is basically the same as that which gives rise to existence and Borel summability of resonances out of the separability in squared parabolic coordinates in the Lo Surdo–Stark effect [7]. A major difference is that here the "single-well" equation is that of Case B. Of course, the non-self-adjoint, stable problem having the same $1/R$ expansion as H_2^+ can be immediately defined (see the subsequent proposition) within the separated formalism out the operators $T_m(\beta'_1, e^{-i\pi}\tau)$, $T_m(\beta_1, \beta'_1(\tau e^{-\pi}), \tau)$ realized below. The result, whose proof is to be obtained in the course of this section, reads as follows:

THEOREM III.2. *Let* $(|m|, j, k) = 0, 1,...$ *be fixed. Then for any* $\mu = \mu(m, j, k) > 0$ *there are* $0 < M = M(m, j, k) < \infty$ *and* $0 < M_1(m, k) < \infty$ *such that:*

(1) *The implicitly defined functions* $\tau' \mapsto \beta'_1(m, k; \tau')$ *exist as holomorphic functions of* τ' *for* $0 < M_1$, $|\arg \tau'| < \pi$, *admit analytic continuation to the Riemann-surface sector* $\mathscr{C}(m, k) = \{\tau' \colon 0 < |\tau'| < M_1|; |\arg \tau'| < \frac{3}{2}\pi - \mu\}$ *across the negative real axis, and* $\lim \beta'_1(m, k; \tau') = \beta(m, k) = k + \frac{1}{2}(|m| + 1)$ *as* $\tau' \to 0$, $\tau' \in \bar{\mathscr{C}}$.

(2) *The implicitly defined functions* $\tau \mapsto \beta_1(m, j; \beta'_1(m, k; \tau e^{-i\pi}), \tau)$, *which will be denoted for convenience as* $\beta_1(m, j, k; \tau)$, *exists as holomorphic functions of* τ *for* $0 < |\tau| < M$, $0 < \arg \tau < \pi$, *admit analytic continuation to the Riemann-surface sector* $\mathscr{D}(m, j, k) = \{\tau \colon 0 < |\tau| < M;\ -\pi/2 + \mu < \arg \tau < \frac{3}{2}\pi - \mu\}$ *across the real axis, and* $\lim \beta_1(m, j, k; \tau) = \beta(m, j) = j + \frac{1}{2}(|m| + 1)$ *as* $\tau > 0$, $\tau \in \bar{\mathscr{D}}(m, j, k)$.

(3) *The functions* $\tau \mapsto \gamma_1(m, j, k; \tau) = \beta_1(m, j, k; \tau) + \beta'_1(m, k; \tau e^{-i\pi})$ *are holomorphic for* $0 < |\tau| < M$, $0 < \arg \tau < \pi$, *and admit analytic continuation to* $\mathscr{D}(m, j, k)$ *as above. The functions* $\tau\gamma_1(m, j, k; \tau)^{-1}$ *are invertible in* $\mathscr{D}(m, j, k)$; *the inverse functions* $\rho \mapsto \Gamma_1(m, j, k; \rho)$ *of* $\tau\gamma_1(m, j, k; \tau)^{-1}$ *are holomorphic for* $0 < |\rho| < M$, $0 < \arg \rho < \pi$, *and admit analytic continuation to* $\mathscr{D}(m, j, k)$ *as above.*

(4) *The functions*

$$\rho \mapsto E_1(m, j, k; \rho) = -\tfrac{1}{2}\,[\gamma_1(m, j, k; \Gamma_1(m, j, k; \rho))]^{-2} \tag{3.14}$$

and holomorphic for $0 < \arg \rho < \pi$, *admit analytic continuation to* $\mathscr{D}(m, j, k)$ *as above, and have the same* $\rho = 1/R$ *expansion as* $E(m, j, k; \rho)$.

(5) *The* $1/R$ *expansion near any eigenvalue* $E(m, j, k)$ *of* H_0 *is Borel summable not to* $E_+(m, j, k; \rho)$ *or to* $E_-(m, j, k; \rho)$, *but to* $E_1(m, j, k; \rho)$ *for* $0 < |\rho| < M$, $-\pi/2 + \mu < \arg \rho < \frac{3}{2}\pi - \mu$.

Remarks. (1) The definition of ρ' as $e^{-i\pi}\rho$ makes $\operatorname{Im} E_1(\cdot, \rho) \leqslant 0$. The opposite choice of phase would have made $\operatorname{Im} F_1(\cdot, \tau) \geqslant 0$.

(2) In terms of the Borel summability in the standard sense (see, e.g., Reed and Simon [15, Sect. XII.4]) statement (5) means that the $1/R$ expansion is Borel summable to $E_1(m, j, k; \rho)$ for $0 < \arg \rho < \pi$, $|\rho| < M$. Thus, for ρ real $E_1(m, j, k; \rho)$ is determined from the Borel sum ((4)) and analytic continuation to the real axis. On the other hand, under the present conditions, the analytic continuation can be explicitly written in terms of the Nevanlinna modified representation of the Borel integral (for details see, e.g., Sokal [26]), namely,

$$\begin{gathered} E_1(m, j, k; e^{i\alpha}\rho) = R \int_0^{\infty} e^{-Rte^{i\alpha}} F_\alpha(t)\, dt, \\ -\pi/2 + \mu < \alpha + \arg \rho < \tfrac{3}{2}\pi - \mu, \end{gathered} \tag{3.15}$$

where $F_\alpha(t)$ is the Borel transform of the $1/R$ expansion computed at $\rho = te^{i\alpha}$. Therefore statement (5) can be considered equivalent to (3.15).

(3) Statement (5), and hence also Remark (2) above, applies to the separation-constant eigenvalues as well. That is, the perturbation series (2.32) coincides with the perturbation series for $\beta'_1(\cdot, \tau e^{-i\pi})$ and is Borel summable to that function and not to $\beta_2^{\pm}(\cdot, \tau)$; the perturbation series (2.31) is Borel summable to $\beta_1(\cdot; \tau)$ and not to $\beta_1(\cdot; \beta_2^{\pm}(\cdot, \tau), \tau)$; and the series for γ is summable not to $\gamma(\cdot, \tau)$ but to $\gamma_1(\cdot; \tau)$.

(4) Interchanging the roles of ρ and ρ', a statement equivalent to (5) is that the ρ' expansion for each eigenvalue $E'(m, j, k; \rho')$ of $H'(\rho')$ is Borel summable to $E_2(m, j, k; \rho') \equiv -\frac{1}{2}\,[\gamma_2(m, j, k; \Gamma_2(m, j, k; \rho'))]^{-2}$. Here $\tau' \mapsto \gamma_2(m, j, k; \tau') = \beta'_1(m, j; \tau') + \beta_2(m, k; \beta'_1(m, j; \tau'), e^{-i\pi}\tau')$, and $\rho' \mapsto \Gamma_2(m, j, k; \rho')$ is the inverse function of $\tau'/\gamma_2(\cdot; \tau')$. Of course the remarks above apply also to this case.

(5) We will see in Proposition IV.1 that $\operatorname{Im} E_1(\cdot, \rho)$ is non-zero for ρ real and small. Since the $1/R$ expansion has real coefficients, the Borel summability implies its divergence.

The first step in proving Theorem III.2 is represented by the analysis of the operator families $T'_m(\beta'_1, \tau')$, $T_m(\beta_1, \beta_2, \tau)$ for suitable complex values of the parameters. For $\theta \in \mathbb{C}$, $|\operatorname{Im} \theta| < \pi/2$, set

$$\begin{aligned} p(u, m, \beta_1, \beta_2, \tau, \theta) = {} & -\frac{2\beta_1 + \beta_1}{e^{\theta}u + 2r} \\ & + \frac{m^2 - 1}{4}\left((e^{\theta}u + 2r)^{-2} - 2e^{-\theta}u^{-1}(e^{\theta}u + 2r)^{-1}\right) \end{aligned} \tag{3.16}$$

and

$$q(u, m; \beta'_1, \tau', \theta) = \frac{\beta'_1}{2r' + e^{\theta}u} + \frac{m^2 - 1}{4}((e^{\theta}u + 2r')^{-2} - 2e^{-\theta}u^{-1}(e^{\theta}u + 2r')^{-1}. \tag{3.17}$$

Hence, if we define the differential expressions

$$t_m(\beta_1, \beta_2, \tau, \theta) = -e^{-2\theta}\frac{d^2}{du^2} + e^{-2\theta}\frac{m^2 - 1}{4u^2} - e^{-\theta}\frac{\beta_1}{u} + p(u, m, \beta_1, \beta_2, \tau, \theta) + \frac{1}{4} \tag{3.18}$$

and

$$t'_m(\beta'_1, \tau', \theta) = -e^{-2\theta}\frac{d^2}{du^2} + e^{-2\theta}\frac{m^2 - 1}{4u^2} - e^{-\theta}\frac{\beta'_1}{u} + q(u, m; \beta'_1, \tau', \theta) + \frac{1}{4} \tag{3.19}$$

by (3.4) and (3.6), we have

$$t_m(\beta_1, \beta_2, \tau, 0) = t_m(\beta_1, \beta_2, \tau); \qquad t'_m(\beta'_1, \tau', 0) = t'_m(\beta'_1, \tau') \tag{3.20}$$

and

$$t^0_m(\beta_1, \theta) = t_m(\beta_1, \beta_2, 0, \theta) = e^{-2\theta}\frac{d^2}{du^2} + e^{-2\theta}\frac{m^2 - 1}{4u^2} - e^{-\theta}\frac{\beta_1}{u} + \frac{1}{4}. \tag{3.21}$$

PROPOSITION III.3. *Let* $(\beta'_1, \tau') \in \Omega \times \mathbb{C}\backslash(\mathbb{R}^+ \cup \{0\})$. Ω *open, bounded, and simply connected in the half-plane* Re $\beta'_1 > 0$. *Then, for* $|m| = 0, 1, \ldots$:

(1) $T'_m(\beta'_1, \tau')$, $T^0_m(\beta'_1)$ *are type-A, real-holomorphic families (in the sense of Kato [16, Sect. VII.1]) of m-sectorial operators in* (β'_1, τ') *jointly and in* β'_1, *respectively, and thus self-adjoint for* $(\tau', \beta'_1) \in \mathbb{R}^+ \times \mathbb{R}^+$.

(2) $\sigma_{ess}(T_m(\cdot)) = \sigma_{ess}(T^0_m(\cdot)) = [\frac{1}{4}, +\infty)$ *for all* (β'_1, τ').

(3) *Given* $\mu_1(m, k) > 0$ *there is* $0 < M_1(m, k) < \infty$ *such that each eigenvalue* $\lambda(m, k; \beta'_1)$ *of* $T^0_m(\beta'_1)$, $(|m|, k) = 0, 1, \ldots$, *is stable as an eigenvalue* $\lambda'(m, k; \beta'_1, \tau')$ *of* $T_m(\beta'_1, \tau')$ *for* $|\tau'| < M_1$, $|\arg \tau'| \leq \pi - \mu_1$.

(4) *Each eigenvalue* $\lambda'(\cdot, \beta'_1, \tau')$ *is holomorphic in* (τ', β'_1) *jointly for* $0 < |\tau'| < M_1$, $|\arg \tau'| < \pi - \mu_1$, *locally in* β'_1, *and admits analytic continuation with respect to* τ' *to the Riemann-surface sector* $\mathscr{D}_1(m, k) = \{\tau' : 0 < |\tau'| < M_1(m, k); |\arg \tau'| < \frac{3}{2}\pi - \mu\}$ *across the negative real axis.*

(5) $\lim \lambda'(m, k; \beta'_1, \tau') = \lambda(m, k; \beta'_1)$ *as* $|\tau'| \to 0$ *within* $\bar{\mathscr{D}}_1(m, k)$, *uniformly with respect to* $\beta'_1 \in \Omega$.

Proof. It is well known that the quadratic form

$$t^0_m(f, g) : (f, g) \mapsto \left\langle \left(-\frac{d^2}{du^2} + \frac{m^2 - 1}{4u^2} \right) f, g \right\rangle_{L^2(0, \infty)},$$

$$(f, g) \in H^1_0[0, +\infty),$$

if $m > 1$, $(f, g) \in H^1(0, \infty)$ and $(f(u), g(u)) = O(u^{1/2})$ as $u \to 0$ for $m = 0$, is symmetric, closed, and positive. The associated self-adjoint operator on $L^2(0, \infty)$ is T^0_m, defined as the action of $-d^2/du^2 + (m^2 - 1)/4u^2$ on $D \equiv \{H^1_0[0, \infty) \cap H^2(0, \infty)$, $m > 0$; $H^2(0, +\infty)$ with boundary condition $f(u) = O(u^{1/2})$ as $u \downarrow 0$, $m = 0\}$. By the Sobolev inequality, the maximal multiplication operator by u^{-1} on $L^2(0, \infty)$ is compact from D to $L^2(0, \infty)$, and the same is true for the maximal multiplication operator by $q(u, m; \beta'_1, \tau', 0)$ in $L^2(0, \infty)$ as long as $|\arg \tau'| < \pi$. Hence by standard results of perturbation theory $T^0_m(\beta'_1)$ and $T'_m(\beta'_1, \tau')$ are closed and m-sectorial, and thus self-adjoint for $(\beta'_1, \tau') \in \mathbb{R}^+ \times \mathbb{R}^+$. Furthermore, clearly $\sigma_{ess}(T^0_m) = [\frac{1}{4}, +\infty)$, and thus by Weyl's theorem, $\sigma_{ess}(T^0_m(\beta'_1)) = \sigma_{ess}(T'_m(\beta'_1, \tau')) = \sigma_{ess}(T^0_m) = [\frac{1}{4}, +\infty)$ for all $(\beta'_1, \tau') \in \Omega \times \{\tau' : |\arg \tau'| < \pi\}$. Moreover, $D(T^0_m(\beta'_1)) = D(T_m(\beta'_1, \tau'))$ is (β'_1, τ')-independent, and the L^2-valued functions $\beta'_1 \mapsto T^0_m(\beta'_1) f$, $(\beta'_1, \tau') \mapsto T'_m(\beta'_1, \tau') f$ are holomorphic in Ω and $\Omega \times \{\tau' : |\arg \tau'| < \pi\}$, respectively, for any $f \in D$. Therefore, the operator families $T^0_m(\beta'_1)$ and $T'_m(\beta'_1, \tau)$ are type-A holomorphic by definition, with the property $(T^0_m(\beta'_1))^* = T^0_m(\bar{\beta}'_1)$, $(T'_m(\beta'_1, \tau'))^* = T'_m(\bar{\beta}'_1, \bar{\tau}')$. This verifies (1) and (2). To see (3), it is enough, by standard arguments of perturbation theory (see, e.g., Simon [27]), to prove that $T'_m(\beta'_1, \tau')$ converges in norm-resolvent sense to $T'_m(\tau'_1)$ as $|\tau|' \to 0$, uniformly with respect to $(\beta'_1, |\arg \tau'|) \in \Omega \times [0, \pi - \mu]$. By the uniform m-sectoriality, $\|(T'_m(\beta'_1, \tau') - z)^{-1}\| \leq C$ for z negative and $|z|$ suitably large and some $C > 0$ independent of $(\beta'_1, \tau') \in \Omega \times \{\tau' : |\tau'| < M; |\arg \tau'| \leq \pi - \mu_1\}$. Since $D(T'_m(\cdot))$ is independent of τ', we can write

$$(T'_m(\beta'_1, \tau') - z)^{-1} - (T^0_m(\beta'_1) - z)^{-1} = (T'_m(\beta'_1, \tau') - z)^{-1} q(u, m; \beta'_1, \tau', 0)(T^0_m(\beta'_1) - z)^{-1}. \tag{3.22}$$

Now the norm of the right side of (3.22) is majorized by $C\|q(\cdot)\, C(T^0_m(\cdot) - z)^{-1}\| \leq C'\|q(u, \cdot)\|_{L^\infty(0, +\infty)} \|(T^0_m(\beta'_1) - z)^{-1}\| \leq C^2 \sup_{u \geq 0} |q(u, m; \beta'_1, \tau', 0)| \to 0$ as $|\tau'| \to 0$ with the stated uniformity in $(\beta'_1, |\arg \tau'|)$. This proves assertion (3). The holomorphy statement of assertion (4) is a well-known consequence of the stability and of the holomorphy of the operator family $T_m(\beta'_1, \tau')$.

To see the existence of the analytic continuation we use the complex-scaling technique of Aguilar, Balslev, and Combes (see, e.g., Reed and Simon [15, XIII.10]). The dilatation map

$$(U(\theta) f)(u) = e^{\theta/2} f(e^{\theta} u), \qquad \theta \in \mathbb{R}, \tag{3.23}$$

is unitary on $L^2(0, +\infty)$ and leaves D invariant. The unitary images of $T^0_m(\beta'_1)$ and $T_m(\beta'_1, \tau')$ are the operators $T^0_m(\beta'_1, \theta)$ and $T'_m(\beta'_1, \tau', \theta)$ defined as the action on D of the differential expressions (3.21) and (3.19). Proceeding as in the verification of assertions (1) and (2), we see that $T^0_m(\beta'_1, \theta)$ extends to a type-A, real-holomorphic family of m-sectorial operators in $(\beta'_1, \theta) \in \Omega \times \{\theta: |\mathrm{Im}\,\theta| < \pi/2\}$, and that $T_m(\beta'_1, \tau', \theta)$ extends to a type-A, real-holomorphic family of m-sectorial operators in $(\beta'_1, \tau', \theta) \in \Omega \times \{(\tau', \theta): |\arg(\tau' e^{\theta})| < \pi\}$. Furthermore, $\sigma_{\mathrm{ess}}(T^0_m(\cdot)) = \sigma_{\mathrm{ess}}(T'_m(\cdot)) = [e^{-2\theta}\xi^2 + \frac{1}{4})$, $\xi \in \mathbb{R}$, and the eigenvalues of both families are independent of θ. The norm-resolvent convergence of assertion (3) holds unchanged also in the present situation provided $|\arg(\tau' e^{\theta})| \leqslant \pi - \mu_1$. Therefore, the eigenvalues $\lambda(m, \beta'_1)$ are stable as eigenvalues $\lambda'(m, \beta'_1, \tau')$ of $T'_m(\beta'_1, \tau', \theta)$ for $|\tau'| < M_1$, $|\arg(\tau' e^{\theta})| \leqslant \pi - \mu_1$. Since $|\mathrm{Im}\,\theta| < \pi/2$, we see that $\lambda'(\cdot, \beta'_1, \tau')$ admits analytic continuation to $|\tau'| < M_1$, $|\arg(\tau')| < \frac{3}{2}\pi - \mu$, a priori many-valued because $\lambda'(\cdot, e^{i\pi}\tau') \neq \lambda'(\cdot, e^{-i\pi}\tau')$, $\tau' > 0$, $\beta'_1 \in \mathbb{R}$. In fact, $\lambda'(\cdot, e^{i\pi}\tau')$ is by definition an eigenvalue of $T'_m(\cdot, \theta)$ for $-\pi/2 < \mathrm{Im}\,\theta < 0$, while $\lambda'(\cdot, e^{-i\pi}\tau')$ is an eigenvalue of $T'_m(\cdot, \theta)$ for $0 < \mathrm{Im}\,\theta < \pi/2$. Since $T'_m(\cdot, \theta)^* = T'_m(\cdot, \bar{\theta})$, $\mathrm{Im}\,\lambda'(\cdot, e^{-i\pi}\tau') = -\mathrm{Im}\,\lambda'(\cdot, e^{i\pi}\tau')$, $\tau' > 0$. This proves (4) and (5). ∎

Proposition III.4. *Let (m, k) be fixed, $\beta'_1 \in \Omega$, $|\arg(\tau e^{\theta})| < \pi$. Let $\lambda'(\cdot, \tau')$, $\tau' \in \mathscr{D}_1(\cdot)$ be the eigenvalue of $T'_m(\cdot, \tau', \theta)$ near the eigenvalue $\lambda(\cdot)$ of $T^0_m(\cdot, \theta)$. Then:*

(1) *The Rayleigh–Schrödinger perturbation expansion $\sum_{n=0}^{\infty} A'_n(\cdot, \beta'_1)(\tau'/2)^n$, $A'_0 = \lambda(\cdot)$, exists and represents a strongly asymptotic expansion (see, e.g., Reed and Simon [15, Sect. XII.4]) for $\lambda'(\cdot, \beta'_1, \tau')$ as $|\tau'| \to 0$, uniformly in $(\beta'_1, |\arg\tau'|) \in \bar{\Omega} \times [0, \frac{3}{2}\pi - \mu_1]$, i.e., given $\mu_1 > 0$ there is $B(\mu_1) > 0$ such that*

$$\begin{aligned} |R_N(\cdot, \tau')| &\equiv \left| \lambda'(\cdot, \tau') - \sum_{n=0}^{N-1} A'_n(\cdot)(\tau'/2)^n \right| \\ &\leqslant B(\mu_1)\, N!\, |\tau'/2|^N, \end{aligned} \tag{3.24}$$

$(\tau', \beta'_1) \in \mathscr{D}_1(\cdot) \times \Omega$, $N = 1, 2, \ldots$.

(2) *The perturbation expansion given above is Borel summable to $\lambda'(\cdot, \beta'_1, \tau')$ for $\tau' \in \mathscr{D}_1(\cdot)$, uniformly in $\beta'_1 \in \Omega$.*

(3) $A'_n(m, k; \beta'_1) = (-1)^n B_n(m, k; \beta'_1)$, $n \in \mathbb{N}$.

Proof. By the Watson–Nevanlinna theorem (for details see Reed and Simon [15, Sect. XII.5] and Sokal [27]), given Proposition III.3(4), (5), assertion (2) is a consequence of (1). We prove (1) by standard arguments of perturbation theory

(see, e.g., Reed and Simon [15, Sects. XII.2–4]). Let $d = d(m, k; \beta'_1)$ be the isolation distance of the eigenvalue $\lambda(\cdot, \beta'_1)$, $0 < v < \frac{1}{2}d$, and let $\Gamma_v = \{z \in \mathbb{C}: |z - \lambda(\cdot)| = v\}$.

Denote by $R'_m(z, \beta'_1, \tau', \theta)$, $R^0_m(z, \beta'_1, \theta)$ the resolvents of $T'_m(\cdot)$, $T^0_m(\cdot)$, respectively. By the norm-resolvent convergence of Proposition III.3 there is a constant $C > 0$ independent of $(\tau', \beta'_1, \theta)$ as long as $\beta'_1 \in \bar{\Omega}$, $|\arg(e^{\theta}\tau')| \leqslant \pi - \mu_1$, $|\tau'| < M_1$, such that

$$\sup_{z \in \Gamma_v} \| R'_m(z, \beta'_1, \tau', \theta) \| \leqslant C, \tag{3.25}$$

and furthermore

$$\| P'_m(\beta'_1; \tau', \theta) - P^0_m(\beta'_1, \theta) \| \to 0 \quad \text{as} \quad |\tau'| \to 0 \tag{3.26}$$

uniformly in $\beta'_1 \in \bar{\Omega}$ and $(|\arg\tau'|, \theta)$, $|\arg(\tau' e^{\theta})| \leqslant \pi - \mu_1$. Here the strong Riemann integrals

$$P'_m(\beta'_1, \tau', \theta) = (2\pi i)^{-1} \int_{\Gamma_v} R'_m(z, \beta'_1, \tau', \theta)\, dz \tag{3.27}$$

and

$$P^0_m(\beta'_1, \theta) = (2\pi i)^{-1} \int_{\Gamma_v} R^0_m(z, \beta'_1, \theta)\, dz \tag{3.28}$$

are the projection operators on the one-dimensional eigenspaces of $\lambda'(\cdot, \beta'_1, \tau')$ and $\lambda(\cdot, \beta'_1)$. If $\phi = \phi(\cdot, \beta'_1, \theta)$ denotes the eigenvector corresponding to $\lambda(\cdot, \beta'_1)$, we have

$$\lambda'(\cdot, \beta'_1, \tau') = \frac{\langle P'_m(\beta'_1, \tau', \theta)\phi, T'_m(\beta'_1, \tau', \theta) P'_m(\beta'_1, \tau', \theta)\phi \rangle}{\langle P'_m(\beta'_1, \tau', \theta)\phi, P'_m(\beta'_1, \tau', \theta)\phi \rangle}. \tag{3.29}$$

Recall now that the Rayleigh–Schrödinger expansion is generated by inserting the geometric expansion of the resolvent in powers of the perturbation, as represented by formulae (2.28), (3.11) with $e^{\theta}u$ in place of u, collecting all the terms having the same power of τ', and performing the integration by the residue method. We also recall that by standard complex-scaling arguments the resulting coefficients $A'_n(\cdot)$ are independent of θ. Now, by standard arguments of singular perturbation theory (see, e.g., Reed and Simon [15, Sects. XII.3, 4] and in particular Morgan and Simon [3] for a specific application to the present case in the non-separated formalism), to see (3.24) it is enough to prove that there are $\sigma(v) > 0$, $C(v) > 0$ independent of $(\beta'_1, \tau', \theta)$, $\beta'_1 \in \bar{\Omega}$, $|\arg(\tau' e^{\theta})| \leqslant \pi - \mu_1$, such that

$$\begin{aligned} \sum_{k_1 + \cdots + k_l = N} \sup_{z \in \Gamma_v} \| R^0_m(z, \beta'_1, \theta)\, F_{k_1}(e^{\theta}u, \beta'_1)\, R^0_m(\cdot) \cdots \\ F_{k_l}(\cdot)\, \phi(\beta'_1, \theta) \| \leqslant C \sigma^N N! \end{aligned} \tag{3.30}$$

and since the number of terms in this sum is dominated by 4^N we need only prove the bound for each term separately. To this end, we first recall that under the present conditions it is well known that there are $\delta_1 > 0$ and $C_1 > 0$ independent of $(\beta'_1, \theta) \in \bar{\Omega} \times \{\theta\colon |\mathrm{Im}\, \theta| \leqslant \pi/2 - \varepsilon,\ \varepsilon > 0\}$ such that $\|e^{\delta_1 u}\phi(\cdot, \beta'_1, \theta)\| \leqslant G'_1$. Furthermore, there is $C_2 > 0$ independent of (β'_1, θ) as above such that

$$\sup_{0 \leqslant \delta \leqslant \delta_1, z \in \Gamma_v} \|e^{\delta u} R^0_m(z, \beta'_1, \theta)\, e^{-\delta u}\| \leqslant C_2. \tag{3.31}$$

To see this, we apply a well-known argument (see, e.g., Hunziker and Pillet [28]): for $f \in D$, we compute

$$e^{\delta u} T^0_m(\beta'_1, \theta)\, e^{-\delta u} f = T^0_m(\beta'_1, \theta)\, f - \delta^2 u + 2e^{-\theta}\delta p f, \qquad p = -i\frac{d}{du}.$$

Now p is obviously $T^0_m(\cdot)$-bounded with relative bound zero, uniformly in $(\beta'_1, \theta) \in \bar{\Omega} \times \{\theta\colon |\mathrm{Im}\, \theta| \leqslant \pi/2 - \varepsilon,\ \varepsilon > 0\}$. Hence (3.13) follows by a standard argument, described, e.g., in Morgan and Simon [3], for δ_1, and hence δ, small enough. Now the rest of the argument goes exactly as in Morgan and Simon [3]. We write

$$\begin{aligned} &R^0_m(z, \beta'_1, \theta)\, F'_{k_1}(e^\theta u, \beta'_1) \cdots F'_{k_l}(\cdot)\, R^0_m(\cdot)\, \phi(\cdot, \beta'_1, \theta) \\ &\quad = \bar{Q}_0 \bar{P}_1 \bar{Q}_1 \cdots \bar{Q}\, e^{\delta u}\phi(\cdot, \beta'_1, \theta) \end{aligned} \tag{3.32}$$

and

$$\bar{P}_i = F'_{k_i}(\cdot)\, e^{-k_i \delta u/N}, \qquad \bar{Q}_i = e^{j_i \delta u/N} R^0_m(\cdot)\, e^{-j_i \delta u/N}, \qquad j_i = \sum_{s=1}^{i} k_s. \tag{3.33}$$

Now $\|\bar{Q}_i\| \leqslant C_2$, and $\|\bar{P}_i\| = \|F'_{k_i}(\cdot)\, e^{-k_i \delta u/N}\|_{L^\infty} \leqslant N^{k_i - 1} C_3$ for some $C_3 > 0$ independent of (β'_1, θ) as above. Thus each term of (3.30) is majorized by $C_3^N C^{N+1} N^N \leqslant C\sigma^N N!$ for some $\sigma(v) > 0$, whence (3.30). Therefore (1), and hence (2), is proved. To see (3), it is enough to remark that $F'(u, \beta'_1, \tau e^{-i\pi}) = G(u, \beta'_1, \tau)$, $\tau > 0$, while the unperturbed operator is the same in both cases and the perturbation expansion is independent of θ. ∎

As an immediate consequence of this proposition we have:

COROLLARY III.5. *The Rayleigh–Schrödinger perturbation expansion* $\sum_{n=0}^{\infty} B_n(m, k; \beta_2)(\tau/2)^n$ *for the eigenvalue* $\mu(m, k; \beta_2, \tau)$ *of* $S_m(\beta_2, \tau)$ *is Borel summable not to* $\mu_\pm(m, k; \beta_2, \tau)$ *but to* $\lambda'(m, k; \beta_2, e^{-i\pi}\tau)$, $\tau > 0$.

The second step in proving Theorem III.2 is represented by the unraveling of the first separation-constant eigenvalues.

PROPOSITION III.6. *Let* $|m| = 0, 1, \ldots,\ \beta'_1 \in \Omega$, $|\arg(\tau' e^{\theta})| < \pi$. *Denote by* $\sigma'(m, \tau', \theta)$ *and* $\sigma_0(m, \theta)$ *the charge spectra of* $T'_m(\cdot)$ *and* $T^0_m(\cdot)$, *respectively, i.e., the sets* $\{\beta'_1 \in \Omega\colon T'_m(\beta'_1, \tau', \theta)$ *has the eigenvalue* $0\}$ *and* $\{\beta'_1 \in \Omega\colon T^0_m(\beta', \theta)$ *has the eigenvalue* $0\}$. *Then*:

(1) $\sigma'(m, \tau', \theta) = \sigma'(m, \tau', 0) \equiv \sigma'(m, \tau')$; $\sigma_0(m, \theta) = \sigma_0(m, 0) \equiv \sigma_0(m)$, *i.e., the charge spectra are independent of* θ.

(2) *For any fixed* $(|m|, k) = 0, 1, \ldots,$ *and any* $\mu_2(m, k) > 0$, *there is* $0 < M_2(m, k) < +\infty$ *such that the condition* $\lambda'(m, k; \beta'_1, \tau) = 0$ *implicitly defines one and only one isolated eigenvalue in* $\sigma'(m, \tau')$ *as a function* $\tau' \mapsto \beta'_1(m, k, \tau')$, *holomorphic for* $0 < |\tau'| < M_2$, $|\arg \tau'| < \pi$, *which admits analytic continuation to the Riemann-surface sector* $\mathscr{D}_2(m, k) = \{\tau'\colon 0 < |\tau'| < M_2;\ |\arg \tau'| < \frac{3}{2}\pi - \mu_1\}$ *across the negative real axis, and is such that* $\beta'_1(m, k; \tau') \to \beta(m, k) = k + \frac{1}{2}(|m| + 1)$ *as* $|\tau'| \to 0$, $\tau' \in \bar{\mathscr{D}}_2(m, k)$.

(3) *The function* $\tau' \mapsto \beta'_1(m, k; \tau')$ *admits an asymptotic expansion to all orders*,

$$\beta'_1(m, k; \tau') \sim \sum_{n=0}^{\infty} L'_m(m, k)(\tau'/2)^n, \qquad L'_0(m, k) = \beta(m, k) \tag{3.34}$$

as $\tau' \to 0$ *within* $\bar{\mathscr{D}}_2(m, k)$. *The coefficients* $L'_m(m, k)$ *can be directly computed through Rayleigh–Schrödinger perturbation theory.*

(4) *The asymptotic expansion* (3.34) *is Borel summable to* $\beta'_1(m, k; \tau')$ *in* $\mathscr{D}_2(m, k)$.

Proof. Assertion (1) is an immediate consequence of dilatation analyticity. To see the subsequent ones, first recall that $\lambda(m, k; \beta'_1) = 0$ if and only if $\beta'_1 = \beta(m, k)$, i.e., $\sigma_0(m) = \bigcup_{k=0}^{\infty} \beta(m, k)$. The corresponding eigenfunctions $\phi(\beta(m, k), \theta) = \phi(m, k, e^\theta u)$ are the Laguerre functions of argument $e^\theta u$. Consider the eigenvalue $\lambda'(m, k; \beta'_1, \tau')$ existing near $\lambda(m, k, \beta'_1)$ for $\beta'_1 \in \Omega$ and $\tau' \in \mathscr{D}_1(m, k)$. By Proposition III.4, uniformly with respect to $\beta'_1 \in \bar{\Omega}$,

$$\lambda'(m, k; \beta'_1, \tau') = \lambda(m, k; \beta'_1) + O(m, k; \tau'/2) \tag{3.35}$$

as $|\tau'| \to 0$ within $\bar{\mathscr{D}}_1(m, k)$. Furthermore (see Buchholz [24]), $\lambda(m, k; \beta'_1) = \frac{1}{4} - (\beta'_1)^2/4[k + \frac{1}{2}(|m| + 1)]^2$ and thus $\beta(m, k) \in \Omega$, $(\partial\lambda/\partial\beta'_1)(m, k; \beta'_1)|_{\beta'_1 = \beta(m,k)} \neq 0$. Hence (3.35) implies, by continuity, that

$$\frac{\partial y}{\partial \beta'_1}(m, k; \beta'_1, \tau') \neq 0$$

for $|\beta'_1 - \beta(m, k)|$ suitably small and $\tau' \in \mathscr{D}_1(m, k)$, $|\tau'|$ suitably small. Since $\lambda'(m, k; \beta(m, k), \tau') \to \lambda(m, k; \beta(m, k)) = 0$ as $\tau' \to 0$ within $\bar{\mathscr{D}}_1(m, k)$, assertion (2) is a direct consequence of the analytic implicit-function theorem (see, e.g., Gallavotti [29, Appendix G]). Furthermore, the analytic implicit-function theorem also implies that $\beta'_1(m, k; \tau')$ has finite derivatives of all orders as $\tau' \in \bar{\mathscr{D}}_2(m, k) \to 0$. To compute these derivatives, viz., the coefficients $L'_n(m, k)$, notice that $\beta(m, k)$ satisfies the ordinary differential equation $e^{\theta}ut^0_m(0, \theta)\,\phi(m, k; e^{\theta}u) = \beta(m, k)\,\phi(m, k; e^{\theta}u)$. Hence if we consider the ODE eigenvalue problem

$$[e^{\theta}ut^0_m(0, \theta) + e^{\theta}uF(m, e^{\theta}u, \beta'_1, \tau')]\,\phi'(m, k; e^{\theta}u, \tau') = \beta'_1\phi'(m, k; e^{\theta}u, \tau') \tag{3.36}$$

on $L^2(\mathbb{R}^+; d\chi)$, $d\chi = u^{-1}du$, with boundary boundary condition $\phi'(m, \cdot) = O(u^{1/2 + |m|/2})$ as $u \downarrow 0$, we generate the coefficients $L'_n(m, k)$ recursively through Rayleigh-Schrödinger perturbation theory. Note that this formal procedure is justified because $\|\phi'(m, k; \tau', \theta)\,u^{-1}\|$ is bounded independently of $|\tau'|$, and $[e^{\theta}u(T^0_m(0, \theta) - z)]^{-1}e^{\theta}uF'_n(m, e^{\theta}u, \beta'_1) = [T^0_m(0, \theta) - z]^{-1}\,F_n(m, e^{\theta}u, \beta'_1)$. Finally, assertion (4) follows by Proposition A.1. ∎

COROLLARY III.7. *Let $(|m|, k) = 0, 1,...$ be fixed, and let $\tau > 0$. Then the separation-constant eigenvalue doublet $\beta_2^{\pm}(m, k, \tau)$ implicitly defined by $\mu_{\pm}(m, k, \beta_2, \tau) = 0$ admits an asymptotic Rayleigh–Schrödinger perturbation expansion*

$$\beta_2^{\pm}(m, k; \tau) \sim \sum_{n=0}^{\infty} L_n(m, k)(\tau/2)^n, \qquad L_0 = \beta(m, k), \tag{3.37}$$

which is Borel summable not to $\beta_2^{\pm}(m, k)$ but to $\beta'_1(m, k, e^{-i\pi}\tau)$.

Proof. The expansion (3.37) can be generated as in Proposition III.6(3) considering this time the ODE eigenvalue problem $[vs^0_m(0) + vG(\beta_2, \tau, v)]\,\psi(m, k; \tau, v) = \beta_2(m, k; \tau, v)$ (see Proposition II.3, (2.29)-(2.30), (3.11)) on $L^2(\mathbb{R}^+, d\chi)$ with boundary condition $\psi(m, \cdot, v) = O(v^{1/2 + |m|/2})$ as $v \downarrow 0$. Here, as usual,

$$s^0_m(\beta_2) = -\frac{d^2}{dv^2} - \frac{\beta_2}{v} + \frac{m^2 - 1}{4v^2} + \frac{1}{4}.$$

By Corollary III.5, we have $L_n(m, k) = (-1)^n L'_n(m, k)$, with $L'_n(m, k)$ as in (3.34). Therefore the assertion is implied by (4) of Proposition III.6.

The analysis of the operator family $T_m(\beta_1, \beta_2, \tau)$ is now straightforward. By exactly the same arguments as in Propositions III.3 and III.4, we obtain:

PROPOSITION III.8. *Let $(\beta_1, \beta_2, \tau) \in \Omega \times \Omega \times \{\tau\colon |\arg \tau| < \pi\}$, Ω as in Proposition III.3. Let $T_m(\beta_1, \beta_2, \tau)$ be the operator family on $L^2(0, +\infty)$ defined by the differential expression $t_m(\beta_1, \beta_2, \tau)$ on D, D as in Proposition III.3. Then:*

(1) *$(\beta_1, \beta_2, \tau) \mapsto T_m(\beta_1, \beta_2, \tau)$, $|m| = 0, 1,...$ is a type-A, real-holomorphic family of m-sectorial operators in $(\beta_1, \beta_2, \tau) \in \Omega \times \Omega \times \{\tau\colon |\arg \tau| < \pi\}$, and thus self-adjoint for $(\beta_1, \beta_2, \tau) \in \mathbb{R}$.*

(2) *$\sigma_{ess}(T_m(\cdot)) = [\frac{1}{4}, +\infty)$ for any $(\beta_1, \beta_2, \tau) \in \Omega \times \Omega \times \{\tau\colon |\arg \tau| < \pi\}$.*

(3) *Given $\mu_3(m, j) > 0$ there is $M_3(m, j) > 0$ such that each eigenvalue $\lambda(m, j, \beta_1)$ of $T^0_m(\beta_1)$ is stable as an eigenvalue $\lambda(m, j; \beta_1, \beta_2, \tau)$ for $|\tau| < M_3$, $|\arg \tau| < \pi$; the function$(\beta_1, \beta_2, \tau) \to \lambda(m, j, \beta_1, \beta_2, \tau)$ is holomorphic in (β_1, β_2, τ), jointly for $0 < |\tau| < M_3$, $|\arg \tau| < \pi$, and locally in $(\beta_1, \beta_2) \in \Omega \times \Omega$, and admits analytic continuation with respect to τ to the Riemann-surface sector $\mathscr{D}_3(m, j) = \{\tau\colon 0 < |\tau| < M_3(m, j);\ |\arg \tau| < \frac{3}{2}\pi - \mu_3\}$ across the negative real axis. Furthermore, $\lim \lambda(m, j, \beta_1, \beta_2, \tau) = \lambda(m, j, \beta_1)$ as $\tau \to 0$ within $\mathscr{D}_3(m, j)$ uniformly in $(\beta_1, \beta_2) \in \bar{\Omega} \times \bar{\Omega}$.*

(4) *The Rayleigh–Schrödinger perturbation expansion*

$$\sum_{n=0}^{\infty} A_n(m, j; \beta_1, \beta_2)(\tau/2)^n, \qquad A_0 = \lambda(m, j, \beta_1),$$

exists, represents a strong asymptotic expansion for $\lambda(m, j; \beta_1, \beta_2, \tau)$ as $\tau \to 0$, $\tau \in \bar{\mathscr{D}}_3(m, j)$, uniformly with respect to $(\beta_1, \beta_2) \in \bar{\Omega} \times \bar{\Omega}$, and is Borel summable to $\lambda(m, i; \beta_1, \beta_2, \tau)$ in $\mathscr{D}_3(m, j)$, uniformly in (β_1, β_2) as above.

These results, together with Proposition III.6, Proposition A.1, and Corollary A.2, immediately imply:

COROLLARY III.9. *For $\tau \in \mathscr{D}_3(m, j)$, consider the eigenvalue $\lambda(m, j; \beta_1, \beta_2, \tau)$ and the β'_1-separation-constant eigenvalue $\tau' \to \beta'_1(m, k; \tau')$ of Proposition III.6, $\tau' \in \mathscr{D}_2(m, k)$, $(|m|, j, k) = 0, 1,...$ Then:*

(1) *The function $\tau \to \lambda(m, j; \beta_1, \beta'_1(m, k, \tau e^{-i\pi}), \tau)$ is holomorphic in (β_1, τ) for $0 < |\tau| < M_4(m, j, k) = \min(M_2(\cdot), M_3(\cdot))$, $0 < \arg \tau < \pi$, locally in $\beta_1 \in \Omega$. Furthermore, $\lambda(\cdot, \beta'_1(\cdot, \tau e^{-i\pi}), \tau)$ admits analytic continuation to the Riemann-surface sector $\mathscr{D}_4(m, j, k) = \{\tau\colon 0 < |\tau| < M_4(\cdot), -\pi/2 + \mu_4(\cdot) < \arg \tau < \frac{3}{2}\pi - \mu_4(\cdot)\}$, $\mu_4(m, j, k) = \max(\mu_1(\cdot), \mu_2(\cdot))$, across the real axis, with $\lim \lambda(m, j; \beta_1, \beta'_1(m, k, \tau e^{-i\pi}), \tau) = \lambda(m, j, \beta_1)$ as $\tau \to 0$ within $\bar{\mathscr{D}}_4(m, j, k)$, uniformly with respect to $\beta_1 \in \bar{\Omega}$.*

(2) *The Rayleigh–Schrödinger perturbation expansion for $\lambda(m, j; \beta_1, \beta'_1(m, k, \tau e^{-i\pi}), \tau)$, viz.,*

$$\lambda(m, j; \beta_1, \beta'_1(m, k, \tau e^{-i\pi}), \tau) \sim \sum_{n=0}^{\infty} A_n(m, j, k; \beta_1)(\tau/2)^n, \tag{3.38}$$

exists, is strongly asymptotic to $\lambda(\cdot, \tau)$ as $\tau \to 0$ within $\bar{\mathscr{D}}_4(\cdot)$, uniform in $\beta_1 \in \bar{\Omega}$, and is Borel summable to $\lambda(m, j, \beta_1, \beta'_1(m, k, \tau e^{-i\pi}), \tau)$ in $\mathscr{D}_4(m, j, k)$, uniformly with respect to $\beta_1 \in \bar{\Omega}$.

Remark. Equation (3.38) is also the perturbation expansion of $\lambda(m, j; \beta_1, \beta_2^{\pm}(m, k; \tau), \tau)$, because $\beta_2^{\pm}(m, k, \tau)$ and $\beta'_1(m, k, e^{-i\pi}\tau)$ have the same perturbation expansion.

The β_1 spectrum is now determined as follows:

PROPOSITION III.10. *For* $(|m|, j, k) = 0, 1, \ldots,$ *consider the eigenvalue* $(m, j; \beta_1, \beta_1'(m, k; \tau e^{-i\pi}), \tau)$ *of* $T_m(\beta_1, \beta_1'(e^{-i\pi}\tau), \tau)$. *Then*:

(1) *The condition that*

$$\lambda(m, j; \beta_1, \beta_1'(m, k; \tau e^{-i\pi}), \tau) = 0 \tag{3.39}$$

implicitly defines a function $\tau \mapsto \beta_1(m, j, k)$, *which is holomorphic for* $0 < |\tau| < M_4(m, j, k)$, $0 < \arg\tau < \pi$, *admits analytic continuation to the Riemann-surface sector* $\mathscr{D}_4(m, j, k)$, *and is such that* $\lim \beta_2(m, j, k; \tau) = \beta(m, i) = i + \frac{1}{2}(|m| + 1)$ *as* $\tau \to 0$ *within* $\mathscr{D}_4(m, j, k)$.

(2) *The implicit function* $\tau \mapsto \beta_1(m, j, k; \tau)$ *admits the Rayleigh–Schrödinger perturbation expansion*

$$\beta_1(m, j, k) \sim \sum_{n=0}^{\infty} L_n(m, j, k)(\tau/2)^n, \qquad L_0 = \beta(m, i) \tag{3.40}$$

as a strongly asymptotic expansion as $\tau \to 0$, $\tau \in \mathscr{D}_4(m, j, k)$. *The expansion* (3.40) *is Borel summable to* $\beta_1(m, j, k; \tau)$ *for* $\tau \in \mathscr{D}_4(m, j, k)$.

Proof. (1) Since $\lambda(m, j, \beta(m, j)) = 0$, proceeding as in Proposition III.6 we have to prove only that

$$\frac{\partial\lambda}{\partial\beta_1}(m, j; \beta_1, \beta_1'(m, k, \tau e^{-i\pi}, \tau)) \neq 0$$

for β_1 in a neighborhood of $\beta(m, j)$ and $\tau \in \mathscr{D}_4(m, j, k)$ with M_4 suitably small. In turn, by Proposition III.8(4) it is enough to check that

$$\frac{\partial}{\partial\beta_1} A_0(m, j, k; \beta_1)\bigg|_{\beta = \beta(m, j)} \neq 0,$$

which is true because $A_0(m, j; k, \beta_1) = \lambda(m, j, \beta_1) = \frac{1}{4} - \beta_1^2/4[j + \frac{1}{2}(|m| + 1)]^2$. Assertion (2) is again proved as in Proposition III.6(3) and Proposition A.1, given Proposition 3.9(1) and (2). We note that by the remark after Proposition III.9 the functions $\tau \mapsto \beta_1(m, j, k; \tau)$ and $\tau \mapsto \beta_1(m, j; \beta_2(m, k; \tau), \tau)$ have the same perturbation expansion (3.40). ∎

Proof of Theorem III.2. Setting $M(m, j, k) = \min\{M_1(\cdot), \ldots, M_4(\cdot)\}$, $\mu(m, j, k) = \max\{\mu_1(\cdot), \ldots, \mu_4(\cdot)\}$, assertion (1) is proved in Proposition III.6, and assertion (2) in Proposition III.10. Assertion (3) follows from (1), (2), and the analytic local-invertibility theorem, because

$$\frac{\partial}{\partial\tau}[\tau\gamma_1(m, j, k; \tau)^{-1}] = (j + k + |m| + 1)^{-1} + O(m, j, k; \rho) \qquad \text{as } \tau \to 0$$

within $\mathscr{D}(m, j, k)$. Finally, note that by Proposition III.4(3), Corollaries III.5, III.7, and III.9, and Proposition III.10, and the analytic local-invertibility theorem, the function $\rho \to -\frac{1}{2}[\gamma_1(m, j, k; \Gamma_1(m, j, k; \rho))]^{-2}$ admits an asymptotic expansion to all orders as $\rho \to 0$ within $\mathscr{D}(m, j, k)$. Hence assertions (4) and (5) are direct consequences of Corollary III.7, Proposition III.10(2), Propositions A.1 and A.2, and Reed and Simon [15, Problem XII.26]. ∎

IV. IMAGINARY PARTS, ASYMPTOTICS, AND THE FORMULA OF BRÉZIN AND ZINN-JUSTIN

As stated in the first section, our program now is to relate the Borel sum $E_1(m, i, k; \rho)$ of the $1/R$ expansion to the fundamental quantities of the problem, viz., the eigenvalue gap and the asymptotics of the coefficients of the $1/R$ series itself. In this section, the quantum numbers m, j, and k are fixed and may have any allowed value. Although eigenvalues, expansion coefficients, wavefunctions, error estimates, etc., all depend on these numbers, to avoid notational complexity that dependence will be indicated only where necessary. Since the coefficients of the $1/R$ expansion are real, Im E_1 must have zero asymptotic expansion as $\rho \to 0$. In fact, the asymptotic behavior of Im E_1 is determined to leading exponential order by the following statement.

THEOREM IV.1. *Let* $E(m, j, k; \rho)$ *be the Borel sum of the* $1/R$ *expansion near the eigenvalue* $E(m, j, k) = -\frac{1}{2}(|m| + j + k)^{-2}$ *of* $-\frac{1}{2}\Delta - |x|^{-1}$ *of magnetic quantum number* m *and parabolic quantum numbers* (j, k), $(|m|, j, k) = 0, 1, \ldots,$ *and let* $n = |m| + j + k + 1$ *be the principal quantum number. Then, as* $|\rho| \downarrow 0$, $\rho \in \mathbb{R}$,

$$\operatorname{Im} E_1(m, j, k; \rho) = -\pi C(m, j, k)\left(\frac{2}{n\rho}\right)^{2|m| + 4k + 2} \times e^{-2/|\rho| n}(1 + O(n, j, k; \rho^{1/2})) \tag{4.1}$$

with

$$C(m, j, k) = n^{-3}[k!(k + |m|)!]^{-2}e^{-2n}. \tag{4.2}$$

Here, and everywhere else, $O(m, j, k, \rho^{1/2})$ *means order* $\rho^{1/2}$ *as* $\rho \to 0$ *with coefficients depending on* (m, j, k). *This theorem will be proved in this section by adapting the* ODE *techniques of Harrell and Simon* [6], *which are in essence rigorously justified* JWKB *estimates. Before turning to that analysis, we note that the asypmtotics of the* $1/R$ *expansion and the formula of Brézin and Zinn-Justin are simple consequences of Theorems* IV.1 *and* III.2 *along with the rigorously known gap estimates of Harrell* [13].

COROLLARY IV.2. *Let* $E_N(m, j, k)$ *be the Nth coefficient of the* $1/R$ *expansion near the eigenvalue* $E(m, j, k)$ *of* H_0. *Then*:

(1) *As* $N \to \infty$,

$$E_N(m, j, k) = C(m, j, k)\, n^N 2^{-N}(N + 4k + 2m + 1)!\,(1 + O(m, j, k; N^{-1/2}))$$
$$= -e^{-2n} n^{N-3}[k!(|m| + k)!]^{-2} 2^{-N}(N + 4k + 2m + 1)!$$
$$\cdot (1 + O(m, j, k; N^{-1/2})). \tag{4.3}$$

(2) *Let* $\rho > 0$, *and* $\Delta E(m, j, k; \rho)$ *be the gap between the two eigenvalues in the doublet near* $E(m, j, k)$ *as* $\rho \downarrow 0$. *Then, as* $\rho \downarrow 0$,

$$-\operatorname{Im} E_1(m, j, k; \rho) = \pi n^3 (\Delta E(m, j, k); \rho)^2 (1 + O(m, j, k; \rho)). \tag{4.4}$$

Remark. Equation (4.4) is the formula of Brézin and Zinn-Justin, rewritten in the language of the Borel sum. Formula (4.6) below shows that the asymptotic behavior of E_N is controlled by the eigenvalue gap as well, which was the numerical discovery of Brézin and Zinn-Justin [5].

Proof. (1) We use a standard approximate dispersion relation argument which goes back to Simon's paper on the anharmonic oscillator [27]. By Theorem III.2(4), the function $\rho \mapsto E_1(m, j, k; \rho)$ is holomorphic for $0 < |\rho| < M$, $0 < \arg \rho < \pi$, and analytic up to the real boundary of this half-circle. If Γ_ε denotes the half-circle $|z| = \varepsilon < M$, $0 \leqslant \arg z \leqslant \pi$, by Cauchy's theorem,

$$E_1(m, j, k; \rho) = \frac{1}{2\pi i} \int_{\Gamma_\varepsilon} \frac{E_1(m, j, k; z)}{z - \rho}\, dz. \tag{4.5}$$

Therefore, by Taylor's theorem and the reality of the perturbation coefficients,

$$E_N(m, j, k) = \frac{1}{2\pi} \int_{-\varepsilon}^{\varepsilon} z^{-N-1} \operatorname{Im} E_1(m, j, k; z)\, dz + O(\varepsilon^{-N}), \tag{4.6}$$

and hence (4.1) yields (4.3). Furthermore, assertion (2) is an immediate consequence of (4.1), (4.2), and the known estimate [13]

$$\Delta E(m, j, k; \rho) = e^{-n} n^{-3} [k!(k + |m|)!]^{-1}$$
$$\cdot \left(\frac{2}{n\rho}\right)^{|m| + 2k + 1} e^{-1/\rho n}(1 + O(\cdot, \rho^{1/2})). \quad ∎ \tag{4.7}$$

To prove Theorem IV.1 it is necessary to estimate the imaginary parts first of $\beta'_1(\cdot, \tau e^{-i\pi})$ and then of $\beta_1(\cdot, \beta'_1(\cdot, e^{-i\pi}\tau), \tau)$, $\tau \in \mathbb{R}$. As already mentioned, we will make use of the JWKB technique of Harrell [30] and Harrell and Simon [6]. We note in passing that a more sophisticated (but so far not rigorously justified) approach based on the Langer–Cherry refinement of the JWKB method [31] makes the computation of all exponential corrections possible. This is the content of the second paper announced in [14].

The first preliminary result is as follows:

PROPOSITION IV.3. *For* $\tau > 0$, $\operatorname{Im} \theta > 0$, *let*

$$q'(m; \beta'_1, \tau, e^\theta u) = \frac{1}{4} - e^{-\theta} \beta'_1 u^{-1} - (2r - e^\theta u)^{-1} \beta'_1$$
$$+ \frac{m^2 - 1}{4} [(2r - e^\theta u)^{-2} + 2e^{-\theta} u^{-1} (2r - e^\theta u)^{-1}] \tag{4.8}$$

and

$$\beta'_1(m, k; \tau e^{-i\pi}) = \beta'_1(m, k; \tau) = \beta'_1(\cdot, \tau). \tag{4.9}$$

Let $t_2 = t_2(m, k, \tau)$ *be the greatest solution in* $0 \leqslant u \leqslant 2r$ *of* $q'(m, k\beta(m, k), \tau, u) = 0$, *and let* $\phi'_1(\cdot, \tau, e^\theta u)$ *denote once again the eigenvector corresponding to* $\beta'_1(\cdot, \tau)$ *in* $\sigma'(m, \tau)$. *Then*:

(1) $\lim_{\operatorname{Im}\theta \downarrow 0} \phi'_1(\cdot, \tau, e^\theta u) = \phi'_1(\cdot, \tau, u)$ *exists, uniformly in* $0 \leqslant u \leqslant t_2$.

(2) *For* $0 < a \leqslant t_2$,

$$\operatorname{Im} \beta'_1(\cdot, \tau) = \frac{\phi'_1(\cdot, \tau, u) \dfrac{d}{du} \bar{\phi}'_1(\cdot, \tau, u)\Big|_{u=a} - \bar{\phi}'_1(\cdot, \tau, u) \dfrac{d}{du} \phi'_1(\cdot, \tau, u)\Big|_{u=a}}{2i \int_0^a |\phi'_1(\cdot, \tau, u)|^2 (u^{-1} + (2r - u)^{-1})\, du}. \tag{4.10}$$

Proof. By Propositions III.5 and III.6, ϕ'_1 is the solution in $L^2(0, +\infty)$ of the ODE

$$\left(-e^{-2\theta} \frac{d^2}{du^2} + q'(m, \beta'_1(\cdot, \tau), \tau, e^\theta u)\right) \phi'_1(\cdot, \tau, e^\theta u) = 0 \tag{4.11}$$

for $0 < \operatorname{Im} \theta < \pi/2$. It is well known from standard techniques of asymptotic integration (see, e.g., Hille [32], Olver [33]) that the subdominant solution of (4.11) as $|u| \to \infty$, $u \in \mathbb{C}$, is unique up to constants as long as $|\arg(e^\theta u)| < \pi/2$. Therefore, we can replace the condition $\phi'_1(\cdot, u) \in L^2(0, +\infty)$ by the condition $\phi'_1(\cdot, u) \in L^2(C, d|u|)$, where C is any contour in the complex half-plane $u \in \mathbb{C}$, $\operatorname{Re} u \geqslant 0$, lying above the singularity at $u = 2re^{-\theta}$. For example, $C = C_1 \cup C_2$; $C_1 = \{u \in \mathbb{C}\colon \operatorname{Im} u = 0,\ 0 \leqslant \operatorname{Re} u \leqslant 2(r - \bar{r}),\ \operatorname{Re} u \geqslant 2(r + \bar{r})\}$; $C_2 = \{u \in \mathbb{C}\colon |u - 2r| = 2\bar{r}$: $\operatorname{Im} u > 0\}$ for some fixed $\bar{r}(m, k) > 0$. Since the regular, subdominant solution of (4.11) is continuous at $\operatorname{Im} \theta = 0$ uniformly with respect to $u \in C$, and the eigenvalues are independent of θ, we may henceforth assume $\operatorname{Im} \theta = 0$. The point $2(r - \bar{r})$ can be taken as the greatest solution $t_2(m, k)$ in $(0, 2r)$ of $q'(m, \beta'_1(\cdot, \tau), \tau, u) = 0$ (the "large turning point"). Formula (4.10) then follows by a standard partial integration argument. In particular

$$\operatorname{Im} \beta_1'(\cdot, \tau) = \frac{\phi_1'(\cdot, t_2) \frac{d}{du} \bar{\phi}_1'(\cdot, u)\Big|_{u=t_2} - \bar{\phi}_1'(\cdot, t_2) \frac{d}{du} \phi_1'(\cdot, u)\Big|_{u=t_2}}{2i \int_0^{t_2} |\phi_1'(\cdot, u)|^2 (u^{-1} + (2r-u)^{-1})\, du}. \quad \blacksquare \tag{4.12}$$

Equation (4.12) is the standard formula for estimating imaginary parts, and in order to evaluate it we shall exhibit a patched-together comparison function $\chi(m, k, \tau, u) = \chi(\cdot, \tau, u)$ such that

$$\phi_1'(\cdot, \tau, u) = \chi(\cdot, \tau, u)(1 + \varepsilon(\cdot, \tau, u)), \tag{4.13}$$

where $|\varepsilon(\cdot, \tau, u)| + |(d\varepsilon/du)(\cdot, \tau, u)| = O(\tau^\alpha)$ for some $\alpha = \alpha(m, k) > 0$, $0 \leqslant u \leqslant t_2$.

Since the subsequent arguments are essentially adaptations to the present case of those of Harrell [30] and Harrell and Simon [6], we shall be somewhat sketchy. We begin by stating the following:

DEFINITION IV.4. Let $\Omega(\tau) \subset \mathbb{C}$ be the closure of an open, bounded, simply connected set for $\tau \geqslant 0$. Let $(u, \tau) \mapsto f(u, \tau)$, $(u, \tau) \mapsto g(u, \tau)$ be the functions from $\Omega(\tau) \times [\bar{\tau}, +\infty)$ to $\mathbb{C}$, $0 < \bar{\tau} < \infty$. Let $f, g \in C^2(\Omega(\tau) \times I_1)$, where I_1 is any compact subinterval of $[\bar{\tau}, +\infty)$, and let f, g be analytic in $u \in \Omega(\tau)$. Then we say that f is uniformly approximated by g in $\Omega(\tau)$ as $\tau \to 0$ if there exist $\alpha > 0$, $\gamma > 0$, $\tau_0 < \bar{\tau}$ independent of (u, τ) such that for all $u \in \Omega(\tau)$ and $\tau < \tau_0$,

$$f(u, \tau) = g(u, \tau)(1 + \varepsilon(u, \tau)), \tag{4.14}$$

where

$$|\varepsilon(u, \tau)| + \left|\frac{d\varepsilon}{du}(u, \tau)\right| < \gamma\tau^\alpha.$$

If $\Omega_1, \ldots, \Omega_j$ are several such domains, then we say that f is uniformly approximated by $g_1, \ldots, g_j$ on their union, provided (4.14) holds on each domain separately, and if C is a contour in such a domain or set of domains, we say that f is uniformly approximated on C by $g_1, \ldots, g_j$.

Remarks. (1) It is easily seen that this is an equivalence relation: in particular we shall make use of the observation that if f is uniformly approximated by g and g is uniformly approximated by h, then f is uniformly approximated by h.

(2) Since Eq. (4.11) for $\tau = 0$, $\theta = 0$ is the confluent hypergeometric equation in Whittaker's form (see, e.g., Buchholz [24]), the standard Picard approximation procedure yielding existence and uniqueness for the ODE Cauchy problem shows that with a suitable choice of normalization $\phi_1'(\cdot, \tau, u)$ is uniformly approximated for $u \in [0, 1]$ by the Whittaker function $W_{\beta(m,k),m/2}(u)$. We remark that $W_{\beta(m,k),m/2}(u)$ is an equivalent way of writing the unperturbed eigenvectors of Remark (3) after Proposition II.2, denoted by $\phi(m, k, u)$ in Proposition III.6: $\phi(m, k, u) = W_{\beta(m,k),m/2}(u)$.

(3) Let $\Omega_1(\tau) = \{u \in \mathbb{C}\colon \operatorname{Re} u \geqslant r^{1/2},\ \operatorname{Im} u \geqslant 0,\ |u - 2r| \geqslant r^{1/2}\}$. Then $\phi_1'(\cdot, \tau, u)$ is uniformly approximated in $\Omega_1(\tau)$ by the JWKB-type function

$$\psi_-(\cdot, \tau, u) = K(\cdot, \tau)\, q'(\cdot, \tau, u) \exp\left(-\int_{t_1}^{u} q'(\cdot, u')^{1/2} du'\right), \tag{4.15}$$

where $t_1(m, k; \tau)$ is the zero of $q'(\cdot, \tau, u)$ near $\frac{1}{2}[\beta_1'(\cdot) + (\beta_1'(\cdot))^2 + (m^2 - 1)/4]^{1/2}$, and

$$K(\cdot, \tau) = r^{\beta_1(\cdot)} \sqrt{2}\, e^{-\sqrt{r/2}} \exp\left(\int_{t_1}^{r} q'(\cdot, u')^{1/2} du'\right). \tag{4.16}$$

The branch of the square root here and elsewhere is taken such that $\operatorname{Re}(q')^{1/2} > 0$ as $u \to \infty$. Formulae (4.15) and (4.16) are immediate conseqences of a theorem of Olver [33] and the estimate of the error control function given in Appendix B.

(4) When there are several domains of uniform approximation they may either touch at isolated points or overlap, and the overall approximating function may have jump discontinuities.

The foregoing remarks show that a uniform approximation has to be constructed only for $1 \leqslant u \leqslant \sqrt{r}$ and $0 < a \leqslant |u - 2r| \leqslant \sqrt{r}$. To this end we apply the variation-of-parameters technique of Harrell and Simon [6]. The result is as follows:

LEMMA IV.5. *Let* $\Omega_2(\tau) = C \cap \{u\colon \operatorname{Re} u \geqslant 2r - \sqrt{r}\}$, *where* C *is as in Proposition* IV.3, *and* $\Omega_3(\tau) = \{u\colon 1 \leqslant u \leqslant \sqrt{r}\}$. *Then*:

(1) *For* $u \in \Omega_3(\tau)$, $\phi_1'(\cdot, \tau, u)$ *is uniformly approximated by* $W_{\beta(m,k),m/2}(u)$ *with* $\alpha = 1/2$.

(2) *For* $u \in \Omega_2(\tau)$, $\phi_1'(\cdot, \tau, u)$ *is uniformly approximated by* $\phi_-(\cdot, \tau, u)$ *with* $\alpha = 1/2$, *where*

$$\phi_-(\cdot, \tau, u) = T(\cdot, \tau)\, W_{-\beta(\cdot),m/2}(u - 2r) + b(\cdot, \tau)\, W_{\beta(\cdot),m/2}(e^{i\pi}(u - 2r)), \tag{4.17}$$

$$T(\cdot, \tau) = 2K(\cdot, \tau)^2 \exp\left(-\int_{t_1}^{t_2} q'(m, \beta_1'(\cdot), \tau, u)\, du\right) \times (1 + O(\cdot, \tau^{1/2})) \qquad \text{as } \tau \to 0; \tag{4.18}$$

with $K(\cdot, \tau)$ *as in* (4.16), *and*

$$T(\cdot, \tau)^{-1} b(\cdot, \tau) = O(r^{\beta_1(\cdot,\tau)} e^{-\sqrt{r}}) \qquad as \quad \tau \to 0. \tag{4.19}$$

Proof. We first sketch the proof of (2). Following the variation-of-parameters technique of Harrell and Simon [6] (the reader is referred to that reference for a fully detailed description), for $u \geqslant 2r + \sqrt{r}$, set

$$\phi_-(\cdot, \tau, u) = K(\cdot, \tau, u)\, q'(m, \beta(m, k), \tau, u)^{-1/4} \cdot \exp\left(\int_{r_1}^{u} q'(m, \beta(m, k), \tau, u')^{1/2} du'\right), \tag{4.20}$$

so that

$$-\phi''_-(\cdot, u) + A(\cdot, u)\,\phi_-(\cdot, u) = 0, \qquad u \geqslant 2r + \sqrt{r}, \tag{4.21}$$

for some function $(\tau, u) \mapsto A(\cdot, \tau, u)$ analytic in u and C^1 in τ. Let $\phi\ (\cdot, u)$ be C^1 at $u = 2r + \sqrt{r}$ and solve

$$\left[-\frac{d^2}{du^2} - \frac{1}{4} + \frac{\beta(m, k)}{u - 2r} + \frac{m^2 - 1}{4(2r - u)^2} + \frac{m^2 - 1}{4}\left[(2r - u)^{-2} + 2u^{-1}(2r - u)^{-1}\right]\right]\phi_-(\cdot, u) = 0, \tag{4.22}$$

where u belongs to C, $2r - \sqrt{r} \leqslant \operatorname{Re} u \leqslant 2r + \sqrt{r}$, i.e., $\bar{r} = \sqrt{r}$. Simple matching at $u = 2r + \sqrt{r}$ with the use of the asymptotic formulae for Whittaker's functions (see, e.g., Abramowitz and Stegun [34], Buchholz [24]) shows that, on $C \cap \{u: 2r - \sqrt{r} \leqslant \operatorname{Re} u\}$,

$$\phi_-(\cdot, \tau, u) = T(\cdot, \tau)\, W_{-\beta(m,k),m/2}(u - 2r) + b W_{\beta(m,k),m/2}(e^{i\pi}(u - 2r)), \tag{4.23}$$

where $T(\cdot, \tau)$ is given by (4.18) and $b(\cdot, \tau)/T(\cdot, \tau)$ satisfies (4.19). Furthermore, let $(u, \tau) \to \phi_+(\cdot, u, \tau)$ be defined as the unique function which satisfies (4.21) and is a simple multiple of $W_{\beta(m,k),m/2}(e^{i\pi}(u - 2r))$ on C. It is straightforward to check that $W(\phi_-, \phi_+) = 1$, where $W(\cdot)$ denotes the Wronskian of (ϕ_-, ϕ_+), and that

$$\begin{aligned} B(\cdot, \tau, u) \equiv q'(\cdot, \tau, u) - A(\cdot, \tau, u) &= 0(\cdot, \tau), && u \in C, \\ &= 0(\cdot, (u - 2r)^{-2}), && u \geqslant 2r + \sqrt{r}. \end{aligned} \tag{2.24}$$

Furthermore, with the aid of the estimates on Whittaker's functions (see Buchholz [24] or Abramowitz and Stegun [34]) it is also easy to check that

$$\int_u^\infty B(\cdot, \tau, u')\,\phi_+(\cdot, \tau, u')\,\phi_-(\cdot, \tau, u')\,du' = O(\cdot, \tau^{1/2}),$$

$$\int_u^\infty B(\cdot, u', \tau)\,\phi_-(\cdot, u', \tau)^2 du' = O(\cdot, \tau^{1/2}),$$

$$\int_u^\infty B(\cdot, u', \tau), \phi_+(\cdot, u', \tau)^2 \int_v^\infty B(\cdot, v, \tau)\,\phi_-^2(\cdot, v, \tau)\,dv\,du' = O(\cdot, \tau^{1/2}). \tag{4.25}$$

Therefore it follows, as in Harrell and Simon [6], that on $\Omega_2(\tau)$

$$\begin{aligned} \phi'_1(\cdot, \tau, u) &= a_-(\cdot, \tau, u)\,\phi_-(\cdot, \tau, u) + a_+(\cdot, \tau, u)\,\phi_+(\cdot, \tau, u), \\ \frac{d}{du}\phi'_1(\cdot, \tau, u) &= a_-(\cdot, \tau, u)\frac{d\phi_-}{du}(\cdot, \tau, u) + a_+(\cdot, \tau, u)\frac{d\phi_+}{du}(\cdot, \tau, u), \end{aligned} \tag{4.26}$$

where $a_-(\cdot, \tau, u) = 1 + O(\cdot, \tau^{1/2})$, $a_+(\cdot, \tau, u) = O(\cdot, \tau^{1/2})$. The same technique also proves that $\phi'_1(\cdot)$ is uniformly approximated by $W_{\beta(m,k),m/2}(u)$ on $[0, \sqrt{r}]$. This time use as comparison functions $\psi_-(\cdot)$ from (4.15), uniquely extended in a C^1-fashion to a linear combination of $W_{\beta(m,k),m/2}(u)$, $W_{-\beta(m,k),m/2}(e^{i\pi}u)$ on $[1, \sqrt{r}]$, and $\psi_+(\cdot) = \text{const}\ W_{-\beta(m,k),m/2}(e^{i\pi}u)$ on $[1, \sqrt{r}]$, extended to be a linear combination of $\psi_-(\cdot)$ and (dominantly) of $q'(\cdot)^{-1/4}\exp(\int_r^u q'(\cdot, u')^{1/2}du')$. Then a straightforward verification of (4.25) and the asymptotic formulae of Whittaker's functions show that $\phi'_1(\cdot, \tau, u)$ is uniformly approximated by $\psi_-(\cdot, \tau, u)$, which is in turn uniformly approximated by $W_{\beta(m,k),m/2}(u)$ on $[1, \sqrt{r}]$. Since we already know that $\phi'_1(\cdot, \tau, u)$ is uniformly approximated by $W_{\beta(m,k),m/2}(u)$ on $[0, 1]$, the lemma is proved. ∎

The estimate of the imaginary part is now easy to obtain:

PROPOSITION IV.6. *Let (m, k) be fixed. Then, as $\tau \downarrow 0$,*

$$\begin{aligned} \operatorname{Im} \beta'_1(m, k; \tau) &= -\pi \frac{T(m, k; \tau)^2}{[k!(|m| + k)!]^2}(1 + O(\tau^{1/2})) \\ &= \frac{-\pi(2r)^{2|m| + 4k + 2}}{[k!(|m| + k)!]^2} e^{-2/\tau}(1 + O(\tau^{1/2})). \end{aligned} \tag{4.27}$$

Remark. In the notation of Section II, by (4.8) formula (4.27) yields the behavior of $\operatorname{Im} \beta'_1(m, k; e^{-i\pi}\tau)$ as $\tau \to 0$. Furthermore, by the approximate dispersion-relation argument recalled in the proof of Corollary IV.2, integrating this time over the boundary of the circle $\Delta_\varepsilon = \{\tau: |\tau| = \varepsilon,\ 0 < \varepsilon < M_1(m, k)\}$ cut along the negative real axis, (4.27) yields the asymptotics of the coefficients $L_N(m, k)$,

$$L_N(m, k) = [k!(|m| + k)!]^{-2}(N + 4k + 2|m| + 1)!(1 + O(m, k; N^{-1/2})). \tag{4.28}$$

By the estimate of Harrell [13], it also yields the formula analogous to that of Brézin and Zinn-Justin (formula (4.4)) for the separation constant β_2,

$$-\operatorname{Im} \beta'_1(m, k; \tau e^{-i\pi}) = \pi\Delta\beta_2(m, k, \tau)^2(1 + O(m, k; \tau^{+1/2})), \tag{4.29}$$

where $\Delta\beta_2(\cdot) = \beta_2^+(\cdot) - \beta_2^-(\cdot)$, $\beta_2^\pm$ being of course implicitly defined by $\mu_\pm(\cdot, \beta_2, \tau) = 0$ (see Corollary III.7).

Proof. $\operatorname{Im}\beta'_1(m,k;\tau)$ is given by (4.12). By definition of $t_2(m,k)$ and Lemma IV.5(1) we have

$$\int_0^{t_2(m,k)} |\phi'_1(m,k;\tau,u)|^2(u^{-1}+(2r-u)^{-1})\,du$$

$$=\left[\int_0^{\infty} W^2_{\beta(m,k),m/2}(u)\,u^{-1}du\right]\cdot(1+0(m,k;\tau^{1/2}))$$

$$=\left[(k!)^2\int_0^{\infty} e^{-u}u^m(L_k^{(m)}(u))^2du\right](1+O(m,k;\tau^{1/2}))$$

$$=k!(k+|m|)!\,[1+O(m,k;\tau^{1/2})], \tag{4.30}$$

where the well-known formulae on integrals of Whittaker and Laguerre functions (see (Buchholz [24, pp. 23, 115]) have been used. Furthermore, by Lemma IV.5(2)

$$\phi'_1(m,k;\tau,t_2)\frac{d}{du}\bar\phi'_1(m,k;\tau)\Big|_{u=t_2}-\bar\phi'_1(m,k;\tau,t_2)\frac{d}{du}\phi'_1(m,k,\tau u)\Big|_{u=t_2}$$

$$=T(m,k;\tau)^2W\{W_{-\beta(m,k),m/2}(u),W_{-\beta(m,k),m/2}(e^{-2\pi i}u)\}(1+O(\cdot,\tau^{1/2})). \tag{4.31}$$

Now, as proved in Appendix B,

$$T(m,k;\tau)=(2r)^{2|m|+1+2k}e^{-2/\tau}(1+O(\cdot,\tau^{3/2})) \tag{4.32}$$

and (see Buchholz [24, p. 27])

$$W\{W_{-\beta(m,k),m/2}(u),W_{-\beta(m,k),m/2}(e^{-2\pi i}u)\}$$

$$=-\frac{2\pi i\,e^{-\pi i\beta(m,k)}}{\left[\Gamma\left(\frac{m+1}{2}+\beta(m,k)\right)\right]\left[\Gamma\left(\beta(m,k)-\frac{m}{2}\right)\right]}$$

$$W\{W_{-\beta(m,k),m/2}(u),W_{\beta(m,k),m/2}(e^{i\pi}u)=-2\pi i/[k!(|m|+k)!]. \tag{4.33}$$

Inserting (4.30)–(4.33) into (4.12), we get (4.27). ∎

COROLLARY IV.7.

$$\operatorname{Im}\beta_1(m,j,\beta'_1(m,k;\tau e^{-i\pi}),\tau)\equiv\operatorname{Im}\beta_1(m,j;\beta'_1(m,k;\tau),\tau)$$
$$\equiv\operatorname{Im}\beta_1(m,j,k;\tau)=-2\tau\operatorname{Im}\beta'_1(m,k;\tau)(1+O(\cdot,\tau))\qquad as\quad \tau\downarrow 0. \tag{4.34}$$

Proof. Denoting the eigenvector $\phi_1(m,j;\beta'_1(\cdot,\tau),\tau)$ corresponding to $\beta_1(m,j,k;\tau)$ simply as $\phi_1(\cdot)$, taking the imaginary part of the ODE $t_m(\beta_1(\cdot,\tau),\beta'_1(\cdot,\tau),\tau)\,\phi_1(\cdot)=0$, multiplying by $\phi_1(\cdot)$, and integrating, we get

$$\operatorname{Im}\beta_1(m,j,k;\tau)=-2\frac{\operatorname{Im}\beta'_1(m,k,\tau)\int_0^\infty|\phi_1(\cdot)|^2(u+2r)^{-1}du}{\int_0^\infty|\phi_1(\cdot)|^2u^{-1}du+\int_0^\infty|\phi_1(\cdot)|^2(u+2r)^{-1}du},$$

whence (4.34) easily follows in the limit $\tau\to 0$. ∎

PROPOSITION IV.8. *As* $\tau\downarrow 0$,

$$\operatorname{Im}\gamma_1(m,j,k;\tau)=\operatorname{Im}\beta'_1(m,j,k;\tau)(1+O(\cdot,\tau)), \tag{4.35}$$

while for $\tau\uparrow 0$,

$$\operatorname{Im}\gamma_1(m,j,k;\tau)=\pi(-1)^m\frac{(j+2k+|m|+1)!\,(j+2k+2|m|+1)!}{j!(k+|m|)!}$$
$$\cdot 16(j+k+|m|+1)^4(2r)^{-2|m|-2-4k}e^{-2/|\tau|}(1+O(\cdot,|\tau|^{1/2})). \tag{4.36}$$

Proof. For $\tau\downarrow 0$, i.e., $\tau>0$, (4.35) is an immediate consequence of (4.32) by the definition of γ_1 (see Theorem III.2). For $\tau<0$, i.e., $\tau=|\tau|\,e^{+i\pi}$, once more by Theorem III.2 we can write

$$\gamma_1(\cdot;\tau)|_{\tau<0}=\beta_1(\cdot;\beta'_1(\tau e^{-i\pi}),\tau)|_{\tau<0}+\beta'_1(\cdot;\tau e^{-i\pi})|_{\tau<0}.$$

Now $\beta'_1(\cdot;\tau e^{-i\pi})|_{\tau<0}=\beta'_1(\cdot;|\tau|)$ is real, and therefore $\operatorname{Im}\gamma_1(\cdot;\tau)|_{\tau<0}=\operatorname{Im}\beta_1(\cdot;\beta'_1(|\tau|),\tau)|_{\tau<0}$, where the right side is defined in Corollary III.10. The argument leading to (4.36) is, up to the obvious modifications, identical to that of IV.5 and Proposition IV.6 applied this time to the limit as $\operatorname{Im}\theta\downarrow 0$ of the equation (see (3.18))

$$t_m(\beta_1,\beta'_1(\cdot;|\tau|),\tau,\theta)\,\phi_1=0,$$

and can therefore be omitted. ∎

Proof of Theorem IV.1. By (4.35), (4.36), and (4.27), as $|\tau|\downarrow 0$, $\tau\in\mathbb{R}$,

$$\operatorname{Im}\gamma_1(m,j,k;\tau)=-\pi\frac{(2r)^{2|m|+2+4k}e^{-2/|\tau|}}{[k!(|m|+k)!]^2}(1+O(\cdot,|\tau|^{1/2})). \tag{4.37}$$

Now the inverse function $\rho\to\Gamma_1(m,j,k;\rho)$ of $\tau\mapsto\tau\gamma_1(m,j,k,\tau)^{-1}$ exists and enjoys the properties stated in Theorem III.2(5). To see (4.1), it is enough to observe that with $n=|m|+j+k+1$, by Propositions III.6(3) and III.10(2), we can write

$$\tau\gamma_1(m,j,k;\tau)^{-1}=\tau n^{-1}+\tau^2+O(\cdot,\tau^3)\qquad\text{as}\quad|\tau|\downarrow 0, \tag{4.38}$$

and thus $\Gamma_1(\cdot,\rho)=n\rho-n^3\rho^2+O(\cdot,\tau^3)$ as $|\tau|\downarrow 0$. Furthermore,

$$\begin{aligned}\operatorname{Im}[-\tfrac{1}{2}\gamma_1(\cdot,\tau)]^{-2} &= [\operatorname{Re}\gamma_1(\cdot,\tau)\operatorname{Im}\gamma_1(\cdot,\tau)]/[(\operatorname{Re}\gamma_1(\cdot,\tau))^2+(\operatorname{Im}\gamma_1(\cdot,\tau))^2]^2\\ &= n^{-3}\operatorname{Im}\gamma_1(\cdot,\tau)(1+O(\cdot,\tau))\end{aligned}$$

by (4.37) and (4.36). Therefore (3.14) and (4.37) immediately yield (4.1). ∎

APPENDIX A

For the sake of completeness, in this appendix we prove some results about Borel summability of composed and implicit functions, because we do not know of any study where they may have been worked out before. We first prove that under certain circumstances Borel summability is stable under composition of functions.

PROPOSITION A.1. *Let* $D=\{z\in\mathbb{C}:\ 0<|z|<M,\ |\arg z|<\pi/2\}$; *let* $x\mapsto f(x)$, $y\mapsto F(y)$ *be analytic in* D, *continuous in* $\bar{D}$, *and let* f, F *admit strongly asymptotic expansions as* $x\to 0$, $y\to 0$, *in* $\bar{D}$, *respectively, of the form*

$$\begin{aligned}&f(x)\sim x\sum_{n=0}^{\infty}a_kx^k,\\ &|R_N(x)|\equiv\left|\frac{f(x)}{x}-\sum_{k=0}^{N-1}a_kx^k\right|\leqslant A^{N+1}N!|x|^N,\qquad N=1,\ldots,\end{aligned}\tag{A.1}$$

$|x|\to 0$ *in* $\bar{D}$, A *independent of* $x\in\bar{D}$,

$$\begin{aligned}&F(y)\sim\sum_{i=0}^{\infty}b_iy^i,\\ &|Q_N(y)|\equiv\left|F(y)-\sum_{i=0}^{N-1}b_iy_i\right|\leqslant A_1^{N+1}N!|y|^N,\qquad N=1,\ldots,\end{aligned}\tag{A.2}$$

$|y|\to 0$ *in* $\bar{D}$, A_1 *independent of* $y\in\bar{D}$.

Then $F\circ f=F(f(x))$ *admits a strongly asymptotic expansion as* $x\to 0$ *in* $\bar{D}$:

$$\begin{aligned}&F(f(x))\sim\sum_{l=0}^{\infty}c_lx^l,\\ &|P_N(x)|\equiv\left|F(f(x))-\sum_{l=0}^{N-1}c_lx^l\right|\leqslant C^{N+1}N!|x|^N,\qquad N=1,\ldots,\end{aligned}\tag{A.3}$$

as $|x|\to 0$ *in* $\bar{D}$, *with* C *independent of* $x\in\bar{D}$.

Remarks. (1) Our definition of strongly asymptotic expansion is that of Reed and Simon [15, Sect. XII. 4]. We recall that by the Watson–Nevanlinna theorem (for further details see Sokal [26]) the stated analyticity bounds of the type (A.1), (A.2), (A.3) imply Borel summability for $0\leqslant x\leqslant A^{-1}$, $0\leqslant y\leqslant A^{-1}$, $0\leqslant x\leqslant C^{-1}$, respectively.

(2) The functions $\rho\mapsto\Gamma_1(m,j,k;\rho)$ and $\tau\mapsto\gamma_1(m,j,k;\tau)$ of Section II fulfill the conditions of f and F, respectively.

Proof. In the sense of formal power series,

$$\left(\sum_{k=0}^{\infty}a_kx^k\right)^2=\sum_{n=0}^{\infty}a_n^{(2)}x^n,\qquad a_n^{(2)}=\sum_{i=0}^{n}a_ia_{n-i},$$

so

$$\begin{aligned}|a_n^{(2)}|\leqslant|2a_na_0|+\sum_{i=1}^{n-1}|a_ia_{n-i}|&\leqslant 2A^{n+2}n!+\sum_{i=1}^{n-1}\frac{i!(n-i)!}{n!}A^{n+2}\\ &\leqslant 3A\cdot A^{n+1}n!\end{aligned}$$

by (A.1), since $i!(n-i)!/n\leqslant 1/n$. Iterating, we get

$$\begin{aligned}&\left(\sum_{n=0}^{\infty}a_kx^k\right)^i=\sum_{n=0}^{\infty}a_n^{(i)}x^n,\qquad i=2,\ldots\\ &|a_n^{(i)}|\leqslant 3A^{(i-1)}A^{n+1}n!,\end{aligned}\tag{A.4}$$

Therefore $F(f(x))$ has the asymptotic expansion

$$\begin{aligned}&F(f(x))\sim\sum_{i=1}^{\infty}b_ix^i\left(\sum_{n=0}^{\infty}a_kx^k\right)^i\sim\sum_{i=1}^{\infty}b_ix^i\sum_{k=0}^{\infty}a_k^{(i)}x^k\sim\sum_{n=0}^{\infty}c_nx^n,\\ &c_n=\sum_{i=0}^{n}a_{n-i}^{(i)}b_i.\end{aligned}\tag{A.5}$$

Now,

$$|c_n|\leqslant\sum_{i=0}^{n}|b_ia_{n-i}^{(i)}|\leqslant A^1A^{n+1}n!+\sum_{i=1}^{n}A^{i+1}(3A)^{i-1}A^{n+1-i}(n-i)!\,i!\tag{A.6}$$

by (A.4), and hence

$$|c_n|\leqslant A^{n+2}n!+A^{n+2}(3A)^{n-1}2(n!)\leqslant(3A)^nA^{n+1}n!.\tag{A.7}$$

Therefore (A.3) is implied by (A.2) if we insert (A.4) and (A.7) in (A.2) itself. ∎

COROLLARY A.2. *Let* $x\mapsto f(x)$ *be as in Proposition* A.1, *with strong asymptotic expansion* $\sum_{k=1}^{\infty}a_kx^k$, *and let* $(z,y,x)\mapsto F(z,y,x)$ *be analytic in* $(z,y,x)\in\{z:|z|\leqslant 1\}\times\{y:\ |y|<1\}\times D$, *continuous in* $\bar{D}$ *uniformly in* (z,y), *and let* $F(z,y,x)$

admit a strongly asymptotic expansion as $x \to 0$ in $\bar{D}$ uniformly with respect to (z, y). Then the function $(z, x) \to F(z, f(x), x)$ is analytic in $\{z: |z| < 1\} \times D$, continuous in $\bar{D}$ uniformly with respect to z, and admits a strongly asymptotic expansions as $x \to 0$ in $\bar{D}$ uniformly with respect to z.

Remark. The functions $(\beta_1, \beta_2, \tau) \mapsto \lambda(\cdot, \beta_1, \beta_2, \tau)$ and $\tau \to \beta'_1(m, k, e^{-in}\tau) - \beta(m, k)$ fulfill the conditions of F and f, respectively.

PROPOSITION A.3. *Let $(y, x) \mapsto F(y, x)$ be as in Proposition A.2, and let $x \mapsto \delta(x) = xf(x)$, where $f(x)$ is analytic in D, continuous in $\bar{D}$, and admits the asymptotic expansion*

$$f(x) \sim \sum_{n=0}^{\infty} c_n x^n \qquad as \quad x \to 0 \text{ in } \bar{D}. \tag{A.8}$$

Then, if $F(\delta(x), x) = 0$, $x \in \bar{D}$, the expansion (A.8) represents a strongly asymptotic expansion for $x \mapsto f(x)$ in $\bar{D}$.

Remarks. (1) The Borel summability statement for the inverse function is a particular case of this statement: it is enough to take $(y, x) \mapsto F(y, x) \equiv F(y) - x$.

(2) The functions $(\beta'_1, \tau') \mapsto \lambda'(m, k; \beta'_1, \tau')$ and $\tau' \mapsto \beta'_1(m, k; \tau')$ satisfy the conditions of F and f, respectively, so that $\tau' \mapsto \delta(m, k; \tau') = \beta'_1(m, k; \tau') - \beta(m, k)$ satisfies the conditions of $x \mapsto \delta(x)$. In fact, it suffices to rewrite the operator $T'_m(\beta'_1, \tau')$ as the action on $D(T'_m(\cdot))$ of the differential expression

$$\tilde{T}'_m = -\frac{d^2}{du^2} + \frac{\delta}{u} + \frac{\delta}{u + 2r'} - \frac{\beta(m, k)}{u} + \frac{\beta(m, k)}{u + 2r'} + \frac{m^2 - 1}{4}\left((2r' + u)^{-2} - 2u^{-1}(2r' + u)^{-1}\right)$$

and to note that all its eigenvalues $\tilde{\lambda}(m, k, \delta, \tau')$ are such that (cf. Proposition III.6) $(\partial\tilde{\lambda}/\partial\delta)(m, k; \delta, \tau')|_{\delta = 0, \tau' = 0} \neq 0$.

Proof. By assumption, $F(\delta, x)$ admits the strongly asymptotic expansion $F(\delta, x) = \sum_{i,k=0}^{\infty} a_{ik} x^i \delta^k$, with

$$|a_{ik}| \leqslant B^k A^{i+1} i! \tag{A.9}$$

for some $B > 0$, $A > 0$. Write

$$f(x)^n = \sum_{k=0}^{\infty} c_k^{(n)} x^k, \qquad c_n^{(0)} = \delta_{0,k}, \qquad c_k^{(1)} = c_k, \qquad k = 0, 1, \ldots, \tag{A.10}$$

$$F(\delta(x), x) \sim \sum_{i,k=0}^{\infty} a_{ik} x^{i+k} \sum_{j=0}^{\infty} c_j^{(k)} x^j \equiv \sum_{n=0}^{\infty} d_n x^n,$$
$$d_n = \sum_{i=0}^{n} \sum_{k=0}^{n-i} a_{ik} c_{n-k-i}^{(k)}. \tag{A.11}$$

We now prove that (A.9) and the equation $F(\delta(x), x) = 0$ imply the existence of constants $D > 0$, $C > 0$ such that

$$|c_n| \leqslant DC^n n!. \tag{A.12}$$

Let us proceed by induction. We have $|c_1| < D$ for some $D > 0$. Assuming (A.12) true for $k \leqslant n - 2$, let us prove it for $k = n - 1$. Notice that if (A.12) is true up to $k = n - 2$, then

$$|c_{n-2}^{(k)}| \leqslant (3D)^{k-1} DC^{n-2}(n-2)!. \tag{A.13}$$

We now compute

$$c_{n-1} = -(a_{01})^{-1}\left(\sum_{i=1}^{n}\sum_{k=1}^{n-i} a_{ik} c_{n-k-i}^{(k)} + \sum_{i=0}^{n} a_{i0} c_{n-i}^{(0)} + \sum_{k=0}^{n} a_{0k} c_{n-k}^{(k)}\right)$$
$$= -(a_{01})^{-1}\left(\sum_{i=1}^{n}\sum_{k=1}^{n-i} a_{ik} c_{n-k-i}^{(k)} + a_{n0} + \sum_{k=2}^{n} a_{0k} c_{n-k}^{(k)}\right).$$

Hence

$$|c_{n-1}| \leqslant |a_{01}|^{-1}\left(\sum_{i=1}^{n}\sum_{k=1}^{n-i} B^k A^{i+1} i!(3D)^{k-1} DC^{n-k-i}(n-k-i)! + A^{n-1} n! + \sum_{k=2}^{n} AB^k(3D)^{k-1} DC^{n-k}(n-k)!\right)$$
$$\leqslant AB|a_{01}|^{-1}\left(\sum_{i=1}^{n} A_i i! \sum_{n=1}^{n-i} (3DB)^{k-1} C^{-k-i+1} \frac{(n-k-i)!}{(n-1)!} + \left(\frac{A}{C}\right)^{n-1}(A/D)\frac{n}{B} + \sum_{k=2}^{n}(3BD)^{k-1} C^{-(k-1)} \frac{(n-k)!}{(n-1)!}\right) DC^{n-1}(n-1)!$$
$$\leqslant AB|a_{01}|^{-1} DC^{n-1}(n-1)!\left(\sum_{i=1}^{n}\left(\frac{A}{C}\right)^i i! \sum_{j=0}^{n-i-1}\left(\frac{3BD}{C}\right)^j \frac{1}{j!} \cdot \frac{j!(n-1-i-j)!(n-i-1)!}{(n-i-1)!(n-1)!} + \left(\frac{A}{D}\right)\left(\frac{A}{C}\right)^{n-1}\frac{n}{B} + \sum_{j=0}^{n-2}\left(\frac{3BD}{C}\right)\left(\frac{3BD}{C}\right)^j \frac{1}{j!}\frac{j!(n-2-j)!}{(n-2)!}\frac{1}{(n-1)}\right)$$
$$\leqslant AB|a_{01}|^{-1} DC^{n-1}(n-1)!\left(\sum_{i=1}^{n}(A/C)^i \frac{i!(n-i-1)!}{(n-1)!}(3e)^{(3BD/C)} + \left(\frac{A}{D}\right)\left(\frac{A}{C}\right)^{n-1}\frac{n}{B} + \frac{3}{(n-1)}\left(\frac{3BD}{C}\right)e^{(3BD/C)}\right)$$

$$\leqslant AB|a_{01}|^{-1}DC^{n-1}(n-1)!\left(\sum_{j=0}^{n-1}\left(\frac{A}{C}\right)^{j+1}(j+1)\frac{j!(n-1-j)!}{(n-1)!}\right.$$
$$\left.\cdot(3e)^{(3BD/C)}+\left(\frac{A}{D}\right)\left(\frac{A}{C}\right)^{n-1}\frac{n}{b}+\frac{3}{(n-1)}\left(\frac{3BD}{C}\right)e^{(3BD/C)}\right)$$
$$\leqslant AB|a_{01}|^{-1}(n-1)!\left(9\left(\frac{A}{C}\right)(3e)^{(3BD/C)}+\left(\frac{A}{D}\right)\left(\frac{A}{C}\right)^{n-1}\frac{n}{B}\right.$$
$$\left.+\frac{9BD}{(n-1)C}e^{(3BD/C)}\right)\leqslant DC^{n-1}(n-1)!,$$

if we choose $1<A$, $B\ll D\ll C$, since by assumption

$$\left|F(\delta,x)-\sum_{i,k=0}^{N-1}a_{ik}x^i\delta^k\right|\leqslant B^NA^{N+1}|\delta|^N|x|^NN!$$

as $x\to 0$, $x\in\bar{D}$, (A.11) and (A.12) imply that

$$\left|f(x)-\sum_{k=0}^{n-1}c_nx^n\right|\leqslant DC^NN!|x|^n \qquad \text{as} \quad x\to 0 \text{ in } \bar{D},$$

which proves the assertion. ∎

Appendix B

In this appendix we compute the tunneling factor $T(\cdot)$ used in (4.17), (4.18) and bound the error-control function needed to justify formulae (4.15) and (4.16).

We begin with the error-control function, which is the total variation of

$$q'(\cdot,u)^{-1/4}\frac{d^2}{du^2}q'(\cdot,u)^{-1/4}=-\frac{1}{4}\left(\frac{d^2}{du^2}q'(\cdot,u)\right)q'(\cdot,u)^{-3/2}$$
$$+\frac{5}{16}\left(\frac{d}{du}q'(\cdot,u)\right)^2q'(\cdot,u)^{-5/2} \tag{B.1}$$

for $r^{1/2}\leqslant u\leqslant 2r-r^{1/2}$. It has to be shown that this quantity tends to 0 as $r\to\infty$, i.e., $\tau\to 0$. Now, from the definition of $q'(\cdot,u)$ in (4.7) with $\theta=0$, it is easy to see that, uniformly in u, $r^{1/2}<u<2r-r^{1/2}$, $q'(\cdot,u)^{-1}=O(1)$, $(d/du)\,q'(\cdot,u)=O(\tau)$, $(d^2/du^2)\,q'(\cdot,u)=O(\tau^{3/2})$ as $\tau\downarrow 0$. Thus

$$q'(\cdot,u)^{-1/4}\frac{d^2}{du^2}q'(\cdot,u)^{-1/4}=O(\tau^{3/2}) \qquad \text{as} \quad \tau\downarrow 0.$$

Since $q'(\cdot,u)$ is a rational function of u and τ, the total variation of this quantity is also the integral of a function $O(\tau^{3/2})$, and is thus $O(\tau^{1/2})$.

Next we estimate $K(\cdot)$ and $T(\cdot)$, defined in (4.16) and (4.18). We claim:

Proposition B.1.

$$T(m,k;\tau)=2\tau^{-(|m|+2k+1)}e^{-1/\tau}(1+O(\cdot,\tau^{1/2})) \qquad \text{as} \quad \tau\downarrow 0.$$

Proof. Because of the uniformity of the approximations, it suffices to determine T by asymptotic matching. The quantity $K(\cdot)$ of (4.16) is determined to leading order by the condition that

$$K(m,k;\tau)\,q'(\cdot,\beta_1'(\cdot\,\tau),\tau,u)^{-1/4}\exp\left(-\int_{t_1}^{u}q'(\cdot,u')\,du'\right)$$
$$=W_{\beta(m,k),m/2}(u)\cdot(1+O(\cdot,\tau^{1/2}))$$

at $u=\sqrt{r}$ (say). Thus we may set

$$K(m,k;\tau)=\tau^{-\beta(m,k)/2}e^{-1/2\tau^{1/2}}\exp\left(\int_{t_1}^{\tau^{-1/2}}q'(\cdot,\tau,u;)\,du'\right), \tag{B.2}$$

with the aid of an expansion of Buchholz [24].

Then $T(\cdot)$ is determined by

$$T(m,k;\tau)=2[K(m,k;\tau)]^2\exp\left(-\int_{t_1}^{r/2}[q'(\cdot,\tau,u')]^{1/2}du'\right)$$
$$\cdot(1+O(\cdot,\tau^{1/2})).$$

Since

$$\int_{t_1}^{r+1/2}q'((\cdot),\tau,u')^{1/2}=\int_{2r-\sqrt{r}}^{2r}q'(\cdot,\tau,u')^{1/2}du',$$

we get

$$T(m,k;\tau)\tau^{\beta(m,k)}e^{-\tau^{-1/2}}\exp\left(-\int_{\sqrt{r}}^{2r-\sqrt{r}}q'(\cdot,u')^{1/2}du'\right)(1+O(\cdot,\tau^{1/2}))$$
$$=\tau^{-\beta(m,k)}e^{-\tau^{-1/2}}\exp\left(-2\int_{\sqrt{r}}^{r}\left(\frac{1}{4}-\beta(\cdot)\,u^{-1}-\beta(\cdot)(2r-u)^{-1}\right.\right.$$
$$\left.\left.+\frac{m^2-1}{4}(u^{-1}+(2r-u)^{-2})\,du\right)(1+O(\cdot,\tau^{1/2}))$$
$$=\tau^{-\beta(\cdot)}e^{-\tau^{-1/2}}\exp\left(-\int_{\sqrt{r}}^{r}(1-2\beta(\cdot)\,u^{-1}-2\beta(\cdot)(2r-u)^{-1})\,du\right)$$
$$\cdot(1+O(\cdot,\tau^{1/2}))$$
$$=\tau^{-\beta(\cdot)}\exp(-\tau^{-1/2})\exp(\tau^{-1}+\tau^{-1/2}+2\beta(\cdot)\ln(\tau^{1/2})$$
$$+2\beta(\cdot)\ln(2\tau^{-1/2}-1))\cdot(1+O(\cdot,\tau^{1/2}))$$
$$=\left(\frac{\tau}{2}\right)^{-2\beta(m,k)}e^{-\tau^{-1}}(1+O(\cdot,\tau^{1/2})). \quad ∎$$

References

1. L. D. Landau and E. M. Lifshitz, "Quantum Mechanics," Pergamon, New York, 1965.
2. M. Aventini and R. Seiler, *Commun. Math. Phys.* **41** (1975), 119–134.
3. J. D. Morgan III and B. Simon, *Int. J. Quantum Chem.* **17** (1980), 1143–1166.
4. E. Brézin, G. Parisi, and J. Zinn-Justin, *Phys. Rev. D* **16** (1977), 408–415.
5. E. Brézin and J. Zinn-Justin, *J. Phys. Lett.* **40** (1979), L511–512.
6. E. M. Harrell II and B. Simon, *Duke Math. J.* **47** (1980), 845–902.
7. S. Graffi and V. Grecchi, *Commun. Math. Phys.* **62** (1978), 83–94.
8. I. W. Herbst, *Commun. Math. Phys.* **64** (1979), 279–301.
9. S. Graffi and V. Grecchi, *Commun. Math. Phys.* **79** (1981), 91–113.
10. I. W. Herbst and B. Simon, *Commun. Math. Phys.* **80** (1981).
11. S. Graffi and V. Grecchi, *Phys. Lett. B* **121** (1983), 910–914.
12. B. Simon, *Int. J. Quantum Chem.* **21** (1982), 1–25.
13. E. M. Harrell II, *Commun. Math. Phys.* **75** (1980), 239–261.
14. R. J. Damburg, R. Kh. Propin, S. Graffi, V. Grecchi, E. M. Harrell II, J. Čížek, J. Paldus, and H. J. Silverstone, *Phys. Rev. Lett.* **52** (1984), 1112–1115.
15. M. Reed and B. Simon, "Methods of Modern Mathematical Physics," Vols. I–IV, Academic Press, New York, 1975–1979.
16. T. Kato, "Perturbation Theory for Linear Operators," Springer-Verlag, New York, 1966.
17. J. M. Combes, P. Duclos, and R. Seiler, *in* "Rigorous Atomic and Molecular Physics, Proceedings, 4th International School of Mathematical Physics, Erice, Italy, 1980," Plenum, New York, 1981.
18. W. Hunziker and E. Vock, *Commun. Math. Phys.* **83** (1982), 281–302.
19. G. G. T. Jacobi, "Gesammelte Werke," Vol. VIII, "Vorlesungen über Dynamik," Berlin, 1884 (reprinted by Chelsea, New York, 1969).
20. M. Born, "Vorlesungen über Atommechanik," Springer-Verlag, Berlin, 1925.
21. M. P. Strand and W. P. Reinhardt, *J. Chem. Phys.* **70** (1979), 3812–3827.
22. J. N. Komarov, L. J. Ponomarev, and S. J. Slavianov, "Coulomb and Spheroidal Wave Functions," Nauka, Moscow, 1965. [In Russian]
23. W. Magnus, F. Oberhettinger, and R. P. Soni, "Special Functions of Mathematical Physics," Springer-Verlag, New York, 1966.
24. H. Buchholz, "The Confluent Hypergeometric Function," Springer-Verlag, New York, 1969.
25. N. Dunford and J. T. Schwartz, "Linear Operators," Vol. II, Interscience, New York, 1963.
26. A. Sokal, *J. Math. Phys.* **21** (1980), 261–268.
27. B. Simon, *Ann. Phys. (N.Y.)* **58** (1970), 76–136.
28. W. Hunziker and C. A. Pillet, *Comm. Math. Phys.* **90** (1983), 219–233.
29. G. Gallavotti, "The Elements of Mechanics," Springer-Verlag, New York, 1982.
30. E. M. Harrell II, *Int. J. Quantum Chem.* **21** (1982), 199–207.
31. H. J. Silverstone, E. M. Harrell II and C. Grot, *Phys. Rev. A* **24** (1981), 1925–1934.
32. E. Hille, "Ordinary Differential Equations in the Complex Domain," Wiley, New York, 1976.
33. F. W. J. Olver, "Asymptotics and Special Functions," Academic Press, New York, 1974.
34. M. Abramowitz and I. A. Stegun (Eds.), "Handbook of Mathematical Functions," NBS Appl. Math. Series 55, National Bureau of Standards, Washington, D.C., 1964.

List of Symbols

$a_{\pm}$	Eq. (4.26)
A	Eq. (4.21)
A_n	below Eq. (3.13)
A'_n	below Eq. (3.13)
B	Eq. (4.24)
B_n	below Eq. (3.13)
B'_n	below Eq. (3.13)
C	Lemma IV.5
$\mathcal{C}$	Thm. III.2
$\mathcal{D}$	Thm. III.2
E	Prop.II.1; Eqs. (2.5), (2.14)
$E_{\pm}$	Prop. II.1
E_n	Eq. (2.33)
E'	Prop. III.1
E'_n	Propo. III.1
f	Eq. (2.10)
F	Eq. (2.27)
F_n	Eq. (2.28)
F_n	Eq. (3.11)
F_s	Eq. (3.15)
g	Eq. (2.10)
G	Eq. (2.29)
G_n	Eq. (2.29)
G'_n	Eq. (3.12)
H	Prop. II.1
H_0	Prop. II.1
$H^2(\mathbb{R}^3)$	Prop. II.1
H_m	Eq. (2.23)
H'	Prop. III.1
j	Prop. II.2
k	Prop. II.2
K	Eq. (4.15)
L_n	Eq. (2.19)
L'_n	below Eq. (3.15)
m	Prop. II.2
M	Props. II.1, II.3
M_n	Prop. II.1
M'_n	below Eq. (3.13)
n	Props. II.1, II.2
p	Eq. (3.16)
p_n	Prop. II.1
P^0_m	Eq. (3.28)
P'_m	Eq. (3.27)
$\bar{P}_i$	Eq. (3.33)
q	Eq. (3.17)
q'	Eq. (4.8)
$\bar{Q}_i$	Eq. (3.33)
r	Eq. (2.5)
R	Eq. (1.1)
R_N	Eq. (3.24)
R^0_m	Eq. (3.28)
R'_m	Eq. (3.25)
s_m	Eq. (2.9)
S_m	Prop. II.2
t_2	Prop. IV.3
t_m	Eq. (2.9)
t^0_m	Eq. (2.15)
T	Eq. (4.18)
T_m	Prop. II.2
T^0_m	Prop. II.2
T_m	Thm. III.2
[illegible]	Eq. (2.8)
U	Eq. (2.24)
v	Eq. (2.8)
V	Eq. (2.24)
W_n	Prop. III.1
$W_{\beta,m;2}$	below Def. IV.4
x_k	Eqs. (1.1), (2.2)
$Z_{A,B}$	Eq. (1.1)
α	Eq. (2.4)
β	Eq. (2.15)
β_k	Eq. (2.5)
β_1	Thm. III.2
γ	Eqs. (2.5), (3.8)
γ_1	Thm. III.2
Γ	Props. II.2, III.1
Γ_1	Thm. III.2
ϵ	Eq. (4.13)
η	Eq. (2.1)
λ	Props. II.2, II.3, III.1
λ'	Prop. III.3
μ	Props. II.3, III.1
μ_1	Prop. III.3
$\mu_{\pm}$	Eq. (2.35)
ξ	Eq. (2.1)
ρ	Prop. II.1
ρ'	Prop. III.1
σ'	Prop. III.6
σ_0	Prop. III.6
τ	Eq. (2.5); Prop. II.3
τ'	below Eq. (3.13)
$\tilde{\tau}$	Prop. II.2
ϕ	Eq. (2.1)
ϕ_1	Prop. IV.3
ϕ_-	Eq. (4.17)
ϕ_+	Eq. (4.25)
ψ	Eqs. (2.3), (2.20)
ψ_-	Eq. (4.15)
χ	Prop. III. ; Eq. (4.13)
ω	Eq. (2.19)
Ω	Eq. (2.19); Prop. III.3

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POTENTIALS HAVING EXTREMAL EIGENVALUES SUBJECT TO p-NORM CONSTRAINTS

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Abstract

+V

We consider the Sturm-Liouville operator $H_V = \frac{-d^2}{dt^2}$ on certain subsets of the real line with various selfadjoint boundary conditions. We find the optimal upper and lower bounds for the eigenvalues of H_V when the potential V obeys a constraint of the form $\|V\|_p \le M$. We characterize the extremizing potentials in these cases where they exist. Analysis of this one-dimensional problem is facilitated by interpreting it in terms of a classical oscillator.

1. Introduction

In this paper we address the problem of finding optimal bounds for the eigenvalues of the operator

$$H_V = \frac{-d^2}{dt^2} + V(t) \tag{1.1}$$

on certain subsets of the real line (finite interval, half-line, line) with a variety of boundary conditions subject to p-norm constraints on the potential function V. To be more precise, having fixed an interval, a set of boundary conditions, and an index $k \ge 0$, we find optimal upper and lower bounds for $E_k(V)$ where V is allowed to range over the set $S = \{V \in L^p(\Omega) \mid \|V\|_p \le M\}$. Here $E_k(V)$ denotes the $(k+1)$th eigenvalue of H_V as defined by the min-max principle [Reed and Simon, 1972-79]. These bounds depend on S only through the constant M and, as will be made clear shortly, give upper and lower bounds for $E_k(V)$ in terms of $\|V\|_p$.

Our interest in such problems was first stimulated by a problem list of A. G. Ramm [1982] in which the problem of maximizing $E_0(V)$, where H_V acts on a finite interval, has Dirichlet boundary conditions, and V is subjected to a 1-norm constraint, was posed. In particular, in an earlier paper [Harrell, 1984], the maximization problem was analyzed for $E_k(V)$ on a finite interval with various selfadjoint boundary conditions, while laying the foundations for a solution to the problem with general p-norm constraints and also for multidimensional problems, i.e., for $H_V = -\Delta + V(x)$ acting on a set $\Omega \subset R^d$, $d \ge 2$, with suitable boundary conditions. Much of the groundwork for the present study was laid in that paper, and henceforth we shall refer to it as article I. In a paper currently in preparation, we shall give the results of our investigations into the multidimensional case, as well as further material and some of the proofs dealing with the one-dimensional case. The multidimensional case turns out to be closely related to the problem of best constants in Sobolev's inequality and certain nonlinear elliptic partial differential equations which have been the subject of much current interest [Brézis and Nirenberg, 1983; Lions, 1982].

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Following the publication of Ramm's problem list, several other authors solved the problem posed above and, in some cases, pursued generalizations, restrictions, or related problems of their own. Solutions of which we are aware are those by Essén [1983], Farris [1982], and Talenti [1983]. Talenti, in particular, solved not only the problem posed by Ramm but also the problem of minimizing $E_0(V)$ under the same hypotheses and of minimizing $E_0(V)$ under the conditions $V \ge 0$, $\|V\|_1 = M$, and $\|V\|_\infty = B$. The extremizing potentials that Talenti finds have more than a passing resemblance to those found by M. G. Krein [1955] in his investigation of a similar problem for the equation of the vibrating string, $y'' + \lambda\rho(x)y = 0$ on $[0,l]$ subject to $y(0) = y(l) = 0$.

Independently of this, there accumulated over the last 15 years or so a body of literature among workers in ordinary differential equations giving lower bounds for the operator H_V in terms of a given p-norm of V. The relevant papers are those by Everitt [1972], Eastham [1972-72], Evans [1981], and Veling [1982 and 1983]. Each of these authors obtained a lower bound for H_V acting on $L^2(0,\infty)$ of the form $-c\|V\|_p^\alpha$ where c and α are constants depending on p. Each had the correct exponent $\alpha = 2p/(2p-1)$, but Veling was the first to find the optimal value of the constant c. All of these authors dealt with a Dirichlet boundary condition at $t = 0$ and, to varying extents, certain other standard boundary conditions. In particular, Veling [1982] gives the optimal lower bound of the form $-c\|V\|_p^\alpha$ for H_V on $L^2(0,\infty)$ with either a Dirichlet or Neumann boundary condition at $t = 0$. Also, Veling [1983] states the optimal bound for H_V on $L^2(R)$. Not surprisingly, there is a close connection between the three bounds discussed by Veling.

There is yet another line of work that is closely related to our current investigation. This work has been pursued in the mathematical physics community in an effort to get accurate bounds on the number of bound states of a Schrödinger operator and the slightly more restricted problem of obtaining optimal conditions for absence of bound states. The work most closely bearing on our own is that of Glaser, Martin, Grosse, and Thirring [1976], Glaser, Grosse, and Martin [1978], and Lieb and Thirring [1976]. These papers treat problems by methods that are similar in many respects to our own, though since they have somewhat different objectives, our results are largely disjoint from theirs.

Finally, in a forthcoming book by Trabowitz [1984] the problem of extremizing $E_k(V)$ for H_V acting on $L^2(0,1)$ with Dirichlet boundary conditions and with V subjected to a 2-norm constraint is posed and its solution is outlined in hints. One finds in this case that the extremizing potentials have explicit representation in terms of elliptic functions. We shall see shortly that the case $p = 3$ also leads to elliptic functions and, moreover, that qualitatively the solutions in the case of general p are very much the same. This situation is brought out most clearly by discussing the general problem in the context of classical mechanics. (At the end of this paper we discuss a few examples and present some remarks about special cases where elliptic functions arise.) It is also worthy of note that elliptic functions arise in the problem of maximizing resonance widths within a suitable class of potentials [Harrell and Svirsky, 1984] and that the potentials for which Hill's equation has been precisely one nonvanishing finite instability interval are elliptic functions [Hochstadt, 1976].

2. General Remarks

Since many of our arguments are not special to one dimension, we find it appropriate to include them in our longer paper [Ashbaugh and Harrell, 1984] and only to summarize them here. In addition we present those results of Harrell [1984] on which we base our current analysis.

In any problem involving maximizing or minimizing a functional, one is immediately confronted with the following questions:

1. (Semiboundedness) Does the appropriate supremum or infimum exist?

2. Can we find (or estimate) this value?

3. (Existence) Is there an optimizing function, i.e., a function at which the functional attains its sup (inf)?

4. (Characterization) What are the optimizing functions?

5. (Uniqueness) Is there a unique optimizing function?

General results [Ashbaugh and Harrell, 1984] give affirmative answers to questions 1, 3, and 5 in most cases of interest. Exceptions for questions 3 and 5 do arise and will be discussed at the appropriate point. Our main thrust in this paper will be toward answering question 4 and, to a lesser extent, 2. It will transpire that our answer to question 4 will often answer question 5 as a byproduct. This is because our approach to characterization is to study the equation

$$-u'' \pm \mathrm{sgn}(u)\,|u|^{(p+1)/(p-1)} = Eu \qquad (2.1)$$

which, together with appropriate boundary conditions, was shown in article I (with the + sign only) to be a necessary condition for $\pm u^{2/(p-1)}$ to be an optimizing potential for $p > 1$. (For additional comments on the sense in which this equation holds and on the domain on which it holds, see Ashbaugh [1984].) Thus, for instance, if we already have existence and can show that equation (2.1) has only one solution of the required type, then uniqueness follows immediately.

One further remark about the formulation of our problem seems appropriate here. While the requirement that the potential function V be locally L^1 is often regarded as the weakest reasonable condition (see, for example, the comments in Eastham and Kalf [1982: p. 4]), we have occasion to consider the operator H_μ, where μ represents a Borel measure. As pointed out to us by Barry Simon, this provides a reasonable operator since one can show that μ is a relatively form-compact perturbation of $H_0 \equiv -d^2/dt^2$ using Fourier transforms. In fact, for H_μ acting on $L^2(\mathbb{R})$ in Fourier transform space, the kernel of $(H_0+1)^{1/2}\mu(H_0+1)^{-1/2}$,

$$K(k_1k_2) = (k_1^2+1)^{-1/2}\hat{\mu}(k_1-k_2)(k_2^2+1)^{-1/2}, \qquad (2.2)$$

is easily shown to be Hilbert-Schmidt since $\hat{\mu}$ is a bounded continuous function. (Essentially we are defining the operator H_μ by means of quadratic forms in Fourier transform space.) The cases where H_μ has other domains are handled similarly by suitable choice of "Fourier transform." Allowing V to be a measure is crucial to the eigenvalue minimization problem when $p = 1$ since the ball of radius $M > 0$ in L^1 has no extreme points, but it is easy to see that an eigenvalue minimizer must be an extreme point using the Rayleigh-Ritz inequality. Thus when $p = 1$, minimizing potentials do not exist. However, if we allow V to lie in the larger class of all finite Borel measures, then we can obtain an existence result. For example, as exhibited by Talenti [1983], the minimizing potential for a finite interval with Dirichlet boundary conditions is a centered δ-function. With slight modifications the above relative compactness argument also applies to $V \in L^p$, $1 \le p \le 2$. This observation is useful in the one-dimensional case since our general methods and results handle only $p \ge 2$.

Even after restricting attention to the one-dimensional case, there are quite a variety of problems to be considered. First, one can consider the problem either of maximization or of minimization over a set $S = \{V \in L^p(\Omega)\ \|V\|_p \le M\}$. Since by the min-max principle it is easy to show that a maximizing (minimizing) potential satisfies $V \ge 0$ ($V \le 0$) and $\|V\|_p = M$, it is a small step to consider what we shall call the misère problem of minimizing within the class $V \ge 0\ \|V\|_p = M$ (maximizing within the class $V \le 0$, $\|V\|_p = M$). We will see, in fact, that the misère problems do not have extremizers and that the optimal bounds are the appropriate $V = 0$ eigenvalues. Second, one has the three choices of domain to consider: finite interval, half-line, and line. Third, one can impose a variety of boundary conditions at the finite endpoints of the domain. Those with which we shall deal are Dirichlet, Neumann, separated (i.e., $\alpha u(t_i) + \beta u'(t_i) = 0$ where t_i is an endpoint), and "compact-support" boundary conditions. Since this last terminology is not standard, we explain: These are the boundary conditions one gets at $\pm l$ if one requires V to have support in the interval $[-l,l]$. In particular, they take the form

$$u'(\pm l) = \pm\sqrt{-E}\,u(\pm l).$$

Lastly, one can concentrate on any eigenvalue $E_k(V)$ for $k = 0,1,2,\ldots$. The ground state $E_0(V)$ is perhaps the most interesting, and in fact we can get more detailed results about it (partly because more tools are available for studying it). The ground state is also unique compared to higher states in that for a given problem certain results will hold for the ground state but for no excited states. For example, the finite-interval $p = 1$ maximization problem has a unique maximizer for $E_0(V)$ but not for $E_k(V)$, $k \ge 1$ [Harrell, 1984]. As a second example, on $\mathbb{R}$ with $p > 1$ there exists a ground-state minimizer (unique up to translations), but minimizers for the higher states do not exist. However, the general method and viewpoint presented here lend a degree of unity to the various cases and problems outlined above. In particular, the method applies to a large extent equally to the ground and excited states.

3. The Classical Oscillator Viewpoint

While we chose time an independent variable with the classical oscillation interpretation in mind, we find it convenient here to set forth other standard notations from the classical mechanics perspective. For a modern and more comprehensive discussion of classical mechanics, we refer the reader to the recent book by Thirring [1978]. By viewing equation (2.1) as Newton's equation for motion in one dimension (u represents position), we can identify the classical potential energy as

$$W(u;E) = \frac{1}{2}Eu^2 \mp \left(\frac{p-1}{2p}\right)u^{2p/(p-1)}. \qquad (3.1)$$

Note that the quantum energy E appears as a coefficient in this classical potential. A first integral for this system is given by

$$\frac{1}{2}\left(\frac{du}{dt}\right)^2 + W(u;E) = h, \qquad (3.2)$$

where we have let h denote the classical (total) energy of our oscillator. Our convention for the ambiguous sign in all equations — (2.1) and (3.1) thus far — is that we take upper signs when considering maximization problems and lower signs when considering minimization problems.

Though we will refer to the above equations as describing an oscillation . for certain choices of the sign referred to above and the sign of E one will not have oscillations or will have oscillations only for suitable initial values. For the most common boundary conditions (Dirichlet, Neumann) only the truly oscillatory solutions will enter, but with more complicated conditions other solutions can sometimes come into play.

We will refer to the curves given parametrically by $(u(t), u'(t))$, where u solves equation (2.1) as trajectories in phase space. Of course, the oscillatory solutions referred to above are just the closed orbits in phase space. In phase space, separated boundary conditions (Dirichlet and Neumann included) can be viewed geometrically as the condition that a trajectory start on a given line through the origin and end on a second line through the origin (possibly the same) at a specified later time. When the interval is finite, we choose it as $[0,l]$, $l > 0$, or sometimes $[-l,l]$; for the half-line we choose $[0,\infty)$.

4. Minimization on the Line and the Half-Line

We begin our detailed discussion with these cases since from the classical oscillator viewpoint the constant h must be 0, which simplifies the analysis. Also these are the cases that have drawn attention previously. Now since u is an L^2 solution to $H_V u = Eu$, where $V = -u^{2/(p-1)} \in L^p$, we can be sure from the theory of Schrödinger operators [Reed and Simon, 1972-79; Richtmeyer, 1978] that u and u' go to 0 as t goes to ∞. Thus on infinite intervals our only concern is with classical oscillator solutions having total energy $h = 0$, and we need only solve the equation

$$\frac{1}{2}\left(\frac{du}{dt}\right)^2 + \frac{1}{2}Eu^2 + \left(\frac{p-1}{2p}\right)u^{2p/(p-1)} = 0. \tag{4.1}$$

This equation is readily integrated, with the result that

$$u(t) = \left(\frac{-pE}{p-1}\right)^{(p-1)/2} \operatorname{sech}^{p-1}\left[\frac{\sqrt{-E}\,(t-c)}{p-1}\right], \tag{4.1}$$

and hence

$$V(t) = \frac{pE}{p-1}\operatorname{sech}^2\left[\frac{\sqrt{-E}\,(t-c)}{p-1}\right]. \tag{4.3}$$

Here c is the constant of integration. For the minimization problem on the line, it represents the expected fact that a minimizing potential cannot be unique because of translation invariance. For half-line problems, the constant would have to be chosen so that u satisfies the boundary condition at the origin. We shall see shortly that this has the interesting consequence that no minimizers exist for certain choices of the boundary condition. But first let us finish our discussion of the standard cases.

For the full line minimization problem one can compute

$$\|V\|_p^p = \frac{p^p(-E)^{(2p-1)/2}}{(p-1)^{p-1}}B(p,\tfrac{1}{2}), \tag{4.4}$$

or, solving for E,

$$E = -\left[\frac{(p-1)^{p-1}}{p^p B(p,\frac{1}{2})}\right]^{2/(2p-1)} \|V\|_p^{2p/(2p-1)}. \tag{4.5}$$

Here $B(p,\frac{1}{2})$ represents a beta function in standard notation. This formula is that given by Veling [1983] except for a misprint of $(1-\vartheta)\vartheta^{\vartheta/(1-\vartheta)}$ as $(1-\vartheta)^{\vartheta/(1-\vartheta)}$.

For the half-line problem with Neumann boundary condition one must take $c = 0$ in equation (4.3). The computation can be carried out as before, yielding

$$E = -2^{2/(2p-1)}\left[\frac{(p-1)^{p-1}}{p^p B(p,\frac{1}{2})}\right]^{2/(2p-1)} \|V\|_p^{2p/(2p-1)}, \tag{4.6}$$

again agreeing with a result of Veling [1982].

We now consider the general boundary condition

$$u'(0) = mu(0) \tag{4.7}$$

From equation (4.2) this reduces to

$$m = \sqrt{-E}\tanh(\sqrt{-E}\,c\,/\,(p-1)) \tag{4.8}$$

which has a solution for c if and only if $\sqrt{-E} > |m|$. Holding E fixed, we see that as $m \to \sqrt{-E}$ from below $c \to \infty$ and that as $m \to \sqrt{-E}$ from above $c \to -\infty$. Thus as $m \to -\sqrt{-E}$ our sech^2-potential well translates off to the left, "leaving" the positive half-axis, and as $m \to \sqrt{-E}$ it translates to the right into the positive half-axis. We can better understand what is happening here if we note that the potential $V = 0$ with boundary condition (4.7) has a negative eigenvalue at $E = -m^2$ if $m < 0$. Thus a fixed $E < 0$ will not be minimal for the operator H_V on $L^2(0,\infty)$ with boundary condition (4.7) for $m < 0$ until m increases to $-\sqrt{-E}$. At that value of m, E will be minimal for $\|V\|_p = M = 0$. For $|m| < \sqrt{-E}$, E will be minimal for $\|V\|_p$ fixed as required by equations (4.3) and (4.6). One could write the relation between E and $\|V\|_p$ for this range of m in terms of the incomplete beta function, but we refrain from doing so here. When m exceeds $\sqrt{-E}$, one no longer has a minimizing potential, but a minimizing sequence of potentials is easily constructed by taking a sequence of V's given by equation (4.5) with c's going to ∞ and suitably modified on $[0,1]$, say, to meet the boundary condition at $t = 0$. This latter situation also includes the case of Dirichlet boundary conditions. In these cases the value E in equation (4.5) is a strict lower bound for the ground state and hence also for the operator H_V.

We close this section with some cursory remarks about higher eigenvalues. To obtain a minimizing sequence of potentials for a higher eigenvalue, one "pastes on" more sech^2-potential wells out near infinity. The modifications required in the pasting can be shown to have vanishing effect as the spacing between consecutive wells is sent to infinity. We note that the potentials in the minimizing sequence for the k-th eigenvalue approach k-fold degeneracy, i.e., the first k eigenvalues come together in the limit. The appropriate eigenfunction in this case is much like the potential (to the power $(p-1)/2$) except that we flip its sign each time we paste on a new piece; on $[0,\infty)$ we also must rescale the left-most bump so that its L^2 norm is the same as all the others. As an illustration one obtains the bound

$$E_1(V) > -2^{-2/(2p-1)}\left[\frac{(p-1)^{p-1}}{p^p B(p,\frac{1}{2})}\right]^{2/(2p-1)} \|V\|_p^{2p/(2p-1)}$$

in the case of the second eigenvalue of H_V acting on $L^2(\mathbb{R})$.

To those familiar with high-energy physics, there is more than a passing similarity between the above construction of minimizing sequences and the construction of a multiple instanton configuration. We also remark that the sech^2 form of our potential is precisely a soliton solution to the Korteweg de Vries (KdV) equation. There is an extensive literature detailing the intimate connections between the KdV equation and the Schrödinger equation; we content ourselves with noting that the article [Lieb and Thirring, 1976] presents some particularly pertinent observations of P. Lax.

5. Minimization on a Finite Interval

When one seeks to find eigenvalue minimizers on a finite interval, one must consider equation (3.2) with all allowed values of the classical energy h. We adopt the following strategy in this discussion: with fixed $p > 1$ and interval $[0,l]$, we pick a possible optimal eigenvalue E and choose suitable boundary conditions; then we look for those values of h that allow u to meet the boundary conditions at $t = 0$ and $t = l$; and finally we determine the value $M = \|V\|_p$ for which $V = -u^{2/(p-1)}$ is a possible minimizer. If at the end of this process we have only one candidate, then, having already proved existence of a minimizer [Ashbaugh and Harrell, 1984], we can conclude that we have found the unique minimizer. Even if we find several candidates, the existence result guarantees that at least one of them will be a minimizer. Existence of minimizers on a finite interval when V is allowed to range over the class of Borel measures μ satisfying $\int d|\mu| \le M$ is shown in our longer paper. This result handles the minimization question when $p = 1$.

We begin our discussion by considering Dirichlet boundary conditions and taking $E < 0$. Then the only h's for which Dirichlet conditions can be met are $h > 0$, and the time required for one excursion (half the period of the orbit) is

$$T(h,E)/2 = \sqrt{2}\int_0^{u_1}[h - W(u;E)]^{-1/2}du, \tag{5.1}$$

where u_1 represents the positive turning point of the motion, i.e., $W(v_1;E) = h$, $u_1 > 0$. To see how $T(h,E)$ varies with h we eliminate h in favor of u_1 while noting that the mapping $h \to u_1$ is an increasing function from $(0,\infty)$ onto $(u_{1,min},\infty)$ where $u_{1,min}$ satisfies $0 = W(u_{1,min};E)$. One has

$$T = 2\sqrt{2}\int^{u_1}[W(u_1;E) - W(u;E)]^{-1/2}du \tag{5.2a}$$

$$= 2\sqrt{2}\int_0^{u_1}[E(u_1^2 - u^2)/2 + (p-1)\{u_1^{2p/(p-1)} - u^{2p/(p-1)}\}/2p]^{-1/2}du$$

$$= 2\sqrt{2}\int_0^{1}[(p-1)u_1^{2/(p-1)}(1-s^{2p(p-1)})/2p + E(1-s^2]^{-1/2}ds \tag{5.2b}$$

Thus one sees that T decreases from ∞ to 0 as h increases from 0 to ∞. Since to accommodate the $(k+1)$th eigenvalue E_k we need

$$(k+1)T(h,E_k)/2 = l \tag{5.3}$$

to be satisfied, we see that any $E < 0$ can be a minimal $(k+1)$-th eigenvalue for any $k \ge 0$. A similar analysis leads to the same conclusion when $E = 0$. When $E > 0$, one finds that the period T decreases from $2\pi/\sqrt{E}$ to 0 as h increases from 0 to ∞. Thus if $E > (k+1)^2\pi^2/l^2$, then E cannot be a minimal E_k, whereas if $E \le (k+1)^2\pi^2/l^2$, it will be attainable as a minimal E_k. If one notes that $E_k(0) = (k+1)^2\pi^2/l^2$, the reasonableness of these conditons is apparent. Actually, to complete this discussion, we must look at the equilibrium solutions, i.e., the civilized points in the phase plane. These solutions are exceptional in that there is not a fixed period associated with them. For the above, the only critical point solution of relevance is $u = 0$, which is trivial to analyze.

With Neumann boundary conditions the same considerations apply for the orbits and their periods as discussed above. However, there are additional orbits having $h < 0$ to be considered in the case of $E < 0$, including another equilibrium solution corresponding to the minimum of $W(u;E)$. This complicates the indexing of the eigenvalues somewhat, but Sturm's theorem on nodes of eigenfunctions suffices to sort things out. The orbits considered previously lead to candidates for minimal E_k, $k \ge 1$, under the condition

$$kT(h,E_k)/2 = l, \tag{5.4}$$

and the newly considered orbits lead to candidates for E_0 since they give

nodeless solutions. Again any $E \le 0$ can be a minimal Neumann E_k, $k \ge 0$, but for $E > 0$, $E > k^2\pi^2/l^2$ precludes E from being a minimal E_k and $E \le k^2\pi^2/l^2$ allows it. That all allowed E's are actually assumed as minimal E_k's for some choice of $M = \|V\|_p$ follows from continuity considerations which are taken up by Ashbaugh and Harrell [1984].

Other choices of separated boundary conditions at $t = 0$ and $t = l$ will force us to consider more complicated conditions than (5.3) or (5.4) for meeting the boundary conditions. In fact, trajectories that are not closed orbits will even enter: the appropriate point of view is that we need to find those trajectories that take time l to pass from one line through the origin to a second line through the origin in phase space. Periodic or antiperiodic boundary conditions lead back to the same orbits as were discussed in the Neumann case, as do separated boundary conditions of "periodic type": $u'(0) = mu(0)$, $u'(l) = mu(l)$, $m \in \mathbb{R}$.

6. Maximization on a Finite Interval

The analysis of the maximization problem differs only in detail from that of the minimization problem. The most significant difference is that the potential $W(u;E)$is now upside down; in particular, $W \to -\infty$ as $u \to \infty$. This has the effect that for all standard boundary conditions only $E \ge 0$ need be considered. By analyzing $T(h,E)$, one finds in this case that $2\pi/\sqrt{E} \le T(h,E) < \infty$ for the permissible values of h. Thus $E < (k+1)^2\pi^2/l^2$ implies that E cannot be an extremal $(k+1)$-th eigenvalue for the Dirichlet problem whereas $E \ge (k+1)^2\pi^2/l^2$ can be. As should be clear, the discussion of this problem parallels almost exactly that of the previous section, so we conclude it here.

7. Misère Problems

We turn now to a brief discussion of the misère problem, that of minimizing (respectively, maximizing) a given eigenvalue when V is constrained to the class $S = \{V \mid V \ge 0, \|V\|_p = M\}$ (resp., $S = \{V \mid V \le 0, \|V\|_p = M\}$). We shall confine the majority of our remarks to the case of the ground state for Dirichlet boundary conditions which we shall denote by $E(V)$.

We begin by considering the minimization problem with $V \ge 0$ where $\Omega \subset \mathbb{R}^d$ is bounded and has smooth boundaries. The case of unbounded domains for this minimization problem is of no interest since $E(V)$ (as defined by the min-max principle) is then always $0 = E(0)$. We shall show that (1) $E(V) > E(0)$ for all $V \in S$ and (2) $\inf_S E(V) = E(0)$. Thus there is no V that is a minimizer for this misère problem. To obtain (1), we simply use the Rayleigh-Ritz inequality for $-\Delta$ with ϕ_V, the normalized ground-state eigenfunction of H_V, as trial function: $E(V) = (\phi_V,(-\Delta+V)\phi_V) = (\phi_V,-\Delta\phi_V) + \int_\Omega V|\phi_V|^2 > E(0)$. To prove (2), note that since the ground state, ϕ_0, of $-\Delta$ on Ω with Dirichlet boundary conditions goes to 0 on $\partial\Omega$ and since $\partial\Omega$ is smooth, we can find a sequence of sets $B_n \subset \Omega$ satisfying (i) $\sup_{B_n}|\phi_0| \le 1/n$ and (ii) $0 < |B_n| < K$, K a constant independent of n. Then with $V_n = M|B_n|^{-1/p}X_{B_n}$ and again using Rayleigh-Ritz, we compute

$$E(V_n) < (\phi_0,(-\Delta+V_n)\phi_0) = E(0) + \int_{B_n}|\phi_0|^2 M|B_n|^{-1/p} \le E(0) + MK^{1-1/p}/n^2,$$

which goes to $E(0)$ with increasing n.

The problem of maximizing over $S = \{V \mid V \le 0, \|V\|_p = M\}$, $p \ge 1$, is more difficult to analyze, but leads to much the same result. That $E(V) \le E(0)$ is again a consequence of Rayleigh-Ritz or, more precisely, the min-max principle. When $E(0)$ is in the discrete spectrum, this inequality is strict; in any event, there is no $V \in S$ for which $-\Delta + V(x)$ has $E(0)$ as an isolated eigenvalue of finite multiplicity. This, together with the fact that $\sup_S E(V) = E(0)$ (to be shown shortly) shows that this misère problem also lacks an optimizer (in all cases in one and two dimensions, and in all "honest" cases in three or more dimensions). If Ω is unbounded, one can construct a sequence $\{V_n\}$ of potentials in S having $E(V_n) \to 0 = E(0)$ by using $V_1 = M|B_n|^{-1/p} X_{B_n}$ where the sets $B_n \subset \Omega$ satisfy $|B_n| \to \infty$. Then we have used wide but shallow square wells in our construction. For bounded domains this avenue is not open to us, so we shall use narrow and deep square wells. We pick a sequence of balls $B_n \subset \Omega$ with $|B_n| \neq 0$ for all n and $|B_n| \to 0$. Then for $p > 1$ and $V_n = -M|B_n|^{-1/p} X_{B_n}$ we have $\|V_n\|_1 = M|B_n|^{1-1/p} \to 0$ as $n \to \infty$; and using the fact that our lower bound for $E(V)$ in terms of $\|V\|_1$ goes to $E(0)$ as $\|V\|_1 \to 0$ [Ashbaugh and Harrell, 1984], we see that $E(V_n) \to E(0)$. We remark that this sequence works equally well for Ω unbounded but has the drawback that it does not cover the case $p=1$. The essential observations in the above discussion are that for Ω unbounded there is a sequence $\{V_n\}$ in S also lying in L^∞ with $\|V_n\|_\infty \to 0$ and that for $p>1$ and arbitrary Ω there is a sequence $\{V_n\}$ in S also lying in L^1 with $\|V_n\|_1 \to 0$. These observations would also have sufficed in dealing with the misère minimization problem except for the case $p=1$. Indeed, except for this case, the argument given above could have been concluded just by choosing the B_n's so that $|B_n| \to 0$.

To complete the discussion, we need to treat the case of a bounded domain when $p = 1$. Just as in the misère minimization problem, our argument now rests on our choice of Dirichlet boundary conditions. The idea is to take a sequence η_n approximating a δ-function located on $\partial\Omega$ and argue that for $V = -M\eta_n$, we have $(\phi_n, V_n \phi_n) \to 0$ as $n \to \infty$ where ϕ_n represents the normalized ground state for $-\Delta + V_n$. However, here we shall give a proof only in the case of dimension $d = 1$. In this case we may take $\Omega = [0,l]$, $l > 0$, and we define a sequence of potentials $V_n = -MnX_{[0,1/n]}$. By standard methods found in any elementary quantum mechanics textbook, one could give an explicit argument showing that $E(V_n) \to E(0) = \pi^2/l^2$. Instead, we note that $E(V_n)$ is the first eigenvalue of the three-dimensional problem for $-\Delta + V_n(r)$; we remark that this is where we make use of the Dirichlet boundary condition. As a function in three-space, we have $\|V_n\|_1 = Mn\frac{4}{3}\pi(1/n)^3 = 4\pi M/3n^2 \to 0$ as $n \to \infty$ and thus, as proved above, $E(V_n) \to E(0)$, where the 0 represents the 0 potential on the ball of radius l in $\mathbb{R}^3$. But, passing back to one dimension, we have $E(0) = \pi^2/l^2$, which completes the proof. Finally, we remark that except when $p = 1$, Dirichlet boundary conditions were not needed; in particular, the last argument works for arbitrary boundary conditions imposed at $t = l$.

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References

Ashbaugh, M. S., and Harrell, E. M. 1984. "Maximal and minimal eigenvalues and their associated nonlinear equations" (in preparation).

Brézis, H., and Nirenberg, L. 1983. "Positive solutions of nonlinear elliptic equations involving critical Sobolev exponents." Comm. Pure Appl. Math. 36:437-477.

Eastham, M. S. P. 1972-1973. "Semi-bounded second-order differential operators." Proc. Roy. Soc. Edinburgh 72A:9-16.

Eastham, M. S. P., and Kalf, H. 1982. *Schrödinger-type Operators with Continuous Spectra*. Pitman Publishing, Boston.

Essén, M. 1983. "On maximizing the first eigenvalue for a second order linear differential operator" (preprint).

Evans, W. D. 1981. "On the spectra of Sturm-Liouville operators with a complex potential." Math. Ann. 255:57-76.

Everitt, W. N. 1972. "On the spectrum of a second order linear differential equation with a p-integrable coefficient." Applicable Analysis 2:143-160.

Farris, M. 1982. "Sturm-Liouville problem with maximal first eigenvalue" (preprint).

Glaser, V., Grosse, H., and Martin, A. 1978. "Bounds on the number of eigenvalues of the Schrödinger operator." Commun. Math. Phys. 59:197-212.

Glaser, V., Martin, A., Grosse, H., and Thirring, W. 1976. "A Family of Optimal Conditions for the Absence of Bound States in a Potential." *Studies in Mathematical Physics*. Ed. E. H. Lieb, B. Simon, and A. S. Wightman. Princeton University Press, Princeton, pp. 169-194.

Harrell, E. M. 1984. "Hamiltonian operators with maximal eigenvalues." J. Math. Phys. 25:48-51.

Harrell, E. M., and Svirsky, R. 1984. ~~Manuscript in preparation~~ "Potentials approximately sharp resonances" (preprint)

Hochstadt, H. 1976. "An inverse problem for a Hill's equation." J. Diff. Equations 20:53-60.

Krein, M. G. 1951. "On Certain Problems on the Maximum and Minimum of Characteristic Values and on the Lyapunov Zones of Stability." *Amer. Math. Soc. Translations*, Ser. 2, Vol. 1. American Math. Soc., Providence, pp. 163-187 (trans. of Prikl. Mat. Meh. 15:323-348).

Lieb, E. H., and Thirring, W. 1976. "Inequalities for the Moments of the Eigenvalues of the Schrödinger Hamiltonian and Their Relation to Sobolev Inequalities." *Studies in Mathematical Physics*. Ed. E. H. Lieb, B. Simon, and A. S. Wightman. Princeton University Press, Princeton, pp. 269-303.

Lions, P. L. 1982. "On the existence of positive solutions of semilinear elliptic equations." SIAM Review 24:441-467.

Ramm, A. G. 1982. Problem list in H. Samelson, "Queries." Notices Amer. Math. Soc. 29:326-329.

Reed, M., and Simon, B. 1972-1979. *Methods of Modern Mathematical Physics*. 4 vols. Academic Press, New York.

Richtmeyer, R. D. 1978. *Principles of Advanced Mathematical Physics*, Vol. I. Springer-Verlag, New York.

Talenti, G. 1983. "Estimates for eigenvalues of Sturm-Liouville problems" (preprint).

Thirring, W. 1978. *A Course in Mathematical Physics, Vol. I: Classical Dynamical Systems*. Trans. E. M. Harrell. Springer-Verlag, New York.

Trubowitz, E. 1984. Book in preparation.

Veling, E. J. M. 1982. "Optimal lower bounds for the spectrum of a second order linear differential equation with a p-integrable coefficient." Proc. Roy. Soc. Edinburgh 92A:95-101.

Veling, E. J. M. 1983. "Stellingen behorende bij het proefschrift Transport by Diffusion" (thesis extract).

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$1/R$ expansion for H_2^+: Calculation of exponentially small terms and asymptotics

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The energy of any bound state of the hydrogen molecule ion H_2^+ has an expansion in inverse powers of the internuclear distance R of the form

$$E(R) \sim \sum_N E^{(N)}(2R)^{-N} + e^{-R/n} \sum_N A^{(N)}(2R)^{-N} + e^{-2R/n} \left[\sum_N B^{(N)}(2R)^{-N} + \ln(R) \text{ terms} \right] \pm i e^{-2R/n} \sum_N C^{(N)}(2R)^{-N} + \cdots .$$

Rayleigh-Schrödinger perturbation theory (RSPT) gives the coefficients $E^{(N)}$ but is otherwise unable to treat the exponentially small series, which in part are characteristic of the double-well aspect of H_2^+. (Here n denotes the hydrogenic principal quantum number.) We develop a quasisemiclassical method for solving the Schrödinger equation that gives all the exponentially small subseries. The RSPT series diverges: for the ground state $E^{(N)} \sim -(N+1)!/e^2$ for large N. The $E^{(N)}$ asymptotics are governed via a dispersion relation by the imaginary $e^{-2R/n}$ series, which itself is given by the square of the $e^{-R/n}$ series times a "normalization integral." That the expansion itself contains imaginary terms might seem inconsistent with the reality of the H_2^+ eigenvalues. In fact, the RSPT series is Borel summable for R complex. The Borel sum has a cut on the real R axis, and its limit from above or below the positive R axis is complex. The imaginary $e^{-2R/n}$ (and higher) series consist of just the counterterms to cancel the imaginary part of the Borel sum. Extensive numerical examples are given. Of interest is a weak (down by a factor N^{-6}) alternating-sign contribution to $E^{(N)}$, which is uncovered both theoretically and numerically. Also of interest is the identification of the Borel sum of the RSPT series with nonphysical boundary conditions. This too is illustrated both theoretically and numerically.

I. INTRODUCTION

This paper is about the expansion of the energy of the hydrogen molecule ion H_2^+ in powers of $(2R)^{-1}$, R being the internuclear distance. Of course, H_2^+ has special importance as a prototype for molecular binding and for double wells, but it is generally regarded as simple, well understood,[1–4] and perhaps not very interesting. Exactly the opposite is true: the study of H_2^+ at large R has revealed several unexpected features.[5,6]

We list in this introduction seven main results. The first is that (i) the energy of any bound state is given formally by an explicitly computable *complex* expansion that is *discontinuous* across the positive R axis,

$$E(R) \sim \sum_N E^{(N)}(2R)^{-N} + e^{-R/n} \sum_N A^{(N)}(2R)^{-N} + e^{-2R/n} \left[\sum_N B^{(N)}(2R)^{-N} + \ln(R) \text{ terms} \right] \pm i e^{-2R/n} \sum_N C^{(N)}(2R)^{-N} + \cdots . \quad (1)$$

Here the $\pm$ is the sign of $\operatorname{Im} R$, and n is the hydrogenic principal quantum number. When R is real, then the sign indicates whether it has become real from above or below the real axis.

More surprising is that (ii) the "sum" of the explicitly complex series (1) is both real and continuous across the positive R axis. The explicit imaginary series is canceled by an implicit imaginary contribution from the sum of the ordinary, real, divergent Rayleigh-Schrödinger perturbation-theory (RSPT) expansion, $\sum_N E^{(N)}(2R)^{-N}$. This remarkable subtlety involves taking the sum of the divergent RSPT series to be the analytic continuation back to the real axis of the Borel sum, which exists for R complex;[6] this is equivalent, as we shall see,[7] to recognizing that $R>0$ is a Stokes line of the expansion. (A similar cancellation in part has been noticed by Zinn-Justin for the double-well oscillator.[8–10])

This paper is also about the method used to generate the solution of the eigenvalue problem by asymptotic expansion—the quasisemiclassical (QSC) method. Through the separability of the H_2^+ eigenvalue equation in prolate spheroidal coordinates,[11] which here involves two separation constants β_1 and β_2, a systematic procedure is developed to generate the RSPT series, the $e^{-R/n}$ double-well gap series, the $e^{-2R/n}$ real and imaginary series, and so forth. Of course ordinary RSPT gets only the first of these series.

The third specific result concerns the relationship between the imaginary $ie^{-2R/n}$ series and the $e^{-R/n}$ "gap" series. These two series arise primarily from the separation constant β_2 for which (iii) the corresponding imaginary series as πi times the square of the corresponding gap series times a normalization constant.

Other main points include the following. (iv) The H_2^+ eigenvalue equation has complex eigenvalues closely associated with the real eigenvalues in the sense that they have the same RSPT, but involve different boundary conditions.[5,6] The "different boundary conditions" can be understood in a simple way by considering the analytic continuation of one of the separated equations of a related, physically interpretable problem:[5,6] an electron moving in the field of a fixed proton and a fixed antiproton. (v) RSPT for β_2 is Borel summable to the complex eigenvalues.[5,6] (vi) The imaginary series determine the large-order behavior of the RSPT coefficients via dispersion relations. (vii) The imaginary series associated with the discontinuity of the separation constant β_1 across the negative real axis has logarithmic terms in $-R$, which lead to $\ln(N)$ terms in the asymptotics of the $\beta_1^{(N)}$ and $E^{(N)}$.

Two empirical facts have been our main motivation. The first is the same-sign factorial divergence of the RSPT series for the ground state:[3,12–14]

$$E^{(N)} \sim -(N+1)! e^{-2} \left[1 + \frac{2}{N+1} - \frac{18}{(N+1)N} + \cdots \right] . \quad (2)$$

Such behavior is consistent with the asymptotic expansion of a *complex* function that is discontinuous across the $R>0$ axis, whose Borel sum would be like

$$-\sum_{N=0}^{\infty} (N+1)! e^{-2}(2R)^{-N} \sim e^{-2} \int_0^\infty t^2 e^{-t}(t-2R)^{-1} dt \quad [0 < |\arg(R)| < 2\pi] \quad (3)$$

$$= \mathrm{P} e^{-2} \int_0^\infty t^2 e^{-t}(t-2R)^{-1} dt \pm i\pi 4R^2 e^{-2R-2} \quad (\operatorname{Im} R = \pm 0) . \quad (4)$$

where P denotes the principal value of the integral. The second empirical fact is an approximate relationship[12] between the double-well energy gap $E_{\rm gap}$, which for the pair consisting of the ground and first excited state is $\sim 4Re^{-R-1}$, and the asymptotics of the RSPT coefficients [Eq. (2)], which by a dispersion relation involves the "$\pm$" discontinuity in Eq. (1). The relationship is

$$\text{discontinuity in Eq. (1)} \sim 2\pi i \left(\tfrac{1}{2} E_{\rm gap}\right)^2 . \quad (5)$$

Our initial goal was to explain both facts, but in the process we have obtained many more results, which have been summarized in Ref. 5. Further, in Ref. 6, the first of two papers announced in Ref. 5, we have collected the mathematically rigorous results: proof of the analyticity of β_1, β_2, and E; proof of Borel summability of the RSPT series for β_1, β_2, and E to eigenvalues of non-self-adjoint versions of the H_2^+ problem; proof of the approximate formula (5); justification of the dispersion relations; and justification of the leading asymptotic behavior of the RSPT coefficients. This paper is the second paper announced in Ref. 5 in which we develop the QSC technique, derive the multiply-exponentially-small series, and obtain the full high-order asymptotics of the RSPT quantities, i.e., all the corrections in formula (2) for the ground state and for excited states as well.

The organization of the paper is briefly as follows. In Sec. II, the Schrödinger equation is separated, and the RSPT solution is sketched. Section III is a long section devoted to the separation constant β_2, which comes from the separated equation that contains the double-well character of H_2^+. In Sec. III A, the quasisemiclassical method is introduced through the form of the wave function, and the separated Schrödinger equation is turned into a Riccati equation. In Sec. III B, the recursive, perturbative solution of the Riccati equation is sketched, and the usual

RSPT is shown to fall out. In Sec. III C, it is shown how the second boundary condition, ignored by RSPT for H_2^+, leads to the double-well gap and to exponentially small (e^{-R}) terms. Sections III D and III E give alternative formulas for quantities that appear first in Sec. III C. How *imaginary* terms occur in the expansion for β_2 is first introduced in Sec. III F and further developed in Sec. III G, where the "gap-squared" formula is discussed. The doubly-exponentially-small series contributing to β_2 is obtained in Sec. III H. The final subsection, III I, is a mathematical diversion from the physical H_2^+ problem: the β_2 equation is solved not on the finite physical interval, but on a semiinfinite interval. As mentioned in (v) above, the resulting eigenvalue turns out to be the Borel sum of the RSPT series, and the series for the discontinuity in the Borel sum across its cut is given by the imaginary series obtained in Sec. III G. Section IV contains the details for the solution of the separation constant β_1. In Sec. V the two separation constants are put back together to get the energy $E(R)$. The details are mostly algebraic, but nontrivial. In Sec. V C the (appropriate) approximate, gap-squared formula of Brézin and Zinn-Justin is shown to be true for exactly two terms for all states, not just the ground state. In Sec. V E the discontinuity in $E(R)$ for R negative is discussed in preparation for the development of the asymptotics of the RSPT coefficients via dispersion relations in Sec. VI. Section VII contains a JWKB-like reformulation of the method that is easier to use for numerical calculations of the various series, which calculations are discussed and illustrated in Secs. VIII–X. Summation of the expansions and comparison with direct numerical solution of the eigenvalue equations are discussed in Sec. XI. All of the quantities discussed are illustrated numerically in extensive tables, and the paper is summarized in Sec. XII.

II. PRELIMINARIES: SEPARATION OF VARIABLES; RSPT RESULTS

The aims of this preliminary section are to give the separated equations for H_2^+ in prolate spheroidal coordinates,[11] to indicate how to carry out RSPT on them, to state the asymptotic RSPT results, and to set out the notation. The RSPT results serve both as part of the motivation and as a point of departure for the QSC treatment that follows in Sec. III. (For the implementation of the separability in terms of operator theory in Hilbert space, see Ref. 6.)

A. Separated equations in prolate spheroidal coordinates

Prolate spheroidal coordinates, with a translation to make the left endpoints for the ξ and η both be 0, are given by[11]

$$\xi \equiv (r_a+r_b)/R-1 \quad (0\le\xi<\infty)\,, \tag{6}$$

$$\eta \equiv (r_a-r_b)/R+1 \quad (0\le\eta\le 2)\,, \tag{7}$$

$$\phi \equiv \arctan(y/x)\,. \tag{8}$$

The dependence of the wave function on ϕ is the familiar and simple $e^{im\phi}$ (m an integer). The dependence on ξ and η is what needs to be determined.

The Schrödinger equation,

$$H\Psi=(-\tfrac{1}{2}\nabla^2-1/r_a-1/r_b+1/R)\Psi=(E+1/R)\Psi\,, \tag{9}$$

yields two equations for the separation constants β_1 and β_2,

$$\left[-\frac{d^2}{d\xi^2}+\frac{1}{4}r^2-r\frac{\beta_1}{\xi}-r\frac{\beta_1+2\beta_2}{\xi+2}+\frac{m^2-1}{\xi^2(\xi+2)^2}\right]\Phi_1=0\,, \tag{10}$$

$$\left[-\frac{d^2}{d\eta^2}+\frac{1}{4}r^2-r\frac{\beta_2}{\eta}-r\frac{\beta_2}{2-\eta}+\frac{m^2-1}{\eta^2(2-\eta)^2}\right]\Phi_2=0\,, \tag{11}$$

with the energy E being obtained from β_1 and β_2 by the formula

$$E=-\tfrac{1}{2}(\beta_1+\beta_2)^{-2}\,. \tag{12}$$

Equation (12) and the familiar expression for the hydrogen-atom energy eigenvalue, $-\frac{1}{2}n^{-2}$, show that $\beta_1+\beta_2$ may be regarded as a "perturbed principal quantum number n." The r in Eqs. (10) and (11) is a scaled version of the internuclear distance R:

$$r\equiv R/(\beta_1+\beta_2)\sim R/n\,. \tag{13}$$

B. Manipulation of the separated equations into standard RSPT form

Despite the nonstandard form of Eqs. (10)–(13), it is straightforward to develop solutions by RSPT. We begin with a scale transformation that makes the unperturbed problem hydrogenic:

$$u=r\xi,\quad v=r\eta\,, \tag{14}$$

$$[-u\,d^2/du^2+\tfrac{1}{4}u+\tfrac{1}{4}(m^2-1)/u]\Phi_1 +uV_1(u,\beta_1+2\beta_2,r)\Phi_1=\beta_1\Phi_1\,, \tag{15}$$

$$[-v\,d^2/dv^2+\tfrac{1}{4}v+\tfrac{1}{4}(m^2-1)/v]\Phi_2 +vV_2(v,\beta_2,r)\Phi_2=\beta_2\Phi_2\,. \tag{16}$$

The expression that occurs in square brackets in Eqs. (15) and (16) is identical with the separated "Hamiltonians" for the hydrogen atom in parabolic coordinates:[15,16] we take it as the unperturbed Hamiltonian for both problems. Notice also that the factors u and v in $u\,d^2/du^2$ and $v\,d^2/dv^2$ imply that the volume elements are $u^{-1}du$ and $v^{-1}dv$. Thus the unperturbed eigenfunctions are identical with the parabolic hydrogenic eigenfunctions, and the unperturbed separation constants are

$$\beta_i=\beta_i^{(0)}=n_i+\tfrac{1}{2}(|m|+1)\quad (i=1,2,\ r=+\infty)\,, \tag{17}$$

where n_1 and n_2 are the usual parabolic quantum numbers.

We continue by expanding the perturbing potentials V_i in power series in $(2r)^{-1}$ (the perturbation expansions for the $\beta_i^{(N)}$ are defined below):

$$V_1(u,\beta_1+2\beta_2,r)=-\frac{\beta_1+2\beta_2}{u+2r}+\tfrac{1}{4}(m^2-1)\times\left[-\frac{2}{u(u+2r)}+\frac{1}{(u+2r)^2}\right] \quad (18)$$

$$=\sum_{N=1}^{\infty}V_1^{(N)}(2r)^{-N}, \quad (19)$$

$$V_1^{(N)}=\tfrac{1}{4}(m^2-1)(N+1)(-u)^{N-2}-\sum_{k=0}^{N-1}(\beta_1^{(k)}+2\beta_2^{(k)})(-u)^{N-k-1}, \quad (20)$$

$$V_2(v,\beta_2,r)=-\frac{\beta_2}{2r-v}+\tfrac{1}{4}(m^2-1)\left[\frac{2}{v(2r-v)}+\frac{1}{(2r-v)^2}\right] \quad (21)$$

$$=\sum_{N=1}^{\infty}V_2^{(N)}(2r)^{-N}, \quad (22)$$

$$V_2^{(N)}=\tfrac{1}{4}(m^2-1)(N+1)v^{N-2}-\sum_{k=0}^{N-1}\beta_2^{(k)}v^{N-k-1}. \quad (23)$$

Given the expansions (18)–(23), it is straightforward to solve Eqs. (15) and (16) by textbook RSPT. The first step is to obtain β_2 as a power series in $(2r)^{-1}$ by solving Eq. (16). The second step is to obtain the series for β_1 from Eq. (15) and the β_2 series. The third step is to obtain r^{-1} as a series in R^{-1} from Eq. (13), which then permits E to be expressed as a series in R^{-1}, the fourth and final step. Note that Eqs. (20) and (23) are strictly valid only when u and v are both less than $2r$. However, the RSPT solution is an asymptotic power series in $1/2r$, and the order-by-order equations, which are obtained for large $2r$, of course hold formally for all values of u and v. To look at it another way, if a nonperturbative solution were to be obtained, then by ignoring the corresponding expansions for u and v greater than $2r$, an error that is exponentially small in r would be introduced into the solution, which would again therefore be of no consequence for the $1/2r$ RSPT.

Note that β_1 and β_2 depend on m only through the magnitude $|m|$ and not on the sign. To simplify the appearance of the formulas, we assume from now on, *without loss of generality*, that $m\geq 0$.

C. RSPT results for the separation constants

The RSPT series for the separation constants have been calculated as outlined above. We shall not go into the relatively uninteresting details. At low order the series appear unremarkable. One finds for the ground state ($n_1=n_2=m=0$), for example, that

$$\beta_1\sim\sum_{N=0}^{\infty}\beta_1^{(N)}(2r)^{-N} \quad (24)$$

$$=0.5-(2r)^{-1}+3(2r)^{-2}+4(2r)^{-3}-15(2r)^{-4}+\cdots, \quad (25)$$

$$\beta_2\sim\sum_{N=0}^{\infty}\beta_2^{(N)}(2r)^{-N} \quad (26)$$

$$=0.5-(2r)^{-1}-(2r)^{-2}-4(2r)^{-3}-23(2r)^{-4}+\cdots. \quad (27)$$

What is especially significant is that at high order the $\beta_i^{(N)}$ for the ground state behave asymptotically as

$$\beta_2\sim-(N+1)!\left[1-\frac{6}{N+1}+\frac{2}{(N+1)N}-\frac{16}{(N+1)N(N-1)}-\cdots\right], \quad (28)$$

$$\beta_1\sim 2N!\left[1-\frac{6}{N}-\frac{8}{N(N-1)}+\frac{48}{N(N-1)(N-2)}+\cdots\right]. \quad (29)$$

The same-sign factorial divergence of the separation-constant coefficients, Eqs. (28) and (29), is the same phenomenon as the factorial divergence[3,13] of $E^{(N)}$, Eq. (2), discovered by Morgan and Simon.[3] This phenomenon is a main motivating fact for this study. In explaining the detailed relationships among the RSPT quantities and the exponentially small quantities associated with the double-well phenomena, we shall focus on the separation constants. It is easier to deal with the separation constants than with E directly, because the separation constants are eigenvalues of ordinary differential equations.

We conclude this section with a remark about the endpoints of the β_2 equation (16), which have been treated rather unequally in RSPT. By this we mean that since the unperturbed problem is defined on the semi-infinite interval, the influence of the second boundary condition is not seen by the perturbation theory. As a consequence typical of double-well problems, the characteristic splitting does not show up: both the symmetric and antisymmetric partners of a double-well pair have the same $1/2r$ RSPT expansion. The quasisemiclassical method developed in the next section deals explicitly with both boundary points and consequently gets the double-well splitting.

III. SOLUTION OF THE β_2 EQUATION BY THE QUASISEMICLASSICAL METHOD

Rayleigh-Schrödinger perturbation theory is unable to calculate the double-well gap. In this section we develop a method for solving the β_2 equation (11) that gives not only the gap, but also smaller more subtle effects, while still yielding within the same formalism the RSPT expansion. The *exact* relationship between the RSPT asymptotics and the square of the gap is found. The final formula we are led to for β_2 is a complex expansion whose explicit imaginary terms for real r are discontinuous across the positive axis. The explanation of this apparently paradoxical representation of a real, continuous function is that the Borel sum of the real RSPT expansion exists and has a cut on the positive r axis,[6] so that the value of the Borel sum continued to the real axis is complex, and the explicitly imaginary terms in the expansion are the counterterms that cancel the imaginary part of the Borel sum. This behavior turns out to be widespread: for examples in familiar functions, such as the Airy Bi function, see Ref. 7.

The Borel sum of the RSPT expansion for β_2 turns out[5,6] not to be the eigenvalue associated with Eq. (16), but to be the eigenvalue of a related problem. Consider Eq. (16) both at $-r$ and with a semi-infinite domain. That is, set $r'=-r$ in V_2 of Eq. (21):

$$V_2(v,\beta_2(-r'),-r')=\frac{\beta_2}{2r'+v}+\tfrac{1}{4}(m^2-1)\times\left[-\frac{2}{v(2r'+v)}+\frac{1}{(2r'+v)^2}\right]. \tag{30}$$

On the semi-infinite interval, $0\le v<\infty$, Eq. (16), with V_2 given by Eq. (30), represents a stable, single-well eigenvalue problem whose RSPT expansion is Borel summable[5,6] to the eigenvalue of that problem. That RSPT expansion is the same as for $\beta_2(r)$ with r replaced by $-r'$. This modified problem [Eq. (16) where V is defined by Eq. (30) on $0\le v<\infty$] arises naturally from the separation of the Schrödinger equation for an electron moving in the field of a proton and an antiproton.[5,6]

To bring out the connection of the Borel sum with the imaginary series for β_2 mentioned in the first paragraph of this section, we also solve here by the QSC method the β_2 eigenvalue problem on the semi-infinite interval $0\le v<\infty$, but without changing the sign of r. To avoid the singularity that would occur at $v=2r$, we make r complex. Then the QSC method yields an expansion for the discontinuity in the Borel sum at the $r>0$ axis that is exactly -2 times the imaginary series that occurs in the finite, $0\le v\le 2r$ β_2 problem, thus clinching the cancellation. (To leading exponential order only, the calculation of the discontinuity has been made completely rigorous. See Sec. IV of Ref. 6.)

The *method* we develop here is semiclassical. It is closest to the methods of Langer[17] and Cherry.[18] It differs from standard semiclassical practice in that a *singular point* of the differential equation, rather than a *classical turning point*, is the "anchor point" for the expansion, and exponentially small, subdominant terms can enter the actionlike function. To emphasize the similarities and differences, and for lack of a better term, we refer to the approach as the quasisemiclassical (QSC) method.

The basic idea of the QSC method is to make the perturbation expansion on the "natural variable" on which depends a function that represents the solution of the differential equation near one boundary or singular point. One converts the linear Schrödinger equation into a nonlinear, fourth-order Riccati equation for the natural variable that is solved perturbatively. To satisfy one boundary condition perturbatively, β_2 must be represented by its RSPT series. To satisfy both boundary conditions, β_2 must have an additional, exponentially small (e^{-r}) series that represents half the double-well gap between the symmetric and antisymmetric states of an associated pair. In fact there are additional series that are $O(e^{-2r})$, $O(e^{-3r})$, etc., that are found by satisfying both boundary conditions to higher exponentially small orders. (We stop at the e^{-2r} series.)

A. The quasisemiclassical wave function

The most direct way to characterize the QSC method is through the form of the wave function. The characteristic of the semiclassical Jeffreys-Wentzel-Kramers-Brillouin (JWKB) method[1] is that the logarithm of the wave function is expanded in a power series in $\hbar$. More precisely, the wave function is put in the form

$$\Psi_{\rm JWKB}=(dS/dx)^{-1/2}e^{iS/\hbar}, \tag{31}$$

$$S=\sum_{N=0}^{\infty}S^{(N)}(x)\hbar^{2N}, \tag{32}$$

where $S^{(0)}$ is the classical action, and where the corrections $S^{(N)}$ ($N\ge 1$) are determined recursively.

The JWKB method fails at the classical turning points, where the $S^{(N)}(x)$ may have singularities. Langer[17] generalized the JWKB method to include the classical turning points in part by solving the differential equation itself at the turning point in terms of Airy functions. Away from a turning point the Airy functions can be expanded asymptotically, and Langer's method goes over into the JWKB method.

The points of special interest in the β_2 equation (11) are $\eta=0$ and 2—which are singular points rather than turning points. (The JWKB method fails even more strongly at singularities.) Near $\eta=0$, Eq. (11) is

$$\left[-\frac{d^2}{d\eta^2}+\frac{1}{4}r^2-r\frac{\beta_2}{\eta}+\frac{m^2-1}{4\eta^2}\right]\Phi_2\sim 0, \tag{33}$$

which up to rescaling is Whittaker's confluent hypergeometric equation, whose solution[19,20] regular at 0 is denoted by $M_{\beta_2,m/2}(r\eta)$. In the spirit of Langer's generalization, we take the solution of Eq. (11) near $\eta=0$ to have the form

$$\Phi_2=\frac{1}{m!}(d\phi/d\eta)^{-1/2}M_{b,m/2}(r\phi). \tag{34}$$

The Whittaker M function here plays the role of the Airy function in Langer's method, while $1/r$ is like $\hbar$. The value of the index b will be clarified later. The problem of determining the solution Φ_2 of Eq. (11) then becomes the problem of determining the function $\phi=\phi(\eta,r)$, which by Eqs. (11), (33), and (34) satisfies the Riccati equation

$$-\left[\frac{d\phi}{d\eta}\right]^2\left[\frac{1}{4}-\frac{b}{r\phi}+\frac{m^2-1}{4r^2\phi^2}\right]-\frac{1}{r^2}\left[\frac{d\phi}{d\eta}\right]^{1/2}\frac{d^2}{d\eta^2}\left[\frac{d\phi}{d\eta}\right]^{-1/2}+\frac{1}{4}-\frac{\beta_2}{r}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]+\frac{m^2-1}{4r^2}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]^2=0\ . \tag{35}$$

Cherry[18] extended Langer's approach by expanding the function corresponding here to ϕ as a power series in a parameter that here is $(2r)^{-1}$:

$$\phi(\eta,r)\sim\sum_{N=0}^{\infty}\phi^{(N)}(\eta)(2r)^{-N}\ . \tag{36}$$

Thus the problem of determining Φ_2 becomes the problem of determining the $\phi^{(N)}$.

The parameter b in the Whittaker function is ultimately determined by making Φ_2 satisfy both boundary conditions. We anticipate that it is equal to the unperturbed value of β_2 to zeroth exponential order:

$$b=\beta_2^{(0)}+O(r^k e^{-r})\quad\text{(for some } k>0)\ . \tag{37}$$

Then $M_{\beta_2^{(0)},m/2}(r\eta)$ is simply the usual RSPT unperturbed wave function,[1,16] i.e., a polynomial in η times $\eta^{m/2+1/2}e^{-r\eta/2}$. This value of b turns out to simplify both the analytic form of the $\phi^{(N)}$ and also the asymptotic analysis of $M_{b,m/2}$ that is needed to match the boundary condition at $\eta=2$. (Later it will also be necessary to add exponentially small terms to b, to ϕ, and to β_2 when the process of satisfying both boundary conditions is extended to higher exponential order.)

B. Equations satisfied by the $\phi^{(N)}$; explicit solution for $\phi^{(0)}$, $\phi^{(1)}$, and $\phi^{(2)}$; RSPT for $\beta_2^{(1)}$

To provide a concrete example and to illustrate how RSPT "falls out," we calculate $\phi^{(0)}$, $\phi^{(1)}$, $\phi^{(2)}$, and $\beta_2^{(1)}$ explicitly.

Put the expansions (36) for ϕ, (26) for β_2, and (37) for b into the Riccati equation (35), which can then be solved recursively. To lowest order in $(2r)^{-1}$, one finds

$$-\tfrac{1}{4}(d\phi^{(0)}/d\eta)^2+\tfrac{1}{4}=0\ , \tag{38}$$

$$d\phi^{(0)}/d\eta=1,\quad \phi^{(0)}=\eta\ . \tag{39}$$

Note that the unperturbed value of ϕ is η, consistent with the discussion above [between Eqs. (33) and (34)] of Φ_2 near $\eta=0$. Moreover, since Φ_2 at $\eta=0$ behaves like

$$\Phi_2\sim\eta^{m/2+1/2}\ , \tag{40}$$

the equivalent condition for ϕ is

$$\phi^{(N)}=O(\eta)\quad\text{as }\eta\to 0\ , \tag{41}$$

which also explains the choice of "integration constant" in Eq. (39).

To first order in $(2r)^{-1}$, Eqs. (35)—(41) yield

$$-\frac{1}{2}\frac{d\phi^{(1)}}{d\eta}+2\beta_2^{(0)}\frac{1}{\eta}-2\beta_2^{(0)}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]=0\ , \tag{42}$$

$$\phi^{(1)}=4\beta_2^{(0)}\ln(1-\tfrac{1}{2}\eta)\ . \tag{43}$$

To second order in $(2r)^{-1}$, Eqs. (35)—(43) yield

$$-\frac{1}{2}\frac{d\phi^{(2)}}{d\eta}-\frac{1}{4}\left[\frac{d\phi^{(1)}}{d\eta}\right]^2+4\beta_2^{(0)}\frac{1}{\phi^{(0)}}\frac{d\phi^{(1)}}{d\eta}-2\beta_2^{(0)}\frac{\phi^{(1)}}{(\phi^{(0)})^2}-(m^2-1)\frac{1}{(\phi^{(0)})^2}-2\beta_2^{(1)}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]+(m^2-1)\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]^2=0\ , \tag{44}$$

$$d\phi^{(2)}/d\eta=-16(\beta_2^{(0)})^2\eta^{-2}\ln(1-\tfrac{1}{2}\eta)-16(\beta_2^{(0)})^2\eta^{-1}(2-\eta)^{-1}+2[-4(\beta_2^{(0)})^2+m^2-1]\frac{1}{(2-\eta)^2}+2[-2\beta_2^{(1)}+m^2-1-4(\beta_2^{(0)})^2]\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]\ , \tag{45}$$

$$\phi^{(2)}=16(\beta_2^{(0)})^2[\eta^{-1}\ln(1-\tfrac{1}{2}\eta)+\tfrac{1}{2}]+2[-4(\beta_2^{(0)})^2+m^2-1][(2-\eta)^{-1}-\tfrac{1}{2}]+2[-2\beta_2^{(1)}+m^2-1-4(\beta_2^{(0)})^2]\ln[\eta/(2-\eta)]\ . \tag{46}$$

Equation (46) would display a singularity in $\phi^{(2)}$ at $\eta=0$ *unless*

$$\beta_2^{(1)}=-2(\beta_2^{(0)})^2+\tfrac{1}{2}(m^2-1)\ , \tag{47}$$

which is precisely the RSPT result. Then instead of Eq. (46), $\phi^{(2)}$ is given by

$$\phi^{(2)}=16(\beta_2^{(0)})^2[\eta^{-1}\ln(1-\tfrac{1}{2}\eta)+\tfrac{1}{2}]+4\beta_2^{(1)}[(2-\eta)^{-1}-\tfrac{1}{2}]\ . \tag{48}$$

The equations for $\phi^{(3)},\phi^{(4)},\ldots$ get progressively more tedious. However, each $\phi^{(N)}$ can be found in closed form; each $\phi^{(N)}$ is analytic and has a zero at $\eta=0$, provided only that $\beta_2^{(N-1)}$ is chosen correctly. In fact it is not hard to show inductively from Eqs. (35), (39), (43), and (48) that $\beta_2^{(N-1)}$ can be chosen to make $\phi^{(N)}$ analytic and zero at $\eta=0$. By the uniqueness of power series, the $\beta_2^{(N)}$—determined so that the QSC Φ_2 satisfy the boundary condition at $\eta=0$—must be identical with the RSPT $\beta_2^{(N)}$. In this way the QSC method contains RSPT.

C. Boundary condition at $\eta=2$ and the double-well gap

A major advantage of the QSC method over RSPT is that the wave function can be made to vanish at $\eta=2$, as will now be demonstrated. The basic idea is to generate QSC wave functions from both $\eta=0$ and 2 and to match them in the middle where the asymptotic expansion for the Whittaker function is valid. A most crucial detail, however, is that the exponentially small shift [Eq. (37)] in the b index of the Whittaker function of Eq. (34) must now be determined. To find this shift, we reexamine the perturbation hypothesis—namely, that β_2 and ϕ can be expanded in power series in $(2r)^{-1}$.

As is well known, the RSPT expansion for β_2 is incomplete in the sense that there is an exponentially small correction of the form[2,4]

$$\beta_2\sim\sum_{N=0}^{\infty}\beta_2^{(N)}(2r)^{-N}+\Delta\beta_2^{[1]}+O(r^ke^{-2r})\quad\text{(for some } k>0)\,, \tag{49}$$

$$\Delta\beta_2^{[1]}\sim\pm\frac{(2r)^{2\beta_2^{(0)}}e^{-r}}{n_2!(n_2+m)!}\,. \tag{50}$$

The notation $\Delta f^{[q]}$ is to signify that part of f that is proportional to e^{-qr}. The quantity $2\Delta\beta_2^{[1]}$ is the double-well splitting [through $O(e^{-r})$] that separates the symmetric and antisymmetric states of a double-well pair, both of which have the same RSPT expansion. To make it possible to calculate the exponentially small terms, it is necessary to add them to the perturbation expansions (24) and (26) for β_1 and β_2, and to permit them to enter the expansions (37) for b and (36) for ϕ. This generalization is a natural but marked departure from the usual semiclassical practice. We put

$$\beta_i\sim\sum_{N=0}^{\infty}\beta_i^{(N)}(2r)^{-N}+\Delta\beta_i^{[1]}+O(r^ke^{-2r})\quad(i=1,2)\,, \tag{51}$$

$$b\sim\beta_2^{(0)}+\Delta b^{[1]}+O(r^ke^{-2r})\,, \tag{52}$$

$$\phi(\eta,r)\sim\sum_{N=0}^{\infty}\phi^{(N)}(\eta)(2r)^{-N}+\Delta\phi^{[1]}+O(r^ke^{-2r})\,. \tag{53}$$

[In Eqs. (51)—(53) and in all subsequent equations, we omit the generic "for some $k>0$," which without danger of confusion may be taken as understood.] It will be seen later that the leading terms of $\Delta\beta_2^{[1]}$ and $\Delta b^{[1]}$ are equal:

$$\Delta\beta_2^{[1]}=\Delta b^{[1]}[1+O(r^{-1})]=\pm\frac{(2r)^{2\beta_2^{(0)}}e^{-r}}{n_2!(n_2+m)!}[1+O(r^{-1})]\,. \tag{54}$$

The crucial role played by the shift in the b index is immediately apparent when, in preparation for matching the wave function (34) with one satisfying the boundary condition at $\eta=2$, the Whittaker M function is expanded asymptotically:[20]

$$\frac{1}{m!}M_{b,m/2}(z)=\frac{e^{\pm\pi i(m/2+1/2-b)}}{\Gamma(\frac12 m+\frac12+b)}W_{b,m/2}(z)+\frac{e^{\mp\pi ib}}{\Gamma(\frac12 m+\frac12-b)}W_{-b,m/2}(ze^{\mp\pi i})\quad(0<\pm\arg z<\pi) \tag{55}$$

$$\sim\frac{e^{\pm\pi i(m/2+1/2-b)}}{\Gamma(\frac12 m+\frac12+b)}z^be^{-z/2}{}_2F_0(\tfrac12+\tfrac12 m-b,\tfrac12-\tfrac12 m-b;;-z^{-1})+\frac{1}{\Gamma(\frac12+\frac12 m-b)}z^{-b}e^{+z/2}{}_2F_0(\tfrac12+\tfrac12 m+b,\tfrac12-\tfrac12 m+b;;+z^{-1})\quad(0<\pm\arg z<\pi) \tag{56}$$

$$\sim(-1)^{n_2}\frac{e^{\mp\pi i\Delta b^{[1]}}}{(n_2+m)!}z^be^{-z/2}+\Delta b^{[1]}(-1)^{n_2+1}n_2!z^{-b}e^{+z/2}\quad(0<\pm\arg z<\pi)\,, \tag{57}$$

where we have used the Γ-function reflection formula[19] and that $b+\frac12-\frac12 m\sim n_2+1+\Delta b^{[1]}$ to get

$$1/\Gamma(\tfrac12+\tfrac12 m-b)=\Gamma(b+\tfrac12-\tfrac12 m)\pi^{-1}\sin[\pi(b+\tfrac12-\tfrac12 m)] \tag{58}$$

$$=(-1)^{n_2+1}n_2!\Delta b^{[1]}[1+O(\Delta b^{[1]})]\,. \tag{59}$$

Note the introduction in Eq. (55) of the Whittaker W functions, primarily for later use, and in Eq. (56) the usual generalized hypergeometric series,[19]

$${}_2F_0(a,b;;z)=1+ab\frac{z}{1!}+a(a+1)b(b+1)\frac{z^2}{2!}+\cdots\,. \tag{60}$$

When $\Delta b^{[1]}\neq0$, there is a *positive exponential term* in Φ_2. Consider for the moment how Φ_2 appears near the point $\eta=2$. The positive exponential in Eqs. (56) and (57) (where $z=r\phi\sim r\eta$) is the term that is *decaying* away from $\eta=2$ (in the direction of $\eta=0$) and near $\eta=2$ should be the most important term. In fact, because of the symmetry of Eq. (11), Φ_2 should be either symmetric or antisymmetric under the transformation $\eta\to2-\eta$, so that both exponentials should be equally weighted. It will turn out that $\Delta b^{[1]}$ has exactly the right value to achieve this symmetry.

It is now straightforward to obtain the leading terms in the asymptotic expansion of Φ_2. Take $\phi^{(0)}$ and $\phi^{(1)}$ from Eqs. (39) and (43), and use Eqs. (34) and (57) to obtain, for Φ_2 anchored at $\eta=0$ (denoted here by $\Phi_{2[0]}$),

$$\Phi_{2[0]} \sim \frac{(-1)^{n_2}(2r)^{\beta_2^{(0)}}}{(n_2+m)!}\eta^{\beta_2^{(0)}}(2-\eta)^{-\beta_2^{(0)}}e^{-r\eta/2}[1+O(r^{-1})]$$
$$+\Delta b^{[1]}(-1)^{n_2+1}n_2!(2r)^{-\beta_2^{(0)}}(2-\eta)^{\beta_2^{(0)}}$$
$$\times\eta^{-\beta_2^{(0)}}e^{+r\eta/2}[1+O(r^{-1})] \,. \tag{61}$$

(Here and in the following, we use "anchored at $\eta=a$" to mean a QSC wave function generated by expansion from the point a.) If instead of starting the expansion at the boundary point $\eta=0$ we had started at $\eta=2$, exactly the same expression would have been obtained for Φ_2 anchored at $\eta=2$ ($\Phi_{2[2]}$), except that η would be replaced by $2-\eta$:

$$\Phi_{2[2]} \sim \frac{(-1)^{n_2}(2r)^{\beta_2^{(0)}}}{(n_2+m)!}$$
$$\times(2-\eta)^{\beta_2^{(0)}}\eta^{-\beta_2^{(0)}}e^{-r+r\eta/2}[1+O(r^{-1})]$$
$$+\Delta b^{[1]}(-1)^{n_2+1}n_2!(2r)^{-\beta_2^{(0)}}\eta^{\beta_2^{(0)}}$$
$$\times(2-\eta)^{-\beta_2^{(0)}}e^{+r-r\eta/2}[1+O(r^{-1})] \,. \tag{62}$$

These two equations represent the *same wave function* only if

$$(\Delta b^{[1]})^2 = \frac{(2r)^{4\beta_2^{(0)}}e^{-2r}}{[n_2!(n_2+m)!]^2}[1+O(r^{-1})] \,, \tag{63}$$

which gives the formula (54) for $\Delta b^{[1]}$.

The complete series for $\Delta b^{[1]}$ is obtained by carrying out the above process to all powers of $(2r)^{-1}$. The formal result is

$$\Delta b^{[1]} = \pm\frac{(2r)^{2\beta_2^{(0)}}e^{-r}}{n_2!(n_2+m)!}(\tfrac{1}{2}\phi_{[0]})^{\beta_2^{(0)}}(\tfrac{1}{2}\phi_{[2]})^{\beta_2^{(0)}}e^{-r(\phi_{[0]}+\phi_{[2]}-2)/2}\left[\frac{{}_2F_0(-n_2,-n_2-m;;-(r\phi_{[0]})^{-1})}{{}_2F_0(n_2+m+1,n_2+1;;+(r\phi_{[0]})^{-1})}\right]^{1/2}$$
$$\times\left[\frac{{}_2F_0(-n_2,-n_2-m;;-(r\phi_{[2]})^{-1})}{{}_2F_0(n_2+m+1,n_2+1;;+(r\phi_{[2]})^{-1})}\right]^{1/2} . \tag{64}$$

By $\phi_{[0]}$ is meant the ϕ for the QSC eigenfunction anchored at $\eta=0$, while $\phi_{[2]}$ corresponds to the QSC eigenfunction anchored at $\eta=2$. In fact here $\phi_{[2]}(\eta,r)=\phi_{[0]}(2-\eta,r)$. The right-hand side of Eq. (64) is $(2r)^{2\beta_2^{(0)}}e^{-r}$ times a series in $(2r)^{-1}$ that is independent of η. [Note that $\phi^{(0)}$, Eq. (39), is independent of $\beta_2^{(0)}$.]

The index shift $\Delta b^{[1]}$ and RSPT can now be put together to give the $O(e^{-r})$ contribution $\Delta\beta_2^{[1]}$ to β_2. Recall that in the preceding subsection (III B) the index b was set equal to $\beta_2^{(0)}$ and then the higher $\beta_2^{(N)}$ ($N\geq 1$) were obtained as functions of $\beta_2^{(0)}$ by requiring that $\phi^{(N+1)}$ vanish as $\eta\to 0$. That process did not depend on the value of $\beta_2^{(0)}$. If now $\beta_2^{(0)}\to\beta_2^{(0)}+\Delta b^{[1]}$, then one can expand out from the RSPT series the part linear in $\Delta b^{[1]}$,

$$\Delta\beta_2^{[1]} = \Delta b^{[1]}\sum_{N=0}^{\infty}\frac{d\beta_2^{(N)}}{d\beta_2^{(0)}}(2r)^{-N} \tag{65}$$
$$= \Delta b^{[1]}[1-4\beta_2^{(0)}(2r)^{-1}+\cdots] \,, \tag{66}$$

where Eq. (47) has been used to calculate $d\beta_2^{(1)}/d\beta_2^{(0)}$. In a similar way it follows that

$$\Delta\phi^{[1]} = \Delta b^{[1]}\sum_{N=0}^{\infty}\frac{d\phi^{(N)}(\eta)}{d\beta_2^{(0)}}(2r)^{-N} \tag{67}$$
$$= r^{-1}\Delta b^{[1]}[2\ln(1-\tfrac{1}{2}\eta)+\cdots] \,, \tag{68}$$

where Eq. (43) has been used to calculate $d\phi^{(1)}/d\beta_2^{(0)}$.

To use Eqs. (65) and (67) relating $\Delta\beta_2^{[1]}$ and $\Delta\phi^{[1]}$ to $\Delta b^{[1]}$, it is necessary to calculate the RSPT $\beta_2^{(N)}$ and the QSC $\phi^{(N)}$ as explicit functions of $\beta_2^{(0)}$. This is easy for low orders but tedious for high orders. An alternative procedure is given in the next subsection.

D. Solution of the Riccati equation directly to $O(e^{-r})$

To avoid solving for $\beta_2^{(N)}$ and $\phi^{(N)}$ as explicit functions of $\beta_2^{(0)}$ to high order, which would be required to use Eqs. (65) and (67) for $\Delta\beta_2^{[1]}$ and $\Delta\phi^{[1]}$, we give an alternative procedure, which is to solve the Riccati equation (35) directly to $O(e^{-r})$.

Let $q(r)$ denote the ratio

$$q(r)\equiv\Delta\beta_2^{[1]}/\Delta b^{[1]} = \sum_{N=0}^{\infty}\frac{d\beta_2^{(N)}}{d\beta_2^{(0)}}(2r)^{-N} \,. \tag{69}$$

We anticipate that $r^{-1}\Delta b^{[1]}$ is a natural factor in $\Delta\phi^{[1]}$, and we accordingly define the ratio

$$\theta(\eta,r)=\Delta\phi^{[1]}/r^{-1}\Delta b^{[1]} \,. \tag{70}$$

Let ϕ in the remainder of this section denote only the zeroth-exponential-order part of ϕ—i.e., the $1/r$ power-series part. In place of ϕ, put $\phi+r^{-1}\Delta b^{[1]}\theta$ into the Riccati equation (35), and put $\beta_2^{(0)}+\Delta b^{[1]}$ for b and $\sum\beta_2^{(N)}(2r)^{-N}+\Delta b^{[1]}q(r)$ for β_2. Expand the equation in powers of $\Delta b^{[1]}$, and keep only the terms first order in $\Delta b^{[1]}$. The result, divided by $r^{-1}\Delta b^{[1]}$, is an equation for $\theta(\eta,r)$ and $q(r)$, given $\phi(\eta,r)$:

$$\left[\frac{d\phi}{d\eta}\right]^2\left[\frac{1}{\phi}-\frac{\beta_2^{(0)}\theta}{r\phi^2}+\frac{(m^2-1)\theta}{2r^2\phi^3}\right]-2\frac{d\phi}{d\eta}\frac{d\theta}{d\eta}\left[\frac{1}{4}-\frac{\beta_2^{(0)}}{r\phi}+\frac{m^2-1}{4r^2\phi^2}\right]-q(r)\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]$$
$$-\frac{1}{2r^2}\frac{d\theta}{d\eta}\left[\frac{d\phi}{d\eta}\right]^{-1/2}\frac{d^2}{d\eta^2}\left[\frac{d\phi}{d\eta}\right]^{-1/2}+\frac{1}{2r^2}\left[\frac{d\phi}{d\eta}\right]^{1/2}\frac{d^2}{d\eta^2}\left[\frac{d\theta}{d\eta}\left[\frac{d\phi}{d\eta}\right]^{-3/2}\right]=0\,. \quad (71)$$

To solve Eq. (71), first expand $q(r)$ and $\theta(\eta,r)$ in power series in $(2r)^{-1}$:

$$q(r)=\sum_{N=0}^{\infty}q^{(N)}(2r)^{-N}\,, \quad (72)$$

$$\theta(\eta,r)=\sum_{N=0}^{\infty}\theta^{(N)}(\eta)(2r)^{-N}\,. \quad (73)$$

From Eq. (71) and $\phi^{(0)}$ [Eq. (39)], one obtains the zeroth-order equation,

$$\tfrac{1}{2}d\theta^{(0)}/d\eta=\eta^{-1}-q^{(0)}[\eta^{-1}+(2-\eta)^{-1}]\,. \quad (74)$$

Since $d\theta^{(0)}/d\eta$ must be finite at $\eta=0$,

$$q^{(0)}=1,\ \ \theta^{(0)}=2\ln(1-\tfrac{1}{2}\eta)\,. \quad (75)$$

Similarly, one obtains the equation

$$d\theta^{(1)}/d\eta=(d/d\eta)[16\beta_2^{(0)}\eta^{-1}\ln(1-\tfrac{1}{2}\eta)]$$
$$-8\beta_2^{(0)}(2-\eta)^{-2}$$
$$-2(4\beta_2^{(0)}+q^{(1)})[\eta^{-1}+(2-\eta)^{-1}]\,. \quad (76)$$

From the regularity condition at $\eta=0$ it follows that

$$q^{(1)}=-4\beta_2^{(0)}\,, \quad (77)$$

$$\theta^{(1)}=16\beta_2^{(0)}[\eta^{-1}\ln(1-\tfrac{1}{2}\eta)+\tfrac{1}{2}]$$
$$-8\beta_2^{(0)}[(2-\eta)^{-1}-\tfrac{1}{2}]\,. \quad (78)$$

Thus the ratios $q(r)$ and $\theta(\eta,r)$ can be calculated by a recursive, perturbative technique directly, rather than through the $\beta_2^{(0)}$ derivatives of the $\phi^{(n)}$ and the $\beta_2^{(N)}$. It is interesting that there is yet another alternative method for calculating $q(r)$—a "normalization-integral" method—that will be given in the next subsection.

E. Normalization-integral formula for $q(r)$

The two methods given previously for $q(r)$ are generalizable to higher exponential orders. A third formula is developed in this section that is less generalizable but simpler in the respect that it uses only the zeroth-exponential-order wave function in the practical evaluation of $q(r)$. The argument starts out with a "current-density" formula and ends up with an expression that looks like a normalization integral.

Let $\Phi^{(+)}$ and $\Phi^{(-)}$ denote the paired solutions of Eq. (11) that differ only in the choice of sign for $\Delta b^{\{1\}}$ in Eq. (64). To $O(e^{-r})$ the difference in the two eigenvalues—i.e., the double-well gap for these two states—is $2\Delta\beta_2^{\{1\}}$. From Eq. (11) one sees by a standard current-density argument that

$$2\Delta\beta_2^{\{1\}}+O(e^{-2r})=\frac{\Phi^{(+)}(d\Phi^{(-)}/d\eta)-\Phi^{(-)}(d\Phi^{(+)}/d\eta)}{r\int_0^{\eta}\Phi^{(+)}\Phi^{(-)}[\eta^{-1}+(2-\eta)^{-1}]d\eta}\,. \quad (79)$$

The numerator is a Wronskian of two functions that solve the same differential equation if terms $O(r^ke^{-r})$ are neglected. From the form of $\Phi^{(\pm)}$ [in terms of the Whittaker M function, Eq. (34)], from Eqs. (55) and (56) [or more simply Eq. (57)] for the asymptotics of the M function, from the Wronksian of the Whittaker functions,[20]

$$W_{b,m/2}(z)\frac{d}{dz}e^{\mp\pi ib}W_{-b,m/2}(ze^{\mp\pi i})$$
$$-e^{\mp\pi ib}W_{-b,m/2}(ze^{\mp\pi i})\frac{d}{dz}W_{b,m/2}(z)=1\,, \quad (80)$$

and from standard error estimates for formulas of this type,[4] it follows that so long as $0\ll\eta\ll2$, i.e., for $\eta=1+\epsilon$ $(\epsilon\sim0)$, the numerator is to first exponential order,

$$2rn_2!\Delta b^{\{1\}}/(n_2+m)!\,. \quad (81)$$

Similarly, also for $0\ll\eta\ll2$, the denominator is to terms $O(r^ke^{-r})$ independent of η and dominated by the exponentially decreasing component, the $W_{b,m/2}$ in Eq. (55). Since for $b=\beta_2^{(0)}$ this W is just an unperturbed wave function, there is no difficulty and insignificant error in replacing the M by the unperturbed W, expanding the integrand as $e^{-r\eta}$ times a power series in $(2r)^{-1}$ and in η, and then taking the upper limit of the integral to be ∞. That is, the denominator is again up to $O(r^ke^{-r})$

$$r[(n_2+m)!]^{-2}\int_0^{\infty}(d\phi/d\eta)^{-1}[W_{\beta_2^{(0)},m/2}(r\phi)]^2$$
$$\times[\eta^{-1}+(2-\eta)^{-1}]d\eta\,. \quad (82)$$

We emphasize that (82) is not meant literally, but instead as an asymptotic power series in $(2r)^{-1}$. Also, ϕ is meant to be the zeroth-exponential-order solution of the Riccati equation (35). Thus one obtains for $q(r)=\Delta\beta_2^{\{1\}}/\Delta b^{\{1\}}$,

$$q(r)=n_2!(n_2+m)!\left[\int_0^{\infty}(d\phi/d\eta)^{-1}[W_{\beta_2^{(0)},m/2}(r\phi)]^2\times[\eta^{-1}+(2-\eta)^{-1}]d\eta\right]^{-1}. \quad (83)$$

Equation (83), being only an integral to be evaluated, is perhaps the most useful practical expression for computing $q(r)$.

F. Imaginary contribution to the index b

As mentioned in the Introduction and in Sec. II C, same-sign factorial divergence suggests a complex, discontinuous Borel sum [cf. Eqs. (3) and (4)]. For the RSPT for β_2, we infer from Eq. (28) that for the ground state, with $r>0$,

$$\sum_{N=0}^{\infty} \beta_2^{(N)}(2r)^{-N} \sim -\sum_{N=0}^{\infty}(N+1)!(2r)^{-N} \quad (84)$$

$$\sim \mathrm{P}\int_0^{\infty} t^2 e^{-t}(t-2r)^{-1}dt \pm i\pi 4r^2 e^{-2r} \quad (\mathrm{Im}r=\pm 0)\ . \quad (85)$$

This motivates us to look for an *explicit* contribution to β_2 that is $O(e^{-2r})$ and that is *imaginary*, to cancel the imaginary term in Eq. (85).

Since the Riccati equation (35) is formally real, explicit imaginary terms in β_2 can only originate in the index b. The value of b through $O(e^{-r})$ was obtained in Sec. III C by matching two QSC wave functions that separately satisfied the boundary conditions at either $\eta=0$ or 2, and that value was real (for real r and η). The imaginary $O(e^{-2r})$ contribution has its computational origin in the complex phase factor multiplying the subdominant contribution to the ordinary asymptotic expansion for the Whittaker M function, Eqs. (55) and (56).

The reader is well aware that the Whittaker M function is real on the real axis, and that the complex expansion (56) is not usually considered valid[21] on the real axis, which is a Stokes line of the expansion.[21] However, there is a sense[7] in which the complex expansion (56) is valid also on the real axis. In fact, the two power-series expansions represented by the $_2F_0$ functions in Eq. (56) are Borel summable,[7] and the overall result is the Whittaker M function in each appropriate half-plane. The positive real axis is a cut of the Borel sum of the power series multiplying $e^{+z/2}$, the dominant expansion. In the limit as $\mathrm{Im}z \to 0$ from above or below, the imaginary part of the Borel sum times $e^{+z/2}$ cancels the explicit imaginary contribution coming from the phase factor multiplying the subdominant expansion. This is the sense in which the sum of the explicitly complex, discontinuous expansion mentioned in the Introduction is real and continuous. The same phenomenon that holds for the Whittaker M function appears to apply to β_2. (See Ref. 6 for a proof that the Borel sum of the RSPT series for β_2 is complex.)

Let us now get on with the details of extending the matching process of Sec. III C to $O(e^{-2r})$. First we extend the notation to include second exponential order [cf. Eqs. (51)—(53)]:

$$\beta_i \sim \sum_{N=0}^{\infty} \beta_i^{(N)}(2r)^{-N} + \Delta\beta_i^{[1]} + \Delta\beta_i^{[2]} + O(r^k e^{-3r}) \quad (i=1,2)\ , \quad (86)$$

$$b \sim \beta_2^{(0)} + \Delta b^{[1]} + \Delta b^{[2]} + O(r^k e^{-3r})\ , \quad (87)$$

$$\phi(\eta,r) \sim \sum_{N=0}^{\infty} \phi^{(N)}(\eta)(2r)^{-N} + \Delta\phi^{[1]} + \Delta\phi^{[2]} + O(r^k e^{-3r})\ . \quad (88)$$

Next we keep the phase factor in Eqs. (55)—(57) and get as a requirement for the matching of the two QSC functions, instead of Eqs. (64) and (63),

$$(\Delta b^{[1]} + \Delta b^{[2]})^2 = e^{\mp 2\pi i \Delta b^{[1]}} \times [\text{right-hand side of Eq. (64)}]^2 \times [1+O(\Delta b^{[1]})] \quad (89)$$

$$= e^{\mp 2\pi i \Delta b^{[1]}} \frac{(2r)^{4\beta_2^{(0)}} e^{-2r}}{[n_2!(n_2+m)!]^2}[1+O(r^{-1})] \quad (\pm \mathrm{Im}r \geq 0)\ . \quad (90)$$

(The $O(\Delta b^{[1]})$ error in Eq. (89) comes from replacing the $\Gamma(\frac{1}{2}m+\frac{1}{2}\pm b)$ [cf. Eq. (55)] by $(n_2+m)!$ and $n_2!$. There is no contribution from this term to $\mathrm{Im}\Delta b^{[2]}$ (this section), but there is a contribution to $\mathrm{Re}\Delta b^{[2]}$ that will be taken care of in Sec. III H.)

The imaginary contribution to $\Delta b^{[2]}$ comes from the expansion of the phase factor. Take the square root of both sides of Eq. (89), then expand the factor $e^{\mp \pi i \Delta b^{[1]}}$:

$$\Delta b^{[1]} + \Delta b^{[2]} = (1 \mp i\pi \Delta b^{[1]}) \times [\text{right-hand side of Eq. (64)}] \times [1+O(\Delta b^{[1]})] \quad (91)$$

$$= (1 \mp i\pi \Delta b^{[1]}) \times \Delta b^{[1]} \times [1+O(\Delta b^{[1]})]\ . \quad (92)$$

Let $\Delta_r b^{[2]}$ and $\Delta_i b^{[2]}$ denote the real and imaginary parts of $\Delta b^{[2]}$ when r is real and positive, and their analytic continuations otherwise:

$$\Delta b^{[2]} = \Delta_r b^{[2]} + i\Delta_i b^{[2]}\ . \quad (93)$$

Then it is immediately seen from Eq. (92) that the second-exponential-order imaginary contribution to b is

$$\Delta_i b^{[2]} = \mp \pi (\Delta b^{[1]})^2 \quad (\pm \mathrm{Im}r \geq 0)\ . \quad (94)$$

This relationship between the asymptotic expansions is exact. It is the key to the Brézin—Zinn-Justin conjecture[12] discussed in the next subsection. Note, moreover, that for the ground state,

$$\Delta_i b^{[2]} \sim \mp \pi 4r^2 e^{-2r} \quad (\mathrm{Im}r=\pm 0)\ , \quad (95)$$

so that $i\Delta_i b^{[2]}$ to leading order is exactly the counterterm to cancel the imaginary part of Eq. (85).

G. Imaginary contribution to β_2. The gap-squared formula

The imaginary series (94) contributing to the index b leads directly to an imaginary series in β_2 that is $O(e^{-2r})$. Denote by $\Delta_r\beta_2^{[2]}$ and $\Delta_i\beta_2^{[2]}$ the real and imaginary series contributing to $\Delta\beta_2^{[2]}$ when r is real and positive:

$$\Delta\beta_2^{[2]}=\Delta_r\beta_2^{[2]}+i\Delta_i\beta_2^{[2]} . \tag{96}$$

By exactly the same argument that led to Eq. (65) for $\Delta\beta_2^{[1]}$, one finds that the imaginary series to second exponential order is obtained from $\Delta_i b^{[2]}$ via

$$\Delta_i\beta_2^{[2]}=\Delta_i b^{[2]}\sum_{N=0}^{\infty}\frac{d\beta_2^{(N)}}{d\beta_2^{(0)}}(2r)^{-N} \tag{97}$$

$$=\Delta_i b^{[2]}q(r) \tag{98}$$

$$=\mp\pi\frac{(2r)^{4\beta_2^{(0)}}e^{-2r}}{[n_2!(n_2+m)!]^2}[1+O(r^{-1})] \quad (\pm\mathrm{Im}r\geq 0) . \tag{99}$$

The importance of $\Delta_i\beta_2^{[2]}$ is the role it plays, via a dispersion relation[6] to be discussed later in Sec. VI, in the asymptotics of the RSPT coefficients $\beta_2^{(N)}$:

$$\beta_2^{(N)}\sim\pi^{-1}2^N\int_0^{\infty+i\epsilon}r^{N-1}\Delta_i\beta_2^{[2]}dr . \tag{100}$$

The $\infty+i\epsilon$ is to indicate that the "$\mathrm{Im}r\geq 0$ sign" is to be used for $\Delta_i b^{[2]}$ in Eq. (94). Since the same ratio $q(r)$ occurs here that occurred for the first-exponential-order quantity $\Delta\beta_2^{[1]}$ [Eqs. (66)–(69)], it is possible to express $\Delta_i\beta_2^{[2]}$ directly in terms of $\Delta\beta_2^{[1]}$ and $q(r)$ via Eq. (94):

$$\Delta_i\beta_2^{[2]}=\mp\pi(\Delta\beta_2^{[1]})^2/q(r) \quad (\pm\mathrm{Im}r\geq 0) , \tag{101}$$

which, because of Eq. (83), can be written as the product of $\mp\pi$, the "half gap" squared, and a normalization integral, taken in the sense of an asymptotic power series as explained in Sec. III E,

$$\Delta_i\beta_2^{[2]}=\mp\pi(\Delta\beta_2^{[1]})^2\frac{\int_0^{\infty}(d\phi/d\eta)^{-1}[W_{\beta_2^{(0)},m/2}(r\phi)]^2[\eta^{-1}+(2-\eta)^{-1}]d\eta}{n_2!(n_2+m)!} \quad (\pm\mathrm{Im}r\geq 0) . \tag{102}$$

Recall that the expansion for $q(r)$ starts out with 1 [cf. Eqs. (66) and (75)]. Equations (101) and (102) express the *exact* relationship between the asymptotics of the $\beta_2^{(N)}$ [via Eq. (100)] and the square of the gap whose leading term was found numerically by Brézin and Zinn-Justin.[9] In fact, that relationship did not involve β_2 but the energy $E(R)$. It will be seen in Sec. VI, however, that the asymptotics of the $E^{(N)}$ are dominated by $\Delta_i\beta_2^{[2]}$, so that the crux of the explanation of the $E^{(N)}$ asymptotics has already been given.

H. Doubly-exponentially-small real series

The matching process described in Sec. III C was carried out there to $O(e^{-r})$ for the index shift $\Delta b^{[1]}$ and in Sec. III F for the $O(e^{-2r})$ imaginary shift $\Delta_i b^{[2]}$. In this section the calculation of the shift in b to any exponential order is sketched, and results are given for the real $O(e^{-2r})$ shift $\Delta_r b^{[2]}$ and the real second-exponential-order $\Delta_r\beta_2^{[2]}$.

The formulas in this section involve the logarithmic derivative of the gamma function,[19] usually defined by ψ:

$$\psi(z)=\frac{d}{dz}\ln\Gamma(z) . \tag{103}$$

The exact form of the matching equation that results from equating the two QSC functions, one anchored at $\eta=0$, the other at $\eta=2$, the $O(e^{-r})$ version of which is Eq. (64), is [cf. Eqs. (34) and (55)–(59)]

$$b=\beta_2^{(0)}+\Delta b , \tag{104}$$

$$\pi^{-2}\sin^2(\pi\Delta b)=\frac{e^{\mp 2\pi i\Delta b}}{[\Gamma(n_2+m+1+\Delta b)\Gamma(n_2+1+\Delta b)]^2}\frac{W_{\beta_2^{(0)}+\Delta b,m/2}(r\phi_{[0]})}{e^{\mp\pi i(\beta_2^{(0)}+\Delta b)}W_{-\beta_2^{(0)}-\Delta b,m/2}(r\phi_{[0]}e^{\mp\pi i})}\times\frac{W_{\beta_2^{(0)}+\Delta b,m/2}(r\phi_{[2]})}{e^{\mp\pi i(\beta_2^{(0)}+\Delta b)}W_{-\beta_2^{(0)}-\Delta b,m/2}(r\phi_{[2]}e^{\mp\pi i})} \quad (\pm\mathrm{Im}r\geq 0) . \tag{105}$$

As with Eq. (64), the η dependence of the right-hand side of Eq. (105) cancels, leaving only a function of r. Now expand Δb in exponentially ordered terms $\Delta b^{[q]}$,

$$\Delta b=\sum_{q=1}^{\infty}\Delta b^{[q]} . \tag{106}$$

The asymptotic equation for Δb, which is the general version of Eq. (64) valid to all exponential orders, is obtained by using the asymptotic expansions [cf. Eqs. (55)–(57)] for the Whittaker functions and taking the square root of both sides of Eq. (105). To put the result in a form that can be solved recursively for the $\Delta b^{[q]}$ after expansion, we add $\pi^{-1}\sin(\pi\Delta b)-\Delta b$ to both sides (after taking the square root). Then for $\mathrm{Im}r\geq 0$ (the complex conjugate holds for the reverse) we obtain

$$\Delta b = -[\pi^{-1}\sin(\pi\Delta b) - \Delta b] \pm \frac{e^{-\pi i \Delta b}(2r)^{2\beta_2^{(0)}+2\Delta b} e^{-r}}{\Gamma(n_2+m+1+\Delta b)\Gamma(n_2+1+\Delta b)} (\tfrac{1}{2}\phi_{[0]})^{\beta_2^{(0)}+\Delta b} (\tfrac{1}{2}\phi_{[2]})^{\beta_2^{(0)}+\Delta b} e^{-r(\phi_{[0]}+\phi_{[2]}-2)/2}$$
$$\times \left[\frac{{}_2F_0(-n_2-\Delta b, -n_2-m-\Delta b;;-(r\phi_{[0]})^{-1})}{{}_2F_0(n_2+m+1+\Delta b, n_2+1+\Delta b;;+(r\phi_{[0]})^{-1})} \right]^{1/2}$$
$$\times \left[\frac{{}_2F_0(-n_2-\Delta b, -n_2-m-\Delta b;;-(r\phi_{[2]})^{-1})}{{}_2F_0(n_2+m+1+\Delta b, n_2+1+\Delta b;;+(r\phi_{[2]})^{-1})} \right]^{1/2} . \tag{107}$$

The leading term of the second-exponential-order real series comes from the expansion of the Γ functions and of $(2r)^{2\Delta b}$, the latter of which leads to $\ln(2r)$ terms. Subsequent terms are down by $1/2r$ and require ϕ through $O(e^{-r})$. Like $\Delta_i b^{\{2\}}$, the real $\Delta_r b^{\{2\}}$ is proportional to the square of the first-exponential-order series. The first few terms of $\Delta_r b^{\{2\}}$ are

$$\Delta_r b^{\{2\}} = (\Delta b^{\{1\}})^2 [2\ln(2r) - \psi(n_2+1) - \psi(n_2+m+1) - 12\beta_2^{(0)}(2r)^{-1} + O(r^{-2})] . \tag{108}$$

The real second-exponential-order contribution $\Delta_r \beta_2^{\{2\}}$ to β_2 can be found from the index shift as in Sec. III C, Eq. (65), except that now second derivatives with respect to $\beta_2^{(0)}$ are required:

$$\Delta\beta_2^{\{2\}} = \Delta b^{\{2\}} \sum_{N=0}^{\infty} \frac{d\beta_2^{(N)}}{d\beta_2^{(0)}}(2r)^{-N} + \tfrac{1}{2}(\Delta b^{\{1\}})^2 \sum_{N=1}^{\infty} \frac{d^2\beta_2^{(N)}}{d(\beta_2^{(0)})^2}(2r)^{-N} . \tag{109}$$

As for the first-exponential-order case in Sec. III D, it is also possible to avoid the second derivatives of the $\beta_2^{(N)}$ by solving the Riccati equation directly to second exponential order, but we omit the details here. The leading terms in the expansion for $\Delta_r \beta_2^{\{2\}}$ are

$$\Delta_r \beta_2^{(2)} = \frac{(2r)^{4\beta_2^{(0)}} e^{-2r}}{(n_2!)^2[(n_2+1)!]^2} \Bigg[2\ln(2r) - \psi(n_2+1) - \psi(n_2+m+1)$$
$$+ \frac{1}{2r} \Big\{ [2\ln(2r) - \psi(n_2+1) - \psi(n_2+m+1)]$$
$$\times [-4\beta_2^{(0)} - 12(\beta_2^{(0)})^2 + m^2 - 1] - 12\beta_2^{(0)} - 2 \Big\} + O(r^{-2}\ln(2r)) \Bigg] . \tag{110}$$

I. The β_2 equation on a semi-infinite interval and the discontinuity in the Borel sum

In this section we treat a different problem: we solve the β_2 eigenvalue equation not on the original finite interval, but on a semi-infinite interval. There are two reasons for considering this modified problem. (i) It has the same RSPT expansion as the original problem, but the Borel sum of the common RSPT expansion *is* the eigenvalue of this modified problem.[5,6] (ii) The positive r axis is a cut of the eigenvalue of the modified problem, and calculation of the discontinuity across the cut gives an immediate, unambiguous meaning to the imaginary second-exponential-order series $\Delta_i \beta_2^{(2)}$ calculated already in Sec. III G, but which comes up again here: it is the discontinuity that determines the dispersion relation and that gives the asymptotics of the RSPT coefficients [cf. Eq. (100) and Sec. VI].

The problem is to solve Eq. (11) with the boundary conditions

$$\Phi_2(\eta) \to 0 \text{ as } \eta \to 0 \text{ and as } \mathrm{Re}(\eta r) \to +\infty, \quad \mathrm{Im}(\eta r) > 0 \tag{111}$$

or equivalently Eq. (16) with the boundary conditions

$$\Phi_2(v) \to 0 \text{ as } v \to 0 \text{ and as } \mathrm{Re}\, v \to +\infty, \ \mathrm{Im}\, r > 0 . \tag{112}$$

The nonstandard aspect of this modified problem is to avoid the singularity on the positive real axis at $\eta = 2$ for Eq. (11) or at $v = 2r$ for Eq. (16), as indicated by the $\mathrm{Im}\, r > 0$ in Eq. (112). The modified eigenvalue problem is related to a standard eigenvalue problem: the ξ (or u) equation when the Schrödinger equation for an electron moving in the field of a proton and an antiproton [change the sign of the $1/r_b$ term in Eq. (9)] is separated in prolate spheroidal coordinates. The u equation is

$$[-u\, d^2/du^2 + \tfrac{1}{4}u + \tfrac{1}{4}(m^2-1)/u]\Phi_1' + uV_1'(u,\beta_1',r')\Phi_1' = \beta_1'\Phi_1' , \tag{113}$$

$$V_1'(u,\beta_1',r') = +\frac{\beta_1'}{2r'+u} + \tfrac{1}{4}(m^2-1)\left[-\frac{2}{u(2r'+u)} - \frac{1}{(2r'+u)^2} \right] \quad (0 \le u < \infty) , \tag{114}$$

where the primes are to distinguish the mixed-charge problem from H_2^+. The modified β_2 problem is the analytic continuation up to $r' = e^{\pm\pi i} r$ of the stable, single-well β_1' problem. (See Sec. IV of Ref. 6 for the use of this approach in estimating rigorously the leading term in the discontinuity.)

Before giving the details of the QSC solution, one can anticipate certain of its characteristics, which depend on how the singularity on the positive v or η axis is avoided. The v case is easier to state but completely equivalent to the η case. By making r complex, the singularity at $v=2r$ [see Eq. (21)] is moved off the positive axis. Note[5,6] that the positive r axis is a cut for $\beta_1'(r)$, where $r'=e^{\pm\pi i}r$. If $\mathrm{Im}\,r>0$, then the direct Borel sum [for which $|\arg(r')|<\pi$] of the RSPT series will be $\beta_1'(e^{-\pi i}r)$, while if $\mathrm{Im}\,r<0$, the direct Borel sum will be $\beta_1'(e^{+\pi i}r)$. Now here is the subtlety: suppose one requires the complete asymptotic expansion for $\beta_1'(e^{-\pi i}r)$ both for $\mathrm{Im}\,r>0$, where the answer has to be exactly RSPT, and for its *analytic continuation to* $\mathrm{Im}\,r<0$, where the answer cannot be exactly RSPT, because for $\mathrm{Im}\,r<0$ the Borel sum of the RSPT series is $\beta_1'(e^{+\pi i}r)$. In the fourth quadrant, the asymptotic expansion for $\beta_1'(e^{-\pi i}r)$ necessarily must have, besides the RSPT terms, additional terms that represent the difference, $\beta_1'(e^{-\pi i}r)-\beta_1'(e^{+\pi i}r)$, below the positive real r axis. In other words, these additional terms represent the discontinuity in the eigenvalue of the modified problem across the cut on the positive r axis.

The major difference in the details for the modified problem versus the original β_2 problem is the choice of Whittaker function for the solution anchored at $\eta=2$. In the original case the choice was an M function to be regular at $\eta=2$. In the present case the solution does not have to be regular at $\eta=2$: instead it must vanish as $\eta\to\infty$. For $\mathrm{Im}\,r>0$, the correct choice for Φ_2 anchored at $\eta=2$ [$\Phi_{2[2]}$] which vanishes at infinity [cf. Eqs. (55)–(57)] is $W_{-b,m/2}(e^{-\pi i}z)$:

$$\Phi_{2[2]}=(-d\phi_{[2]}/d\eta)^{-1/2}e^{-\pi i b}W_{-b,m/2}(e^{-\pi i}r\phi_{[2]}) \quad (\mathrm{Im}\,r>0)\,. \qquad (115)$$

The details of the calculation of both $\phi_{[0]}$ and $\phi_{[2]}$ are exactly the same as before. Only the value of the index b needs clarification.

The index b must be chosen to make the two QSC wave functions the same. The asymptotic behavior for the QSC function anchored at $\eta=0$ is given by Eq. (61). It always has a term with a negative exponential factor $e^{-r\eta/2}$. If the index shift $\Delta b\neq 0$, it will also have a term with a positive exponential factor $e^{+r\eta/2}$. The QSC wave function anchored at $\eta=2$ in the present case has only a negative exponential factor:

$$\Phi_{2[2]}\sim(-d\phi_{[2]}/d\eta)^{-1/2}(r\phi_{[2]})^{-b}e^{+r\phi_{[2]}/2}\times{}_2F_0(\tfrac{1}{2}m+\tfrac{1}{2}+b,\tfrac{1}{2}-\tfrac{1}{2}m+b;;+(r\phi_{[2]})^{-1}) \qquad (116)$$

$$\sim(2r)^{-b}\eta^{b}(2-\eta)^{-b}e^{r-r\eta/2}[1+O(r^{-1})]\,. \qquad (117)$$

Comparison of Eq. (117) with Eq. (61) shows that the two solutions can be identical (except for normalization) only if $\Delta b\equiv 0$, in which case the solution anchored at $\eta=0$ has no positive exponential factor, and $b=\beta_2^{(0)}$. Thus when $\mathrm{Im}\,r>0$, there is no additional, exponentially small contribution to the expansion for β_2 for the modified problem, i.e., $\beta_1'(e^{-\pi i}r)$, as has been shown rigorously.[5,6]

Now consider the analytic continuation of the QSC function based on the Whittaker $W_{-b,m/2}$, across the positive real axis to $\mathrm{Im}\,r<0$. Since $\arg(e^{-\pi i}r)<-\pi$ when $\arg(r)$ is negative, the asymptotic expansion (116) is no longer valid. To get the correct expansion for the Whittaker function the argument of the $r\phi_{[2]}$ must first be brought within the range $(-\pi,\pi)$ by the circuital relation[20]

$$e^{-\pi i b}W_{-b,m/2}(e^{-\pi i}r\phi_{[2]})=e^{+\pi i b}W_{-b,m/2}(e^{+\pi i}r\phi_{[2]})-\frac{2\pi i W_{b,m/2}(r\phi_{[2]})}{\Gamma(b+\frac{1}{2}+\frac{1}{2}m)\Gamma(b+\frac{1}{2}-\frac{1}{2}m)} \qquad (118)$$

$$\sim(2r)^{-b}\eta^{-b}(2-\eta)^{-b}e^{r-r\eta/2}-\frac{2\pi i}{(n_2+m)!n_2!}(2r)^{b}\eta^{-b}(2-\eta)^{b}e^{-r+r\eta/2}\,. \qquad (119)$$

Since both exponentials now appear, they must also appear in the M-based QSC function anchored at $\eta=0$. Consequently Δb cannot vanish. The exact matching equation to determine Δb, the analog of Eq. (105), is

$$\pi^{-1}\sin(\pi\Delta b)=\frac{2\pi i e^{+\pi i\Delta b}}{[\Gamma(n_2+m+1+\Delta b)\Gamma(n_2+1+\Delta b)]^2}\frac{W_{\beta_2^{(0)}+\Delta b,m/2}(r\phi_{[0]})}{e^{+\pi i(\beta_2^{(0)}+\Delta b)}W_{-\beta_2^{(0)}-\Delta b,m/2}(r\phi_{[0]}e^{+\pi i})}\times\frac{W_{\beta_2^{(0)}+\Delta b,m/2}(r\phi_{[2]})}{e^{+\pi i(\beta_2^{(0)}+\Delta b)}W_{-\beta_2^{(0)}-\Delta b,m/2}(r\phi_{[2]}e^{+\pi i})} \quad (\mathrm{Im}\,r<0)\,. \qquad (120)$$

[Note that even though Eq. (120) appears to be η dependent, as before the η dependence cancels out, and Δb depends only on r.]

Compare the matching formula here [Eq. (120)] with Eq. (105). It is easily seen that the lowest nonvanishing exponential order of the right-hand side of Eq. (120) is the second, that it is purely imaginary, and that it is $2\pi i$ times the square of the previously determined half-gap index shift $\Delta b^{[1]}$ of Eqs. (63) and (64):

$$\Delta b(\text{modified }\beta_2\text{ equation})=+2\pi i(\Delta b^{[1]})^2+O(r^k e^{-4r}) \quad (\mathrm{Im}\,r<0,\ \arg r'<-\pi) \qquad (121)$$

$$=2i\Delta_i b^{[2]}+O(r^k e^{-4r}) \quad (\mathrm{Im}\,r<0,\ \arg r'<-\pi)\,. \qquad (122)$$

Thus the index shift on analytic continuation from the first to the fourth quadrant is nonvanishing in second exponential order and is exactly 2 times the second-exponential-order imaginary index shift already calculated for the original β_2 problem. Since the mechanism by which the lowest-order nonvanishing imaginary index shift induces an imaginary contribution to β_2 is exactly the same for both the original and modified problems, Eqs. (97)–(102), a second-exponential-order contribution completely analogous to Eq. (122) holds for the modified β_2:

$$\beta_1'(e^{-\pi i}r) \sim \sum_{N=0}^{\infty} \beta_2^{(0)}(2r)^{-N} + 2i\Delta_i\beta_2^{[2]} + O(r^k e^{-4r})$$

$$(\mathrm{Im} r < 0, \arg r' < -\pi) . \quad (123)$$

As anticipated, by analytic continuation directly across the positive r axis, one finds a purely imaginary $O(e^{-2r})$ series in addition to the RSPT series. At the real axis, this series represents to lowest exponential order the discontinuity at the cut of the Borel sum of the RSPT series,

$$\beta_1'(e^{-\pi i}r) - \beta_1'(e^{+\pi i}r) \sim 2\pi i(\Delta b^{[1]})^2 q(r) , \quad (124)$$

and as such is the dominating factor in the dispersion relation that gives the asymptotic behavior of the RSPT coefficients, to be discussed further in Sec. VI. Since the RSPT series coefficients are real and the discontinuity is purely imaginary, the imaginary parts of the Borel sums just above and below the positive real axis are equal in magnitude and opposite in sign:

$$\mathrm{Im}\left[\lim_{\mathrm{Im} r \to \pm 0}\left[\text{Borel sum of } \sum \beta_2^{(N)}(2r)^{-N}\right]\right]$$

$$\sim \pm\pi(\Delta b^{[1]})^2 q(r) . \quad (125)$$

The explicit imaginary series found for the original β_2 problem [Eqs. (94)–(102)] is exactly this result (125), but with opposite sign. This clearly demonstrates the cancellation of the explicit imaginary second-exponential-order series with the implicit imaginary part of the Borel sum of the double-well problem, the phenomenon of a complex expansion with a real sum, mentioned in the Introduction.

IV. THE β_1 EQUATION

Although most of the interesting results for H_2^+ come from the β_2 equation, yet the β_1 equation adds its own distinctive twist in the form of a branch cut in the *negative r* direction and in the form of logarithmic terms.[22] Both $\beta_1^{(N)}$ and $E^{(N)}$ get asymptotic contributions with *alternating signs* and with a $\ln N$ dependence, but the relative magnitudes with respect to the dominant, same-sign behavior are down by several powers of N.

Before discussing these unique contributions, we dispense first with the terms in β_1 that are "induced" by the exponentially small terms $\Delta\beta_2 = \Delta\beta_2^{[1]} + \Delta\beta_2^{[2]} + \cdots$ already in β_2. Consider $\Delta\beta_2$ to be a shift of $\beta_2^{(0)}$. Then the induced effect on $\Delta\beta_1$ is expressed by the Taylor series

$$(\Delta\beta_1)_{\mathrm{ind}} = \sum_{k=1}^{\infty} \frac{(\Delta\beta_2)^k}{k!}\left[\frac{\partial}{\partial\beta_2^{(0)}}\right]^k \sum_{N=0}^{\infty} \beta_1^{(N)}(2r)^{-N} . \quad (126)$$

The dependence of $\beta_1^{(N)}$ on $\beta_2^{(0)}$ is determined through Eqs. (15) and (18)–(20). The use of partial derivatives in Eq. (126) is to indicate that the $\beta_2^{(N)}$ $(N \geq 1)$ are to be held constant. An alternative method to obtain $(\Delta\beta_1)_{\mathrm{ind}}$ is to regard the terms $-2u(u+2r)^{-1}(\Delta\beta_2^{[1]} + \Delta\beta_2^{[2]} + \cdots)$ in Eq. (18) as a second, independent perturbation. The effect on $\Delta\beta_1$ can then be calculated by double RSPT. In particular, the leading real first-exponential-order series and the leading imaginary second-exponential-order series, $\Delta\beta_1^{[1]}$ and $i\Delta_i\beta_1^{[2]}$, can be obtained by the standard perturbation formula first order in the exponentially small perturbation but infinite order in the $1/r$ perturbation. That is, with the ordinary RSPT wave function for Φ_1 in powers of $(2r)^{-1}$, Φ_{RSPT}, the induced exponentially small contributions to β_1 in leading exponential order are

$$(\Delta\beta_1^{[1]} + i\Delta_i\beta_1^{[2]})_{\mathrm{ind}} = \frac{-2(\Delta\beta_2^{[1]} + i\Delta_i\beta_2^{[2]})\int_0^{\infty}\Phi_{\mathrm{RSPT}}^2(u+2r)^{-1}du}{\int_0^{\infty}\Phi_{\mathrm{RSPT}}^2[u^{-1}+(u+2r)^{-1}]du} . \quad (127)$$

Here Φ_{RSPT} refers to the solution of Eq. (15) by RSPT in powers of $(2r)^{-1}$. Both integrals are to be evaluated order by order in powers of $(2r)^{-1}$. In short, the induced exponentially small contributions to β_1 are straightforward to obtain but are otherwise unremarkable.

The more interesting exponentially small contributions to β_1 come from a cut in the negative r direction, which is suggested by the singularity in Eq. (15) [cf. also Eq. (18)] at $u = -2r$. Associated with this cut is a dispersion relation that implies alternating-sign asymptotic contributions to $\beta_1^{(N)}$ and to $E^{(N)}$, both proportional to $(N - 4n_2 - 3m - 5)!$ [which is $(n_2 + 4m + 6)$ powers of N down from the asymptotics of the $\beta_2^{(N)}$].

One obtains an explicit formula for the discontinuity in β_1 across the cut by connecting a QSC wave function anchored at the origin, which we denote by $\Phi_{[0]}$, with one with the correct behavior at infinity, but that is anchored at $u = -2r$, which we denote by $\Phi_{[-2]}$. As in the semi-infinite treatment of the β_2 equation in Sec. III I, the role of the QSC function anchored at a singularity that is not an endpoint is to provide control of analytic continuation around that singularity. As in Sec. III I, where β_2 is analytically continued across $r > 0$, here when β_1 is analytically continued across $r < 0$, the Borel sum of the RSPT series switches branches and is discontinuous across the cut. A doubly-exponentially-small imaginary series appears that explicitly cancels the implicit discontinuity in the sum of the RSPT series. Unlike the semi-infinite β_2 case, there is here a new technical feature—the first index of the W Whittaker function is necessarily a power series in $(2r)^{-1}$. This feature leads to *logarithmic* terms in the expansion for $\Delta\beta_1^{[2]}$.

A. QSC wave function at $\xi = 0$

Near $\xi = 0$, Eq. (10) is Whittaker's equation [cf. Eq (33)],

$$[-(d/d\xi)^2+\tfrac{1}{4}r^2-r\beta_1/\xi+\tfrac{1}{4}(m^2-1)/\xi^2]\Phi_{[0]}\sim 0\ , \tag{128}$$

and the QSC wave function regular at the origin has the form

$$\Phi_{[0]}=\frac{1}{m!}(d\phi_{[0]}/d\xi)^{-1/2}M_{b_{[0]},m/2}(r\phi_{[0]})\ . \tag{129}$$

The function $\phi_{[0]}$, which plays the "action" role, depends on both ξ and r: $\phi_{[0]}=\phi_{[0]}(\xi,r)$. The boundary condition at $\xi=0$ is

$$\phi_{[0]}(0,r)=0\ . \tag{130}$$

$\phi_{[0]}$ satisfies the Riccati equation [cf. Eq. (35)],

$$-\left[\frac{d\phi_{[0]}}{d\xi}\right]^2\left[\frac{1}{4}-\frac{b_{[0]}}{r\phi_{[0]}}+\frac{m^2-1}{4r^2\phi_{[0]}^2}\right]-\frac{1}{r^2}\left[\frac{d\phi_{[0]}}{d\xi}\right]^{1/2}\frac{d^2}{d\xi^2}\left[\frac{d\phi_{[0]}}{d\xi}\right]^{-1/2}+\frac{1}{4}-\frac{\beta_1}{r\xi}-\frac{\beta_1+2\beta_2}{r(\xi+2)}+\frac{m^2-1}{r^2\xi^2(\xi+2)^2}=0\ . \tag{131}$$

Expanding β_1 and $\phi_{[0]}$ in powers of $(2r)^{-1}$ and solving recursively, one finds that

$$\phi_{[0]}=\sum_{N=0}^{\infty}\phi_{[0]}^{(N)}(\xi)(2r)^{-N}\ ,$$
$$\beta_1=\sum_{N=0}^{\infty}\beta_1^{(N)}(2r)^{-N}\ , \tag{132}$$

$$\phi_{[0]}^{(0)}=\xi\ , \tag{133}$$

$$\phi_{[0]}^{(1)}=-4(\beta_1^{(0)}+2\beta_2^{(0)})\ln(1+\tfrac{1}{2}\xi)\ , \tag{134}$$

$$\beta_1^{(0)}=b_{[0]}\ , \tag{135}$$

$$\beta_1^{(1)}=-2b_{[0]}(\beta_1^{(0)}+2\beta_2^{(0)})-\tfrac{1}{2}(m^2-1)\ , \tag{136}$$

and so forth. The value of $b_{[0]}$ is to be obtained by matching $\Phi_{[0]}$ with the QSC function that behaves correctly at ∞. The $\beta_1^{(N)}$ are determined so that the $\phi_{[0]}^{(N+1)}$ are analytic and zero at $\xi=0$, just as was the case for the $\beta_2^{(N)}$ in Sec. III B. The $\beta_1^{(N)}$ will turn out to be the RSPT coefficients.

B. QSC wave function at $\xi=-2$

Near $\xi=-2$, Eq. (10) is again a Whittaker equation,

$$[-(d/d\xi)^2+\tfrac{1}{4}r^2-r(\beta_1+2\beta_2)/(\xi+2)+\tfrac{1}{4}(m^2-1)/(\xi+2)^2]\Phi_{[0]}\sim 0\ . \tag{137}$$

The QSC wave function that is exponentially small as $r\xi\rightarrow+\infty$ (but singular at $\xi=-2$) is [cf. Eq. (115)]

$$\Phi_{[-2]}=(d\phi_{[-2]}/d\xi)^{-1/2}W_{b_{[-2]},m/2}(r\phi_{[-2]})\ , \tag{138}$$

with boundary condition

$$\phi_{[-2]}(-2,r)=0\ . \tag{139}$$

The Riccati equation for $\phi_{[-2]}$ is nominally the same as for $\phi_{[0]}$, Eq. (131), and is not repeated here. One solves for $\phi_{[-2]}$ as an expansion,

$$\phi_{[-2]}=\sum_{N=0}^{\infty}\phi_{[-2]}^{(N)}(\xi)(2r)^{-N}\ . \tag{140}$$

In contrast with the method of solution for $\phi_{[0]}$, however, both $\beta_1^{(N)}$ and $\beta_2^{(N)}$ are already fixed and cannot be adjusted to make $\phi_{[-2]}^{(N+1)}$ vanish at $\xi=-2$. Here that role is taken by the index $b_{[-2]}$ on the Whittaker W function. The index $b_{[-2]}$ is given by an expansion in $(2r)^{-1}$,

$$b_{[-2]}=\sum_{N=0}^{\infty}b_{[-2]}^{(N)}(2r)^{-N}\ . \tag{141}$$

One finds that

$$\phi_{[-2]}^{(0)}=\xi+2\ , \tag{142}$$

$$\phi_{[-2]}^{(1)}=-4\beta_1^{(0)}\ln(-\tfrac{1}{2}\xi)\ , \tag{143}$$

$$b_{[-2]}^{(0)}=\beta_1^{(0)}+2\beta_2^{(0)}\ , \tag{144}$$

$$b_{[-2]}^{(1)}=2(\beta_1^{(1)}+\beta_2^{(1)}) \tag{145}$$

$$=-4(\beta_1^{(0)}+\beta_2^{(0)})^2=-4n^2\ , \tag{146}$$

and so forth.

C. Determination of $b_{[0]}$ by matching $\Phi_{[0]}$ and $\Phi_{[-2]}$

The index $b_{[0]}$ is evaluated by the condition that the two QSC functions be the same. Two cases are considered: r large, but with small phase; and r large, but with phase more negative than $-\pi$. In the former case one gets RSPT, while in the latter there is in addition an imaginary second-exponential-order series.

The logic is by now familiar. When $r\phi_{[0]}$ and $r\phi_{[-2]}$, viz., $r\xi$ and $r(\xi+2)$, are large, the asymptotic expansions for the Whittaker functions give

$$\Phi_{[-2]}\sim r^{b_{[-2]}}(\xi+2)^{b_{[-2]}}(-\tfrac{1}{2}\xi)^{\beta_1^{(0)}}e^{-r(\xi+2)/2}\ , \tag{147}$$

$$\Phi_{[0]}\sim\frac{e^{\pm i\pi(m/2+1/2-b_{[0]})}}{\Gamma(\tfrac{1}{2}m+\tfrac{1}{2}+b_{[0]})}(r\xi)^{b_{[0]}}\times[(\xi+2)/2]^{\beta_1^{(0)}+2\beta_2^{(0)}}e^{-r\xi/2}$$
$$+\frac{1}{\Gamma(\tfrac{1}{2}m+\tfrac{1}{2}-b_{[0]})}(r\xi)^{-b_{[0]}}\times[(\xi+2)/2]^{-\beta_1^{(0)}-2\beta_2^{(0)}}e^{+r\xi/2}\ . \tag{148}$$

[The $\pm$ corresponds to the sign of $\arg(r\phi_{[0]})$.] The elimination of the positive exponential $e^{+r\xi/2}$ series from $\Phi_{[0]}$ requires that $\tfrac{1}{2}m+\tfrac{1}{2}-b_{[0]}$ be zero or a negative integer.

$$b_{[0]}=n_1+\tfrac{1}{2}m+\tfrac{1}{2}\quad (n_1=0,1,2,\ldots)\,. \tag{149}$$

Thus $b_{[0]}$ is the unperturbed eigenvalue of Eq. (15). [Cf. also Eq. (17).]

To get at the cut in $\beta_1(r)$ on the negative r axis, we now consider the possibility that r becomes negative. It turns out that $b_{[0]}$ has a different expansion when $\arg r<-\pi$. Notice from Eq. (18) that the singularity at $u=-2r$, which originally occurs at an unphysical value of the physical variable u, moves into the physical domain when r is negative. Note also that to keep the physical variable u approximately positive as r is made negative, ξ will also have to be made negative, but in the opposite sense of r, since $u=r\xi$. Further, it will be convenient to match the two QSC Φ's in the region between their "anchor" points, $\xi=0$ and -2. Consequently the primary region of interest for ξ is near -1, and for $2+\xi$ near $+1$. The dominant term $r\xi$ in $r\phi_{[0]}$ will be large and stay approximately positive, while the dominant term $r(\xi+2)$ in $r\phi_{[2]}$ will become large and approximately negative. The negative z axis, however, is a branch cut for the Borel sum of the asymptotic series for $W_{b,m/2}(z)$. The asymptotic expansion for $W_{b,m/2}(z)$ above the negative z axis and its *analytic continuation* across the negative z axis will differ by an exponentially small expansion that cancels the discontinuity in the Borel sum.

To make this last point more precise, let $z=e^{-\pi i}z'$, and let z' be approximately real and positive. When $\arg z=-\pi-\epsilon$ ($\epsilon>0$), the standard asymptotic expansion for $W_{b,m/2}(z)$ is not applicable. The correct expansion may be obtained by first applying the circuital relation[20] (here $\arg z'=-\epsilon<0$),

$$W_{b,m/2}(z'e^{-\pi i})=e^{-2\pi i b}W_{b,m/2}(z'e^{\pi i})-2\pi i\frac{e^{-\pi i b}W_{-b,m/2}(z')}{\Gamma(\tfrac{1}{2}+\tfrac{1}{2}m-b)\Gamma(\tfrac{1}{2}-\tfrac{1}{2}m-b)}\,, \tag{150}$$

and then by using the asymptotic expansions for the standard domains. As a consequence, $\Phi_{[-2]}$ will now have a positive exponential series, and $b_{[0]}$ will be different from $n_1+\tfrac{1}{2}m+\tfrac{1}{2}$. Let

$$b_{[0]}=\beta_1^{(0)}+\Delta b_{[0]}\,. \tag{151}$$

Also define $\delta b_{[-2]}$ by

$$\delta b_{[-2]}=b_{[-2]}-b_{[-2]}^{(0)}=\sum_{N=1}^{\infty}b_{[-2]}^{(N)}(2r)^{-N}+O(\Delta b_{[0]})\,. \tag{152}$$

Note that Δ has been used exclusively to denote exponentially small quantities. In this case $\delta b_{[-2]}$ is not exponentially small, and δ has been used instead of Δ.

To determine $\Delta b_{[0]}$, one obtains the following matching equation, which is the analog of Eqs. (105) and (120), and which is a simple consequence of Eqs. (55), (58), and (150):

$$\pi^{-1}\sin(\pi\Delta b_{[0]})=\frac{2\pi i(-1)^m e^{+\pi i\Delta b_{[0]}}}{\Gamma(n_1+m+1+\Delta b_{[0]})\Gamma(n_1+1+\Delta b_{[0]})}$$
$$\times\pi^{-2}\sin^2(\pi\delta b_{[-2]})\Gamma(n_1+2n_2+2m+2+\delta b_{[-2]})\Gamma(n_1+2n_2+m+2+\delta b_{[-2]})$$
$$\times\frac{W_{\beta_1^{(0)}+\Delta b_{[0]},m/2}(r\phi_{(0)})}{e^{+\pi i(\beta_1^{(0)}+\Delta b_{[0]})}W_{-\beta_1^{(0)}-\Delta b_{[0]},m/2}(r\phi_{[0]}e^{+\pi i})}\,\frac{e^{-\pi i b_{[-2]}}W_{-b_{[-2]},m/2}(r\phi_{[-2]}e^{\pi i})}{e^{-2\pi i b_{[-2]}}W_{b_{[-2]},m/2}(r\phi_{[-2]}e^{2\pi i})}\quad (\mathrm{Im}\,r<-\pi)\,. \tag{153}$$

Since r is essentially negative, set $r=-r'$:

$$r'=e^{\pi i}r\quad (\arg r'=\epsilon<0)\,. \tag{154}$$

The right-hand side of Eq. (153) is $O(r'^k e^{-2r'})$ and is also to this order purely imaginary. Consequently we can write

$$\Delta b_{[0]}=i\Delta_i b_{[0]}^{(2)}+O(r'^k e^{-4r'})\,, \tag{155}$$

where

$$\Delta_i b_{[0]}^{(2)}=2\pi(-1)^m\frac{\sin^2(\pi\delta b_{[-2]})}{\pi^2}(2r')^{2\beta_1^{(0)}-2b_{[-2]}^{(0)}-2\delta b_{[-2]}}e^{-2r'}$$
$$\times\frac{\Gamma(n_1+2n_2+2m+2+\delta b_{[-2]})\Gamma(n_1+2n_2+m+2+\delta b_{[-2]})}{n_1!(n_1+m)!}$$
$$\times(\tfrac{1}{2}e^{-\pi i}\phi_{[0]})^{2\beta_1^{(0)}}(\tfrac{1}{2}\phi_{[-2]})^{-2b_{[-2]}}e^{r'(\phi_{[0]}-\phi_{[-2]}+2)}\frac{{}_2F_0(-n_1,-n_1-m;;+(r'\phi_{[0]})^{-1})}{{}_2F_0(n_1+m+1,n_1+1;;-(r'\phi_{[0]})^{-1})}$$
$$\times\frac{{}_2F_0(n_1+2n_2+m+2+\delta b_{[-2]},n_1+2n_2+2m+2+\delta b_{[-2]};;-(r'\phi_{[-2]})^{-1})}{{}_2F_0(-n_1-2n_2-m-1-\delta b_{[-2]},-n_1-2n_2-2m-1-\delta b_{[-2]};;+(r'\phi_{[-2]})^{-1})} \tag{156}$$

$$\sim 2\pi(-1)^m 16n^4\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(2r')^{-4\beta_2^{(0)}-2}e^{-2r'}$$

$$\times\left[1-\frac{1}{2r'}\{8n^2\ln(2r')-4n^2+12(\beta_2^{(0)})^2-(m^2-1)-8n+12\beta_2^{(0)}\right.$$

$$\left.-4n^2[\psi(n_1+2n_2+m+2)+\psi(n_1+2n_2+2m+2)]\}+O[r'^{-2}(\ln r')^2]\right]. \tag{157}$$

The complete evaluation of Eq. (156) is somewhat more tedious than the preceding similar cases because of the necessity for expanding the $\delta b_{[-2]}$ series out from the two Γ functions, the $\sin^2$, the $(\frac{1}{2}\phi_{[-2]})^{-2b_{[-2]}}$, and the $(2r')^{\delta b_{[-2]}}$, the last of which leads to subseries proportional to powers of $(2r')^{-1}\ln(2r')$. It is possible to avoid expanding out the generalized hypergeometrics. Since the expression is really independent of ξ, it can be evaluated at a special value of ξ. If $\xi=\infty$, then the generalized hypergeometrics are evaluated at 0 where they are unity.

After evaluating $\Delta_i b\{^2_0\}$, the corresponding imaginary doubly-exponentially-small contribution to the discontinuity of β_1 on the negative axis can be obtained via

$$\Delta_i\beta_1^{\{2\}}=\Delta_i b\{^2_0\}\sum_{N=0}^{\infty}\frac{d\beta_1^{(N)}}{d\beta_1^{(0)}}(-2r')^{-N}. \tag{158}$$

As for the β_2 cases, there are also other methods that avoid derivatives of the RSPT series, but we shall not go into the details here.

V. EXPANSION FOR $E(R)$ FROM THE EXPANSIONS FOR $\beta_1(r)$ AND $\beta_2(r)$

A. Preliminaries

The asymptotic expansion for $E(R)$ in terms of $(2R)^{-1}$ can be obtained from Eq. (12) for E in terms of β_1 and β_2, from Eqs. (24) and (26) for the RSPT expansions, and from the various equations of Secs. III and IV for the exponentially small series contributing to β_1 and β_2, but only after r has been found explicitly as a function of R from the implicit Eq. (13), $R(r)=r[\beta_1(r)+\beta_2(r)]$. The process is mainly algebraic. The main complication is that the transformation itself from r to R contains exponentially small terms. The purpose of this section is to clarify the process and to sketch the necessary steps.

Note that β_1 and β_2 appear in E and $R(r)$ only as the sum $\beta_1+\beta_2$, which we denote by γ:

$$\gamma(r)=\beta_1(r)+\beta_2(r), \tag{159}$$

$$\gamma^{(N)}=\beta_1^{(N)}+\beta_2^{(N)}, \tag{160}$$

$$\Delta\gamma^{\{q\}}=\Delta\beta_1^{\{q\}}+\Delta\beta_2^{\{q\}}\quad(q=1,2,\ldots), \tag{161}$$

and so forth. Further, we denote by γ_0 the formal power series

$$\gamma_0(r)=\sum_{N=0}^{\infty}\gamma^{(N)}(2r)^{-N}. \tag{162}$$

In the expression of r as a function of R, there will be a power-series contribution that we denote by r_0, and that is the formal power-series solution of

$$\frac{1}{2r_0}=\frac{\gamma_0(r_0(R))}{2R}. \tag{163}$$

By means of Lagrange's formula,[19] the solution can in fact be immediately written:

$$\frac{1}{2r_0}=\frac{n}{2R}+\sum_{N=1}^{\infty}\left[\frac{n}{2R}\right]^{N+1}\sum_{\substack{i_1,i_2,\ldots,i_N\\(i_1+2i_2+\cdots+Ni_N=N)}}\frac{N!(\gamma^{(1)}/n)^{i_1}(\gamma^{(2)}/n)^{i_2}\cdots(\gamma^{(N)}/n)^{i_N}}{\left[N+1-\sum_k i_k\right]!i_1!i_2!\cdots i_N!} \tag{164}$$

$$=\frac{n}{2R}+\left[\frac{n}{2R}\right]^2\frac{\gamma^{(1)}}{n}+\left[\frac{n}{2R}\right]^3\left[\frac{\gamma^{(2)}}{n}+\frac{(\gamma^{(1)})^2}{n^2}\right]+\cdots. \tag{165}$$

Here n is the usual principal quantum number. Note that $\gamma^{(0)}=n$, $\gamma^{(1)}=-2n^2$, and that the "natural" expansion parameter is $n/2R$. In a similar fashion the RSPT expansion for $E(R)$ can be written

$$\sum_{N=0}^{\infty}E^{(N)}(2R/n)^{-N}=-\tfrac{1}{2}\gamma_0^{-2}(r_0) \tag{166}$$

$$=\frac{-1}{2n^2}+n^{-2}\sum_{N=1}^{\infty}\left[\frac{n}{2R}\right]^N\sum_{\substack{i_1,i_2,\ldots,i_N\\(i_1+2i_2+\cdots+Ni_N=N)}}\frac{(N-3)!(\gamma^{(1)}/n)^{i_1}(\gamma^{(2)}/n)^{i_2}\cdots(\gamma^{(N)}/n)^{i_N}}{\left[N-2-\sum_k i_k\right]!i_1!i_2!\cdots i_N!} \tag{167}$$

$$=\frac{-1}{2n^2}+\left[\frac{n}{2R}\right]\frac{\gamma^{(1)}}{n^3}+\left[\frac{n}{2R}\right]^2\left[\frac{\gamma^{(2)}}{n^3}-\frac{\frac{1}{2}(\gamma^{(1)})^2}{n^4}\right]+\cdots. \tag{168}$$

The aim now is to express the exponentially small series in E, namely $\Delta E^{[1]}$, $\Delta E^{[2]}$, etc., entirely in terms of $\gamma_0(r_0)$, $\Delta\gamma^{[1]}(r_0)$, $\Delta\gamma^{[2]}(r_0)$, etc. That is, the $\Delta E^{[q]}$ should be put into a form in which the exponentially small contributions Δr to $r=r_0+\Delta r$ are expanded out explicitly as a function of r_0, and the remaining r_0 dependence can be replaced by its power series in R, Eq. (164). In fact, by two successive expansions of $E=-\frac{1}{2}\gamma^{-2}$ [Eq. (12)], the first with respect to $\Delta\gamma$, the second with respect to $\Delta(r^{-1})$, one obtains

$$E=E_{\rm RSPT}+\Delta E=E_{\rm RSPT}+\Delta E^{[1]}+\Delta E^{[2]}+\cdots \tag{169}$$

$$=-\tfrac{1}{2}\gamma_0^{-2}(r)+\Delta\gamma(r)\gamma_0^{-3}(r)-\tfrac{3}{2}[\Delta\gamma(r)]^2\gamma_0^{-4}(r)+\cdots \tag{170}$$

$$\begin{aligned}=&-\tfrac{1}{2}\gamma_0(r_0)^{-2}-\tfrac{1}{2}\Delta(r^{-1})[(d/dr_0^{-1})\gamma_0(r_0)^{-2}]-\tfrac{1}{4}[\Delta(r^{-1})]^2[(d/dr_0^{-1})^2\gamma_0(r_0)^{-2}]+\cdots\\&+\Delta\gamma_0(r_0)[\gamma_0(r_0)^{-3}]-\tfrac{3}{2}[\Delta\gamma_0(r_0)]^2[\gamma_0(r_0)^{-4}]+\cdots+\Delta(r^{-1})(d/dr_0^{-1})[\Delta\gamma(r_0)\gamma_0(r_0)^{-3}]+\cdots\,.\end{aligned} \tag{171}$$

The $\Delta(r^{-1})$ can be expressed directly in terms of ΔE, Eq. (169); the ΔE can then be obtained recursively, as will be shown in the next several paragraphs:

$$r^{-1}=R^{-1}\gamma=R^{-1}(-2E)^{-1/2}=r_0^{-1}+\Delta(r^{-1})\,, \tag{172}$$

$$\begin{aligned}\Delta(r^{-1})=&R^{-1}\Delta E[(-2E_{\rm RSPT})^{-3/2}]\\&+\tfrac{3}{2}R^{-1}(\Delta E)^2[(-2E_{\rm RSPT})^{-5/2}]+\cdots\end{aligned} \tag{173}$$

$$\begin{aligned}=&\Delta E[r_0^{-1}\gamma_0(r_0)^2]\\&+\tfrac{3}{2}(\Delta E)^2[r_0^{-1}\gamma_0(r_0)^4]+\cdots\,,\end{aligned} \tag{174}$$

where $E=E_{\rm RSPT}+\Delta E$ has been expanded around $E_{\rm RSPT}=-\frac{1}{2}\gamma_0(r_0)^{-2}$.

B. First exponential order

From Eqs. (171) and (174) the following preliminary formula for $\Delta E^{[1]}$ can be obtained:

$$\Delta E^{[1]}=\frac{\Delta\gamma^{[1]}(r_0)}{\gamma_0^3(r_0)-r_0^{-1}\gamma_0^2(r_0)(d/dr_0^{-1})\gamma_0(r_0)}\,. \tag{175}$$

The final formula for $\Delta E^{[1]}$ results from inserting Eq. (164) for r_0 into Eq. (175) and using the appropriate equations for $\Delta\gamma^{[1]}(r_0)$ developed in previous sections: Eqs. (64), (65), (69), (83), (126), (127), and (159)–(161). The first few terms are

$$\begin{aligned}\Delta E^{[1]}=\pm&\frac{(2R/n)^{2\beta_2^{(0)}}e^{-R/n-n}}{n^3n_2!(n_2+m)!}\\&\times\left[1+\left[\frac{n}{2R}\right][2n\beta_1^{(0)}-4(\beta_2^{(0)})^2\right.\\&\left.+\beta_2^{(1)}+2n^2]+O(R^{-2})\right]\,.\end{aligned} \tag{176}$$

C. Imaginary second exponential order; more on the approximate formula of Brézin and Zinn-Justin

In exactly the same way that Eq. (175) was obtained, one gets for the imaginary second-exponential-order series, i.e., the imaginary part of $\Delta E^{[2]}$ when R is real and positive,

$$\Delta E^{[2]}=\Delta_rE^{[2]}+i\Delta_iE^{[2]}\,, \tag{177}$$

$$\Delta_iE^{[2]}=\frac{\Delta_i\gamma^{[2]}(r_0)}{\gamma_0^3(r_0)-r_0^{-1}\gamma_0^2(r_0)(d/dr_0^{-1})\gamma_0(r_0)}\,. \tag{178}$$

When the series (164) for r_0 is substituted into the denominator and into the appropriate expressions for $\Delta_i\gamma^{[2]}$, then one gets the desired formula for $\Delta_i(E)^{[2]}$. Up to two terms (but not to three) the formula is, except for sign, πn^3 times the square of $\Delta E^{[1]}$, Eq. (176):

$$\Delta_iE^{[2]}=\mp\pi n^3(\Delta E^{[1]})^2[1+O(R^{-2})]\quad(\pm{\rm Im}R\geq0)\,. \tag{179}$$

Apart from the adjustment by the factor n^3, this result is the approximation of Brézin and Zinn-Justin,[12] demonstrated to be valid to only two terms for the ground state by Čížek, Clay, and Paldus[13] numerically, and by Damburg and Propin analytically.[14] In fact, it is not difficult to see that the exact relationship is

$$\mp\pi n^3\frac{\Delta_iE^{[2]}}{(\Delta E^{[1]})^2}$$

$$=\frac{n^3(d/d\beta_2^{(0)})\gamma_0(r_0)}{\gamma_0(r_0)^3-r_0^{-1}\gamma_0(r_0)^2(d/dr_0^{-1})\gamma_0(r_0)} \tag{180}$$

$$=1-(2r_0)^{-2}4\beta_2^{(0)}n+O(r^{-3}) \tag{181}$$

$$=1-(2R/n)^{-2}4\beta_2^{(0)}n+O(R^{-3})\,. \tag{182}$$

Thus, exactly two terms are given correctly by the gap-squared formula for *every* state.

D. Real second exponential order

The extraction of the real second-exponential-order series for $\Delta_rE^{[2]}$ is more tedious, as can be seen from the following equation obtained from Eqs. (171) and (174), and in which all quantities are to be evaluated at $r=r_0$, the power series given by Eq. (164):

$$\Delta_r E^{\{2\}}=\gamma_0^{-3}\Delta_r\gamma^{\{2\}}-\tfrac{3}{2}\gamma_0^{-4}(\Delta\gamma^{\{1\}})^2+\gamma_0^{-1}\Delta_r E^{\{2\}}r_0^{-1}(d\gamma_0/dr_0^{-1})$$
$$+\Delta E^{\{1\}}[\gamma_0^{-1}r_0^{-1}(d\Delta\gamma^{\{1\}}/dr_0^{-1})-3\gamma_0^{-2}\Delta\gamma^{\{1\}}r_0^{-1}(d\gamma_0/dr_0^{-1})]$$
$$+(\Delta E^{\{1\}})^2\{\tfrac{3}{2}r_0^{-1}(d\gamma_0/dr_0^{-1})+\tfrac{1}{2}\gamma_0 r_0^{-2}[d^2\gamma_0/(dr_0^{-1})^2]-\tfrac{3}{2}r_0^{-2}(d\gamma_0/dr_0^{-1})^2\}\ . \tag{183}$$

The leading term comes from $\Delta E^{\{1\}}\gamma_0^{-1}r_0^{-1}(d\Delta\gamma^{\{1\}}/dr_0^{-1})$, since $r^{-1}(d/dr^{-1})e^{-r}=re^{-r}$. Consequently we obtain for the first few terms of $\Delta_r E^{\{2\}}$

$$\Delta_r E^{\{2\}}=\frac{\Delta E^{\{1\}}\Delta\gamma^{\{1\}}(r_0-2\beta_0^{(0)})}{\gamma_0-r_0^{-1}(d\gamma_0/dr_0^{-1})}[1+O(r^{-2})]+\frac{\Delta_r\gamma^{(2)}-\frac{3}{2}\gamma_0^{-1}(\Delta\gamma^{\{1\}})^2}{\gamma_0^3-\gamma_0^2 r_0^{-1}(d\gamma_0/dr_0^{-1})} \tag{184}$$

$$=R(\Delta E^{\{1\}})^2\gamma_0[1-(2r_0)^{-1}(3+2\beta_2^{(0)})+O(r_0^{-2})]+n^{-3}\Delta_r b^{\{2\}}[1+O(r_0^{-2})]\ , \tag{185}$$

and finally,

$$\Delta_r(E)^{\{2\}}=nR(\Delta E^{\{1\}})^2\left\{1-\frac{n}{2R}[3+2\beta_2^{(0)}+2n^2+2n\psi(n_2+1)+2n\psi(n_2+m+1)]+\frac{n}{2R}[4n\ln(2R/n)]+O(R^{-2})\right\}. \tag{186}$$

Note the term $(n/2R)\ln(2R/n)$.

E. Discontinuity in $E(R)$ for R negative

The last expression we obtain in this section is for the discontinuity of E across the negative R axis, namely, $E(e^{-\pi i}R')-E(e^{+\pi i}R')$, with $\arg R'=0$. The contributing expressions are Eqs. (156)–(161), (171), and (174). By the same logic that led to Eqs. (175) and (178) for $\Delta E^{\{1\}}$ and $\Delta_i E^{\{2\}}$, one can see that with $r_0'=-r_0$,

$$E(e^{-\pi i}R')-E(e^{+\pi i}R')$$
$$=\frac{i\Delta_i\beta_2^{\{2\}}}{\gamma_0^3(-r_0')-r_0'^{-1}\gamma_0^2(-r_0')(d/dr_0'^{-1})\gamma_0(-r_0')} \tag{187}$$
$$=in^{-3}\Delta_i b_{\{0\}}^{\{2\}}[1+O(r_0'^{-2})] \tag{188}$$
$$=2\pi i(-1)^m 16n\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(2R'/n)^{-4\beta_2^{(0)}-2}e^{-2R'/n+2n}$$
$$\times\left\{1-\frac{n}{2R'}[8n^2\ln(2R'/n)+12(\beta_2^{(0)})^2-(m^2-1)-8\beta_1^{(0)}+4\beta_2^{(0)}\right.$$
$$\left.-4n^2[\psi(n_1+2n_2+2m+2)+\psi(n_1+2n_2+m+2)]-12n\beta_1^{(0)}-4n-8n\beta_2^{(0)}]+O[R'^{-2}(\ln R')^2]\right\}. \tag{189}$$

Again, notice the term $(n/2R')\ln(2R'/n)$.

VI. DISPERSION RELATIONS AND ASYMPTOTICS OF THE RSPT COEFFICIENTS

Dispersion relations are pertinent to the large-N behavior of the RSPT coefficients, whose asymptotic behavior they permit to be expressed as moments of the discontinuity of the imaginary part of the eigenvalue across the real axis. Dispersion relations arise from Cauchy's integral formula by enlargement of the contour to wrap around a branch cut. (These are standard arguments. See, e.g., Simon.[23])

Consider first the β_2 RSPT series, whose Borel sum is $\beta_1'(re^{-i\pi})$ for $\mathrm{Im}\, r\geq 0$ (see Sec. III I). One is led to the formula (see Sec. IV of Ref. 6 for a rigorous discussion)

$$\beta_1'(re^{-\pi i})=\frac{1}{2\pi i}\int_0^\infty\frac{\beta_1'(re^{-\pi i})-\beta_1'(re^{+\pi i})}{z-r}dz\ , \tag{190}$$

where again, this integral is meant only in the sense of power-series expansion. The discontinuity in β_1' is given by Eq. (124), which is ∓ 2 times the imaginary series entering the expansion for β_2 when $\pm\mathrm{Im}\, r\geq 0$. This fact, along with the expansion of the denominator $(z-r)$ in a geometric series, gives [cf. Eq. (100)]

$$\beta_2^{(N)}\sim-\int_0^\infty(2z)^{N-1}\Delta b^{\{1\}}(z)^2 q(z)d(2z) \tag{191}$$
$$\sim\pi^{-1}\int_0^{\infty+i\epsilon}(2z)^{N-1}\Delta_i\beta_2^{\{2\}}(z)d(2z)\quad(\epsilon>0) \tag{192}$$
$$\sim-\frac{(N+4n_2+2m+1)!}{(n_2!)^2[(n_2+m)!]^2}$$
$$\times\left\{1-\frac{12(\beta_2^{(0)})^2+4\beta_2^{(0)}-m^2+1}{N+4n_2+2m+1}+O(N^{-2})\right\}. \tag{193}$$

In this way the discontinuity in $\beta_1'(re^{-\pi i})$, which is imaginary and of second exponential order, determines the asymptotics of the RSPT $\beta_2^{(N)}$.

Similar considerations apply to the RSPT series for β_1, which is Borel summable to the eigenvalue of the modified Eq. (15) when $\beta_1'(re^{-\pi i})$ is used for β_2. (See again Ref. 6 for the rigorous details.) Since, however, $\beta_1(r)$ also has a cut for negative r, as well as the cut for positive r induced by the cut in $\beta_1'(re^{-\pi i})$, there are two terms in the dispersion relation:

$$\beta_1(r)=\frac{1}{2\pi i}\int_0^\infty \frac{\beta_1(z)-\beta_1(ze^{2\pi i})}{z-r}dz+\frac{1}{2\pi i}\int_{\infty e^{\pi i}}^0 \frac{-\beta_1(ze^{-2\pi i})+\beta_1(z)}{z-r}dz \tag{194}$$

$$=\frac{1}{2\pi i}\int_0^\infty \frac{\beta_1(z)-\beta_1(ze^{2\pi i})}{z-r}dz+\frac{1}{2\pi i}\int_0^\infty \frac{\beta_1(z'e^{-\pi i})-\beta_1(z'e^{+\pi i})}{z'+r}dz' . \tag{195}$$

As for the β_1' (i.e., β_2) dispersion relation, the discontinuity on the positive axis, $\beta_1(z)-\beta_1(ze^{2\pi i})$, is imaginary and of second exponential order: it is $\mp 2i$ times the $(\Delta_i\beta_1^{[2]})_{\text{ind}}$ of Eqs. (126) and (127). The discontinuity on the negative axis is given by Eqs. (156)–(158). Just as for $\beta_2^{(N)}$, one obtains for $\beta_1^{(N)}$

$$\beta_1^{(N)}\sim\pi^{-1}\int_0^{\infty+i\epsilon}(2z)^{N-1}[\Delta_i\beta_1^{[2]}(z)]_{\text{ind}}d(2z)+(2\pi)^{-1}\int_0^\infty(-2z')^{N-1}\Delta_i\beta_1^{[2]}(z')d(2z') \quad (\epsilon>0) \tag{196}$$

$$\sim\frac{(N+4n_2+2m)!}{(n_2!)^2[(n_2+m)!]^2}\left[4\beta_1^{(0)}-\frac{48\beta_1^{(0)}(\beta_2^{(0)})^2+12(\beta_1^{(0)})^2-(1+4\beta_1^{(0)})(m^2-1)}{N+4n_2+2m}+O(N^{-2})\right]$$
$$+(-1)^{m+N-1}16n^4\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(N-4n_2-2m-5)!$$
$$\times\left[1+\frac{4n^2-12(\beta_2^{(0)})^2+m^2-1+12n-12\beta_2^{(0)}}{N-4n_2-2m-5}\right.$$
$$\left.-\frac{4n^2[2\psi(N-4n_2-2m-5)-\psi(n_1+2n_2+2m+2)-\psi(n_1+2n_2+m+2)]}{N-4n_2-2m-5}+O[N^{-2}(\ln N^2)]\right] . \tag{197}$$

Note that the dominant asymptotic behavior coming from the positive cut is a same-sign $(N+4n_2+2m)!$, but that buried a factor of N^{5+8n_2+4m} down is an alternating-sign contribution that also involves a $\ln N$ dependence, since $\psi(N)\sim\ln N+O(N^{-1})$. Because of its relative smallness, the alternating-sign contribution is not immediately apparent from a numerical table of the $\beta_1^{(N)}$, but careful numerical analysis can detect it.

Similar considerations apply to the RSPT series for $E(R)$, which is Borel summable[5,6] to $-\frac{1}{2}[\beta_1'(r_0e^{-i\pi})+\beta_1(r_0,\beta_1'(r_0e^{-\pi i}))]^{-2}$. That is, instead of the *real* β_2 of Eq. (11), one puts into both Eqs. (10) and (12) the analytic continuation of the β_1' of Eqs. (113) and (114). There are two cuts in this Borel sum, with the key second-exponential-order quantities given by Eqs. (172), (173), and (182). The resulting asymptotics for the $E^{(N)}$ are

$$E^{(N)}\sim\pi^{-1}\int_0^{\infty+i\epsilon}(2z/n)^{N-1}\Delta_iE^{[2]}(z)d(2z/n)$$
$$+(2\pi i)^{-1}\int_0^\infty(2z'/n)^{N-1}[E(R'e^{-\pi i})-E(R'e^{+\pi i})]d(2z'/n) \tag{198}$$

$$\sim-\frac{e^{-2n}}{n^3(n_2!)^2[(n_2+m)!]^2}(N+4n_2+2m+1)!\left[1+\frac{4n\beta_1^{(0)}-8(\beta_2^{(0)})^2+2\beta_2^{(1)}+4n^2}{N+4n_2+2m+1}+O(N^{-2})\right]$$
$$+(-1)^{m+N-1}e^{2n}16n^4\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n^3n_1!(n_1+m)!}(N-4n_2-2m-5)!$$
$$\times\left[1+\frac{12n^2-12(\beta_2^{(0)})^2+m^2-1+12n-12\beta_2^{(0)}-4n\beta_2^{(0)}}{N-4n_2-2m-5}\right.$$
$$\left.-\frac{4n^2[2\psi(N-4n_2-2m-5)-\psi(n_1+2n_2+2m+2)-\psi(n_1+2n_2+m+2)]}{N-4n_2-2m-5}+O(N^{-2}(\ln N)^2)\right] . \tag{199}$$

Again, note the alternating-sign contribution that is down by a factor of N^{6+8n_2+4m} from the dominant same-sign $(N+4n_2+2m+1)!$ behavior. The alternating-sign contribution is not readily apparent from a table of the $E^{(N)}$, but careful numerical analysis can detect it. In fact, it was this unsuspected alternating-sign contribution that was responsible for the prior difficulty in carrying out the Bender-Wu analysis of the numerical $E^{(N)}$ for the ground state.[13] This point will be discussed in more detail in Secs. IX and X.

VII. JWKB-LIKE FORMULATION

The purpose of this section is to simplify the practical procedure for calculating the $O(e^{-r})$ and imaginary $O(e^{-2r})$ expansions for β_1 and β_2. The procedure so far involves three steps: (i) solution of a Riccati equation for ϕ, e.g., Eq. (35); (ii) determination of the index shift, e.g., $\Delta b^{[1]}$ of Eq. (64); (iii) determination of the ratio $q(r)$ by, e.g., Eq. (69) or (83). What complicates the procedure is the presence of ϕ^{-1} and ϕ^{-2} in the Riccati equation, which is the consequence of starting from the Whittaker confluent hypergeometric function. The alternative is to start from an exponential function—i.e., the JWKB-like form—which leads to a much simpler Riccati equation, but which then requires a "connection formula" and an alternative method to calculate $q(r)$.

The JWKB-like form for the QSC wave function Φ_2 [cf. Eqs. (31) and (32)] is

$$\Phi_2=(dS/d\eta)^{-1/2}(Ae^{-rS/2}+Be^{+rS/2}) , \tag{200}$$

where $S=S(\eta,r)$ satisfies the Riccati equation,

$$\frac{1}{4}\left[\frac{dS}{d\eta}\right]^2=\frac{1}{4}-\frac{\beta_2}{4}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]+\frac{m^2-1}{4r^2}\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]^2-\frac{1}{r^2}\left[\frac{dS}{d\eta}\right]^{1/2}\frac{d^2}{d\eta^2}\left[\frac{dS}{d\eta}\right]^{-1/2} . \tag{201}$$

We assume for $S(\eta,r)$ an expansion of the form

$$S(\eta,r)\sim\sum_{N=0}^{\infty}S^{(N)}(\eta)(2r)^{-N}+O(r^ke^{-r}) , \tag{202}$$

where in fact the $S^{(N)}(\eta)$ can be obtained directly from the QSC wave function by using the asymptotic expansion (56) for the Whittaker function and then rearranging terms appropriately. For instance, Eqs. (200) and (61) imply that

$$A(dS/d\eta)^{-1/2}e^{-rS/2}=\frac{(-1)^{n_2}(2r)^{\beta_2^{(0)}}}{(n_2+m)!}\times\eta^{\beta_2^{(0)}}(2-\eta)^{-\beta_2^{(0)}}e^{-r\eta/2}[1+O(r^{-1})] . \tag{203}$$

Then,

$$S=c+\eta+(2r)^{-1}4\beta_2^{(0)}\ln\left[\frac{2-\eta}{\eta}\right]+O(r^{-2}) , \tag{204}$$

$$A=(-1)^{n_2}e^{+rc/2}(2r)^{2\beta_2^{(0)}}/(n_2+m)! , \tag{205}$$

where c is a constant (with respect to η) related to the normalization (see below).

The main point, however, is not to obtain the $S^{(N)}$ from the $\phi^{(N)}$, but figuratively the reverse, because the $S^{(N)}$ are much easier to obtain directly from Eq. (201) than the $\phi^{(N)}$ from Eq. (35). For instance, given already that $dS^{(0)}/d\eta=1$, then for $N\geq1$, $S^{(N)}$ satisfies

$$dS^{(N)}/d\eta=-\tfrac{1}{2}\sum_{k=1}^{N-1}(dS^{(k)}/d\eta)(dS^{(N-k)}/d\eta)-4\beta_2^{(N-1)}[\eta^{-1}+(2-\eta)^{-1}]+2\delta_{N,2}(m^2-1)[\eta^{-1}+(2-\eta)^{-1}]^2-8[(dS/d\eta)^{1/2}(d^2/d\eta^2)(dS/d\eta)^{-1/2}]^{(N-2)} , \tag{206}$$

from which it follows that (see also immediately below)

$$dS^{(1)}/d\eta=-4\beta_2^{(0)}[\eta^{-1}+(2-\eta)^{-1}] , \tag{207}$$

$$S^{(1)}=+4\beta_2^{(0)}\ln\left[\frac{2-\eta}{\eta}\right] , \tag{208}$$

$$dS^{(2)}/d\eta=-8(\beta_2^{(0)})^2[\eta^{-1}+(2-\eta)^{-1}]^2-4\beta_2^{(1)}[\eta^{-1}+(2-\eta)^{-1}]+2(m^2-1)[\eta^{-1}+(2-\eta)^{-1}]^2 \tag{209}$$

$$\beta_2^{(1)}=-2(\beta_2^{(0)})^2+\tfrac{1}{2}(m^2-1) , \tag{210}$$

$$S^{(2)}=-4\beta_2^{(1)}[\eta^{-1}-(2-\eta)^{-1}] , \tag{211}$$

and so forth. There are two tricky points. The first is that the Riccati equation (201) involves only derivatives of S, and not S itself. The integration constants implicit in Eqs. (208) and (211) are therefore not determined by the Riccati equation; they will be explained in the next paragraph. The second point is that, apart from $S^{(1)}$, the $S^{(N)}$ for $N\geq2$ cannot have a $\ln\eta$ dependence. That is, $\beta_2^{(N-1)}$ has the value that eliminates the η^{-1} term from the recursive Eq. (206) for $S^{(N)}$. A most important practical consequence turns out to be that for $N\geq2$, $dS^{(N)}/d\eta$ is a polynomial $P_N(\eta^{-1})$ in η^{-1} of degree N, with no constant or first-order term, plus a similar polynomial in $(2-\eta)^{-1}$. Moreover, because of the symmetry of Eqs. (201) and (206) with respect to $\eta\rightarrow2-\eta$, it follows that

$$dS^{(N)}/d\eta=P_N(\eta^{-1})+P_N[(2-\eta)^{-1}] . \tag{212}$$

Thus, the $S^{(N)}$ for $N\geq2$ have a much simpler structure than the $\phi^{(N)}$ in that they are polynomials requiring only $N-1$ coefficients, and they have no complicated logarithmic terms.

Now we return to the integration-constant problem, which affects both the absolute normalization, which cannot be determined from the differential equation anyway, and the relative weights of the $e^{\pm rS/2}$ components, which is a connection-formula problem solved here easily because the overall Schrödinger equation is symmetric under $\eta\rightarrow2-\eta$. The solution is to make $S^{(N)}$ satisfy

$$S^{(N)}(2-\eta)=S^{(N)}(\eta) , \tag{213}$$

and to take A/B in Eq. (200) to be ±1. This then fixes also $S^{(0)}$,

$$S^{(0)}=\eta-1\ , \tag{214}$$

as well as the integration constants for all $S^{(N)}$.

However, there are still two major remaining problems: how to get $\Delta\beta_2^{[1]}$ and $\Delta_i\beta_2^{[2]}$ from Φ_2 in JWKB form. In Sec. III the procedure depended first on calculating the Whittaker index shift, which does not occur here, and second, the ratio $q(r)$. Here we can obtain $\Delta\beta_2^{[1]}$ from the two functions $\Phi_2^{(\pm)}$,

$$\Phi_2^{(\pm)}=(dS/d\eta)^{-1/2}(e^{-rS/2}\pm e^{+rS/2})\ , \tag{215}$$

via the standard current density formula, Eq. (79), which here becomes

$$2\Delta\beta_2^{[1]}=-2\Big/\int_0^{\eta}(dS/d\eta)^{-1}(e^{-rS}-e^{rS})\times[\eta^{-1}+(2-\eta)^{-1}]d\eta\quad(0\ll\eta\ll 2)\ . \tag{216}$$

By the same argument as in Sec. III E, Eq. (216) can be put in the form

$$\Delta\beta_2^{[1]}=-e^{-r}\Big/\int_0^{\infty}(dS/d\eta)^{-1}e^{-r(S+1)}\times[\eta^{-1}+(2-\eta)^{-1}]d\eta\ , \tag{217}$$

where the integral in Eq. (217) is meant only in the sense of a series in $(2r)^{-1}$, obtained by appropriate expansion of the integrand, followed by integration term by term.

The determination of the imaginary second-exponential-order series $\Delta_i\beta_2^{[2]}$ could also be obtained from the JWKB function by a current-density formula, if one had the requisite connection formula. Unfortunately, we have not found a way to get the right formula without going directly through the Whittaker function. However, we can get $\Delta_i\beta_2^{[2]}$ via Eq. (101) from the square of $\Delta\beta_2^{[1]}$ and from $q(r)$, the latter of which can be solved for directly in the JWKB approach. Note that $q(r)=d\beta_{2,\mathrm{RSPT}}/d\beta_2^{(0)}$ is a series in $(2r)^{-1}$ [Eq. (69)]. Let

$$T^{(N)}(\eta)\equiv dS^{(N)}(\eta)/d\beta_2^{(0)}\ . \tag{218}$$

Then T and $q(r)$ satisfy an equation obtained by differentiating the Riccati equation (201) with respect to $\beta_2^{(0)}$:

$$\frac{1}{2}\frac{dS}{d\eta}\frac{dT}{d\eta}=-r^{-1}q(r)\left[\frac{1}{\eta}+\frac{1}{2-\eta}\right]-r^{-2}\frac{1}{2}\frac{dT}{d\eta}\left[\frac{dS}{d\eta}\right]^{-1/2}\frac{d^2}{d\eta^2}\left[\frac{dS}{d\eta}\right]^{-1/2}+r^{-2}\frac{1}{2}\left[\frac{dS}{d\eta}\right]^{-1/2}\frac{d^2}{d\eta^2}\left[\frac{dS}{d\eta}\right]^{-3/2}\frac{dT}{d\eta}\ . \tag{219}$$

Further, by taking the $\beta_2^{(0)}$ derivative of the recursive Eq. (206), one obtains

$$dT^{(N)}/d\eta=-\sum_{k=0}^{N-1}(dT^{(k)}/d\eta)(dS^{(N-k)}/d\eta)-4q^{(N-1)}[\eta^{-1}+(2-\eta)^{-1}]-4[(dT/d\eta)(dS/d\eta)^{-1/2}(d^2/d\eta^2)(dS/d\eta)^{-1/2}-(dS/d\eta)^{1/2}(d^2/d\eta^2)(dS/d\eta)^{-3/2}(dT/d\eta)]^{(N-2)}\ . \tag{220}$$

One then finds (recall that $q^{(0)}=1$) that

$$T^{(0)}=0\ , \tag{221}$$

$$dT^{(1)}/d\eta=-4[\eta^{-1}(2-\eta)^{-1}]\ , \tag{222}$$

$$T^{(1)}=+4\ln\left[\frac{2-\eta}{\eta}\right]\ , \tag{223}$$

$$dT^{(2)}/d\eta=-16\beta_2^{(0)}[\eta^{-1}+(2-\eta)^{-1}]^2-4q^{(1)}[\eta^{-1}+(2-\eta)^{-1}]\ , \tag{224}$$

$$q^{(1)}=-4\beta_2^{(0)}\ , \tag{225}$$

$$T^{(2)}=16\beta_2^{(0)}[\eta^{-1}-(2-\eta)^{-1}]\ , \tag{226}$$

and so forth. As is by now a familiar argument, the value of $q^{(N-1)}$ is obtained by eliminating the η^{-1} term in the equation [Eq. (220)] for $dT^{(N)}/d\eta$ for $N\geq 2$. In such a way $q(r)$ can be obtained, and consequently $\Delta_i\beta_2^{[2]}$ via Eq. (101).

Finally, we consider the two contributions to β_1: $(\Delta\beta_1^{[1]}+i\Delta_i\beta_1^{[2]})_{\mathrm{ind}}$ and $i\Delta_i\beta_1^{[2]}(-r)$ (the discontinuity at negative r). The induced terms are needed to high order. They can be calculated from Eq. (127) with the RSPT wave function, and thus require no further comment. The discontinuity for negative r, on the other hand, will not be taken further than the few orders given here explicitly, and so the JWKB approach will not be sketched.

This now completes the theoretical discussion of the computation of the asymptotic expansions for β_1, β_2, and E. In the remaining sections we give numerical illustrations of the various terms in the expansions, their asymptotics, and their interrelations.

VIII. NUMERICAL CHARACTERIZATION OF THE β_2 SERIES

In this section we tabulate and discuss the asymptotics for the various series contributing to the asymptotic expansion of β_2. First we list in Tables I–III the terms of the RSPT series, the exponentially small gap series $\Delta\beta_2^{[1]}$, and the doubly-exponentially-small imaginary series $\Delta_i\beta_2^{[2]}$, all through fifty-first order in $(2r)^{-1}$, for the ground state (for which $n_2=0$ and $m=0$) and for two excited states for which n_2 and m are (1,0) and (0,1). We

TABLE I. Coefficients for the RSPT series, the $\Delta\beta_2^{[1]}$ series, and the $\Delta_i\beta_2^{[2]}$ series, as defined by Eqs. (26), (227), and (228) of the text, for the ($n_2=0, m=0$) ground state of β_2.

Order N	$\beta_2^{(N)}$	Coefficient $c^{(1)(N)}$	$c^{(2)(N)}$
0	5.00000 00000 00000 00000 00000 000 $\times 10^{-1}$	1.00000 00000 00000 00000 00000 000 $\times 10^{0}$	1.00000 00000 00000 00000 00000 000 $\times 10^{0}$
1	-1.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-4.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-6.00000 00000 00000 00000 00000 000 $\times 10^{0}$
2	-1.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-3.00000 00000 00000 00000 00000 000 $\times 10^{0}$	2.00000 00000 00000 00000 00000 000 $\times 10^{0}$
3	-4.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-2.00000 00000 00000 00000 00000 000 $\times 10^{1}$	-1.60000 00000 00000 00000 00000 000 $\times 10^{1}$
4	-2.30000 00000 00000 00000 00000 000 $\times 10^{1}$	-1.46000 00000 00000 00000 00000 000 $\times 10^{2}$	-1.31000 00000 00000 00000 00000 000 $\times 10^{2}$
5	-1.64000 00000 00000 00000 00000 000 $\times 10^{2}$	-1.24000 00000 00000 00000 00000 000 $\times 10^{3}$	-1.18600 00000 00000 00000 00000 000 $\times 10^{3}$
6	-1.36200 00000 00000 00000 00000 000 $\times 10^{3}$	-1.18390 00000 00000 00000 00000 000 $\times 10^{4}$	-1.18100 00000 00000 00000 00000 000 $\times 10^{4}$
7	-1.27440 00000 00000 00000 00000 000 $\times 10^{4}$	-1.24324 00000 00000 00000 00000 000 $\times 10^{5}$	-1.27960 00000 00000 00000 00000 000 $\times 10^{5}$
8	-1.31707 00000 00000 00000 00000 000 $\times 10^{5}$	-1.41649 00000 00000 00000 00000 000 $\times 10^{6}$	-1.49465 40000 00000 00000 00000 000 $\times 10^{6}$
9	-1.48424 40000 00000 00000 00000 000 $\times 10^{6}$	-1.73543 12000 00000 00000 00000 000 $\times 10^{7}$	-1.86934 68000 00000 00000 00000 000 $\times 10^{7}$
10	-1.80783 02000 00000 00000 00000 000 $\times 10^{7}$	-2.27232 04200 00000 00000 00000 000 $\times 10^{8}$	-2.49095 24400 00000 00000 00000 000 $\times 10^{8}$
11	-2.36476 47200 00000 00000 00000 000 $\times 10^{8}$	-3.16578 38160 00000 00000 00000 000 $\times 10^{9}$	-3.52338 30400 00000 00000 00000 000 $\times 10^{9}$
12	-3.30587 16700 00000 00000 00000 000 $\times 10^{9}$	-4.67728 16692 00000 00000 00000 000 $\times 10^{10}$	-5.27508 14163 00000 00000 00000 000 $\times 10^{10}$
13	-4.92007 90504 00000 00000 00000 000 $\times 10^{10}$	-7.30893 64286 40000 00000 00000 000 $\times 10^{11}$	-8.33998 05415 40000 00000 00000 000 $\times 10^{11}$
14	-7.77049 28925 20000 00000 00000 000 $\times 10^{11}$	-1.20530 61361 62700 00000 00000 000 $\times 10^{13}$	-1.38965 93049 57800 00000 00000 000 $\times 10^{13}$
15	-1.29869 09942 92800 00000 00000 000 $\times 10^{13}$	-2.09349 93948 78760 00000 00000 000 $\times 10^{14}$	-2.43608 16100 60240 00000 00000 000 $\times 10^{14}$
16	-2.29119 96110 22270 00000 00000 000 $\times 10^{14}$	-3.82297 63917 58058 00000 00000 000 $\times 10^{15}$	-4.48542 46645 03802 00000 00000 000 $\times 10^{15}$
17	-4.25726 70215 18900 00000 00000 000 $\times 10^{15}$	-7.32739 10035 20413 60000 00000 000 $\times 10^{16}$	-8.66093 78935 33990 80000 00000 000 $\times 10^{16}$
18	-8.31362 93369 26679 00000 00000 000 $\times 10^{16}$	-1.47167 45118 75833 30200 00000 000 $\times 10^{18}$	-1.75113 16654 27886 86800 00000 000 $\times 10^{18}$
19	-1.70286 51859 52650 20000 00000 000 $\times 10^{18}$	-3.09248 48922 41491 97040 00000 000 $\times 10^{19}$	-3.70189 81237 24444 08640 00000 000 $\times 10^{19}$
20	-3.65163 71245 95240 29140 00000 000 $\times 10^{19}$	-6.78854 08446 99841 64988 00000 000 $\times 10^{20}$	-8.17064 74365 64111 78302 00000 000 $\times 10^{20}$
21	-8.18363 62546 55226 91640 00000 000 $\times 10^{20}$	-1.55445 81687 12466 66800 80000 000 $\times 10^{22}$	-1.88020 75120 84454 55611 40000 000 $\times 10^{22}$
22	-1.91352 06010 34558 15834 84000 000 $\times 10^{22}$	-3.70764 85296 68338 29993 46200 000 $\times 10^{23}$	-4.50486 43609 14752 88996 53200 000 $\times 10^{23}$
23	-4.66085 99868 46674 53748 97600 000 $\times 10^{23}$	-9.19903 08925 25069 64112 14480 000 $\times 10^{24}$	-1.12231 29845 29462 33492 30384 000 $\times 10^{25}$
24	-1.18087 09875 31777 21528 18974 000 $\times 10^{25}$	-2.37105 59152 59105 74586 84410 000 $\times 10^{26}$	-2.90371 73545 26023 57510 80214 000 $\times 10^{26}$
25	-3.10768 72059 67308 72311 17543 200 $\times 10^{26}$	-6.34097 00820 77188 20855 34988 320 $\times 10^{27}$	-7.79251 53228 08283 84083 62822 960 $\times 10^{27}$
26	-8.48401 03159 03761 99466 43713 720 $\times 10^{27}$	-1.75738 83051 43272 09774 64771 848 $\times 10^{29}$	-2.16661 87672 77887 09157 84670 735 $\times 10^{29}$
27	-2.39970 72843 52675 68333 74424 069 $\times 10^{29}$	-5.04182 10457 38398 35811 33937 983 $\times 10^{30}$	-6.23434 80127 14026 00283 15075 752 $\times 10^{30}$
28	-7.02431 79168 22741 72523 31191 884 $\times 10^{30}$	-1.49571 64288 09167 61657 52989 120 $\times 10^{32}$	-1.85459 34956 33853 10071 88516 430 $\times 10^{32}$
29	-2.12551 33457 46545 09323 16169 555 $\times 10^{32}$	-4.58365 26145 22014 91608 59148 195 $\times 10^{33}$	-5.69801 46494 80673 26407 95454 135 $\times 10^{33}$
30	-6.64185 83025 05175 43644 14212 211 $\times 10^{33}$	-1.44962 62146 16932 19240 75245 053 $\times 10^{35}$	-1.80636 35257 23279 36841 49310 267 $\times 10^{35}$
31	-2.14120 94328 88922 08476 96351 560 $\times 10^{35}$	-4.72699 60495 98641 44352 22329 589 $\times 10^{36}$	-5.90342 08831 68021 20850 61900 585 $\times 10^{36}$
32	-7.11497 97941 70213 53743 47647 260 $\times 10^{36}$	-1.58789 82879 84635 97550 95887 989 $\times 10^{38}$	-1.98723 43570 83596 13745 71503 926 $\times 10^{38}$
33	-2.43476 01998 75947 84045 16985 059 $\times 10^{38}$	-5.49048 73994 89535 01901 11200 699 $\times 10^{39}$	-6.88476 83858 90553 46760 93238 203 $\times 10^{39}$
34	-8.57333 80341 53255 41652 72258 532 $\times 10^{39}$	-1.95258 70796 48423 03941 78559 903 $\times 10^{41}$	-2.45295 71861 49525 55312 40654 798 $\times 10^{41}$
35	-3.10396 56319 28989 55910 55864 809 $\times 10^{41}$	-7.13671 83784 92300 82039 52528 491 $\times 10^{42}$	-8.98116 61087 52749 84174 69544 320 $\times 10^{42}$
36	-1.15461 29420 60619 29018 30718 129 $\times 10^{43}$	-2.67897 35693 68627 74424 09797 058 $\times 10^{44}$	-3.37687 21026 81779 45823 79481 983 $\times 10^{44}$
37	-4.40964 88093 35437 27416 23730 083 $\times 10^{44}$	-1.03211 43799 72823 92389 66487 791 $\times 10^{46}$	-1.30300 74990 96156 42092 56503 281 $\times 10^{46}$
38	-1.72794 59793 86441 83558 55102 283 $\times 10^{46}$	-4.07848 00503 49129 07760 85440 066 $\times 10^{47}$	-5.15649 19022 80787 89237 58353 474 $\times 10^{47}$
39	-6.94287 54341 60981 32809 73866 808 $\times 10^{47}$	-1.65201 67304 14025 34334 48890 893 $\times 10^{49}$	-2.09157 84455 26994 94656 43290 908 $\times 10^{49}$
40	-2.85870 36167 95211 42358 58706 384 $\times 10^{49}$	-6.85524 00386 77524 26835 40750 117 $\times 10^{50}$	-8.69071 33574 32356 42848 37178 851 $\times 10^{50}$
41	-1.20550 51343 76258 72332 02260 750 $\times 10^{51}$	-2.91260 01443 40255 49058 66339 557 $\times 10^{52}$	-3.69707 50313 60110 25599 19234 567 $\times 10^{52}$
42	-5.20355 49106 85414 14568 64618 160 $\times 10^{52}$	-1.26636 09070 46195 03421 76231 613 $\times 10^{54}$	-1.60935 99125 18770 97479 16088 058 $\times 10^{54}$
43	-2.29791 48686 18532 42916 00762 910 $\times 10^{54}$	-5.63158 90714 31873 69861 52625 228 $\times 10^{55}$	-7.16506 99757 94250 99220 85582 926 $\times 10^{55}$
44	-1.03765 25193 10435 21015 42299 284 $\times 10^{56}$	-2.56028 91040 18442 42650 46072 008 $\times 10^{57}$	-3.26099 00973 70612 52788 02117 622 $\times 10^{57}$
45	-4.78900 15564 75344 94313 70950 205 $\times 10^{57}$	-1.18940 07060 37608 89247 32088 544 $\times 10^{59}$	-1.51648 59630 26241 83995 46170 311 $\times 10^{59}$
46	-2.25794 09433 59019 65094 16354 837 $\times 10^{59}$	-5.64356 23561 95807 13378 84812 863 $\times 10^{60}$	-7.20266 80972 58068 07728 82973 260 $\times 10^{60}$
47	-1.08708 24854 82559 41046 75467 189 $\times 10^{61}$	-2.73386 47676 07054 08529 73618 875 $\times 10^{62}$	-3.49243 55429 46068 17903 53647 809 $\times 10^{62}$
48	-5.34207 78495 67110 04754 84898 385 $\times 10^{62}$	-1.35150 99684 21553 94756 34420 727 $\times 10^{64}$	-1.72808 26951 32021 67269 69848 230 $\times 10^{64}$
49	-2.67841 86985 57226 31974 80156 238 $\times 10^{64}$	-6.81564 40356 14582 87447 90262 544 $\times 10^{65}$	-8.72227 43608 43794 99073 75189 599 $\times 10^{65}$
50	-1.36960 98468 21709 74345 22170 539 $\times 10^{66}$	-3.50488 21329 08820 26687 38878 986 $\times 10^{67}$	-4.48909 20002 24446 57754 83776 332 $\times 10^{67}$
51	-7.14005 39439 56397 53456 22192 581 $\times 10^{67}$	-1.83720 85116 61938 24749 17709 789 $\times 10^{69}$	-2.35500 24637 87773 35815 26898 324 $\times 10^{69}$

use the notation $c^{[1](N)}$ and $c^{[2](N)}$ for the series coefficients for the two exponentially small quantities [cf. also Eqs. (54) and (99)]:

$$\Delta\beta_2^{[1]} = \pm\frac{(2r)^{2\beta_2^{(0)}} e^{-r}}{n_2!(n_2+m)!}\sum_{N=0}^{\infty} c^{[1](N)}(2r)^{-N}\,, \qquad (227)$$

$$\Delta_i\beta_2^{[2]} = \mp\pi\frac{(2r)^{4\beta_2^{(0)}} e^{-2r}}{[n_2!(n_2+m)!]^2} \times \sum_{N=0}^{\infty} c^{[2](N)}(2r)^{-N} \quad (\pm\mathrm{Im}\, r \geq 0)\,. \qquad (228)$$

Notice that the coefficients (at least those with fewer than the maximum number of significant digits) appear to be

TABLE II. Coefficients for the RSPT series, the $\Delta\beta_2^{[1]}$ series, and the $\Delta_i\beta_2^{[2]}$ series, as defined by Eqs. (26), (227), and (228) of the text, for the ($n_2=1, m=0$) excited state of β_2.

Order N	Coefficient $\beta_2^{(N)}$	$c^{(1)(N)}$	$c^{(2)(N)}$
0	1. 50000 00000 00000 00000 00000 000 x 10 ^{0}	1. 00000 00000 00000 00000 00000 0 x 10 ^{0}	1. 00000 00000 00000 00000 00000 0 x 10 ^{0}
1	-5. 00000 00000 00000 00000 00000 000 x 10 ^{0}	-2. 00000 00000 00000 00000 00000 0 x 10 ^{1}	-3. 40000 00000 00000 00000 00000 0 x 10 ^{1}
2	-1. 50000 00000 00000 00000 00000 000 x 10 ^{1}	7. 90000 00000 00000 00000 00000 0 x 10 ^{1}	3. 82000 00000 00000 00000 00000 0 x 10 ^{2}
3	-1. 24000 00000 00000 00000 00000 000 x 10 ^{2}	-1. 40000 00000 00000 00000 00000 0 x 10 ^{2}	-1. 80000 00000 00000 00000 00000 0 x 10 ^{3}
4	-1. 40100 00000 00000 00000 00000 000 x 10 ^{3}	-1. 44900 00000 00000 00000 00000 0 x 10 ^{3}	2. 75900 00000 00000 00000 00000 0 x 10 ^{3}
5	-1. 89080 00000 00000 00000 00000 000 x 10 ^{4}	-2. 71800 00000 00000 00000 00000 0 x 10 ^{4}	-1. 28420 00000 00000 00000 00000 0 x 10 ^{4}
6	-2. 87790 00000 00000 00000 00000 000 x 10 ^{5}	-5. 29102 00000 00000 00000 00000 0 x 10 ^{5}	-2. 29554 00000 00000 00000 00000 0 x 10 ^{5}
7	-4. 79032 80000 00000 00000 00000 000 x 10 ^{6}	-1. 07178 00000 00000 00000 00000 0 x 10 ^{7}	-5. 00120 00000 00000 00000 00000 0 x 10 ^{6}
8	-8. 55929 01000 00000 00000 00000 000 x 10 ^{7}	-2. 25598 17700 00000 00000 00000 0 x 10 ^{8}	-1. 11861 67700 00000 00000 00000 0 x 10 ^{8}
9	-1. 62192 49080 00000 00000 00000 000 x 10 ^{9}	-4. 92147 11960 00000 00000 00000 0 x 10 ^{9}	-2. 57053 15820 00000 00000 00000 0 x 10 ^{9}
10	-3. 23250 68706 00000 00000 00000 000 x 10^{10}	-1. 10988 94357 40000 00000 00000 0 x 10^{11}	-6. 06569 00350 00000 00000 00000 0 x 10^{10}
11	-6. 73608 46023 20000 00000 00000 000 x 10^{11}	-2. 58205 23355 44000 00000 00000 0 x 10^{12}	-1. 46892 76000 40000 00000 00000 0 x 10^{12}
12	-1. 46142 79030 98600 00000 00000 000 x 10^{13}	-6. 18612 91921 55800 00000 00000 0 x 10^{13}	-3. 64875 11428 09800 00000 00000 0 x 10^{13}
13	-3. 29060 69379 17680 00000 00000 000 x 10^{14}	-1. 52432 98050 56760 00000 00000 0 x 10^{15}	-9. 29198 45888 50280 00000 00000 0 x 10^{14}
14	-7. 67143 36414 01820 00000 00000 000 x 10^{15}	-3. 85941 36242 03950 00000 00000 0 x 10^{16}	-2. 42511 91536 09848 40000 00000 0 x 10^{16}
15	-1. 84843 79970 80646 24000 00000 000 x 10^{17}	-1. 00330 60726 60789 13600 00000 0 x 10^{18}	-6. 48485 69907 24364 80000 00000 0 x 10^{17}
16	-4. 59699 61209 97360 74900 00000 000 x 10^{18}	-2. 67663 65632 22320 18290 00000 0 x 10^{19}	-1. 77635 67105 06533 32930 00000 0 x 10^{19}
17	-1. 17879 08355 26013 11180 00000 000 x 10^{20}	-7. 32537 77992 96708 57596 00000 0 x 10^{20}	-4. 98393 90973 42652 50038 00000 0 x 10^{20}
18	-3. 11421 63901 20289 86921 00000 000 x 10^{21}	-2. 05610 83355 15227 58653 66000 0 x 10^{22}	-1. 43219 30202 07219 22611 42000 0 x 10^{22}
19	-8. 47114 92481 05832 81940 88000 000 x 10^{22}	-5. 91784 77055 13196 97774 55200 0 x 10^{23}	-4. 21508 26751 34774 24225 84800 0 x 10^{23}
20	-2. 37139 51306 64353 18768 28460 000 x 10^{24}	-1. 74636 02638 88521 58796 86698 0 x 10^{25}	-1. 27053 00054 98321 50863 56998 0 x 10^{25}
21	-6. 82900 54018 38489 37056 42440 000 x 10^{25}	-5. 28348 72967 01142 31949 67652 0 x 10^{26}	-3. 92228 94820 09263 65812 74534 0 x 10^{26}
22	-2. 02232 39028 84232 49825 83059 240 x 10^{27}	-1. 63868 19398 02560 95274 51599 7 x 10^{28}	-1. 24013 69787 85037 54869 30185 5 x 10^{28}
23	-6. 15665 56058 51913 21565 96472 080 x 10^{28}	-5. 20985 42615 91068 09353 90167 0 x 10^{29}	-4. 01576 13158 67891 81492 67074 6 x 10^{29}
24	-1. 92622 25172 07042 01876 03172 196 x 10^{30}	-1. 69776 42417 31158 08294 82577 0 x 10^{31}	-1. 33173 39805 98400 16783 83876 6 x 10^{31}
25	-6. 19158 27043 12407 71637 60630 245 x 10^{31}	-5. 67028 20309 90721 47662 47606 1 x 10^{32}	-4. 52261 32888 36149 44369 21485 5 x 10^{32}
26	-2. 04405 42323 48321 89800 46461 406 x 10^{33}	-1. 94066 31196 26219 37173 29205 7 x 10^{34}	-1. 57268 35502 19543 78418 88854 0 x 10^{34}
27	-6. 92841 54288 88016 64480 78189 018 x 10^{34}	-6. 80524 07901 98263 84893 67740 8 x 10^{35}	-5. 59907 95879 18291 13573 03960 2 x 10^{35}
28	-2. 41031 48241 35442 14985 99921 841 x 10^{36}	-2. 44456 11469 58322 27853 54574 2 x 10^{37}	-2. 04053 92869 53159 10947 16949 2 x 10^{37}
29	-8. 60303 70969 35033 61034 45996 990 x 10^{37}	-8. 99343 52514 02760 98447 98358 7 x 10^{38}	-7. 61101 86968 89220 24321 04967 5 x 10^{38}
30	-3. 14920 34143 86974 19796 00692 752 x 10^{39}	-3. 38773 08077 53251 59474 22324 9 x 10^{40}	-2. 90478 93346 26683 11651 43846 8 x 10^{40}
31	-1. 18180 88928 18561 80957 86905 142 x 10^{41}	-1. 30626 55389 85574 10499 99715 9 x 10^{42}	-1. 13410 82383 50151 69426 32699 2 x 10^{42}
32	-4. 54478 68051 15425 64706 98675 558 x 10^{42}	-5. 15424 58570 19095 02936 34729 7 x 10^{43}	-4. 52842 75237 74185 49325 41237 6 x 10^{43}
33	-1. 79026 95612 40790 23279 03640 787 x 10^{44}	-2. 08053 21720 25534 63296 61777 0 x 10^{45}	-1. 84871 98441 10222 11599 98361 1 x 10^{45}
34	-7. 22069 78673 35164 79148 63644 151 x 10^{45}	-8. 58852 10932 50696 42439 84301 2 x 10^{46}	-7. 71431 74222 19582 71894 45968 7 x 10^{46}
35	-2. 98066 04197 44885 29279 22693 454 x 10^{47}	-3. 62453 24148 46241 86913 83649 4 x 10^{48}	-3. 28923 03154 46304 15004 74978 2 x 10^{48}
36	-1. 25873 95363 48933 92704 37018 582 x 10^{49}	-1. 56324 71918 70763 86589 89602 0 x 10^{50}	-1. 43260 38556 26793 60235 53027 7 x 10^{50}
37	-5. 43586 22112 53563 50247 58601 235 x 10^{50}	-6. 88805 25148 76714 26733 14015 2 x 10^{51}	-6. 37170 76617 73232 33429 33518 5 x 10^{51}
38	-2. 39956 11218 76005 14118 81227 428 x 10^{52}	-3. 09962 46018 18145 40738 35073 6 x 10^{53}	-2. 89298 01806 22921 36021 74676 4 x 10^{53}
39	-1. 08230 75925 96434 51732 05279 466 x 10^{54}	-1. 42402 25909 58260 78956 41689 7 x 10^{55}	-1. 34046 94982 60535 48097 75340 5 x 10^{55}
40	-4. 98601 23372 61673 79697 98421 501 x 10^{55}	-6. 67686 03852 12598 42070 65582 9 x 10^{56}	-6. 33655 04597 44654 11445 74583 0 x 10^{56}
41	-2. 34515 66937 30906 89225 10321 332 x 10^{57}	-3. 19396 11943 63196 89651 27737 1 x 10^{58}	-3. 05490 11323 29236 55442 10253 5 x 10^{58}
42	-1. 12575 13315 75148 07995 20637 080 x 10^{59}	-1. 55827 96259 78061 30025 50082 9 x 10^{60}	-1. 50160 31266 46630 39406 28205 1 x 10^{60}
43	-5. 51322 35319 95889 34088 37293 762 x 10^{60}	-7. 75137 20404 41128 23447 33637 7 x 10^{61}	-7. 52305 62992 97730 94890 80388 6 x 10^{61}
44	-2. 75363 26072 06983 29451 35466 885 x 10^{62}	-3. 92998 57306 41202 55583 30987 1 x 10^{63}	-3. 84046 85805 09093 46782 66425 9 x 10^{63}
45	-1. 40214 42335 29008 28314 25014 531 x 10^{64}	-2. 03023 93933 85626 80333 32386 9 x 10^{65}	-1. 99708 65621 87354 15592 29038 2 x 10^{65}
46	-7. 27644 06986 88205 51053 60561 273 x 10^{65}	-1. 06835 38389 14209 33412 91094 4 x 10^{67}	-1. 05756 45263 27929 37460 55075 4 x 10^{67}
47	-3. 84717 93139 33494 80978 96448 920 x 10^{67}	-5. 72486 63011 85086 61970 23238 2 x 10^{68}	-5. 70152 90109 74236 32455 17242 9 x 10^{68}
48	-2. 07168 93981 50953 44764 69212 890 x 10^{69}	-3. 12299 89365 32400 27393 64589 9 x 10^{70}	-3. 12845 65088 91508 89186 25437 9 x 10^{70}
49	-1. 13587 70317 33535 64658 77546 574 x 10^{71}	-1. 73385 01676 79170 84494 86717 2 x 10^{72}	-1. 74664 95254 45916 75763 02557 9 x 10^{72}
50	-6. 33916 49503 26059 31915 32049 022 x 10^{72}	-9. 79410 14748 54531 37172 30127 7 x 10^{73}	-9. 91981 41758 09251 08270 34313 5 x 10^{73}
51	-3. 59998 13761 20306 92394 57989 742 x 10^{74}	-5. 62748 11044 41740 67063 02348 3 x 10^{75}	-5. 72942 93811 75222 29516 04585 1 x 10^{75}

integers. The coefficients are estimated to be accurate to the precision reported, with uncertainty only in the last digit. Notice that for the ($n_2=1$, $m=0$) state, only 27 digits have been reported for the coefficients $c^{[1](N)}$ and $c^{[2](N)}$, two fewer than the 29 reported for the (0,0) and (0,1) states. The numerical error seems to depend on n_2.

It is interesting to examine numerically the prediction of the asymptotics of the $\beta_2^{(N)}$ by the dispersion relation [Eqs. (192) and (193)], which in the more general notation of Eq. (228) becomes

TABLE III. Coefficients for the RSPT series, the $\Delta\beta_2^{[1]}$ series, and the $\Delta_i\beta_2^{[2]}$ series, as defined by Eqs. (26), (227), and (228) of the text, for the ($n_2=0, m=1$) excited state of β_2.

Order N	Coefficient $\beta_2^{(N)}$	$c^{(1)(N)}$	$c^{(2)(N)}$
0	1. 00000 00000 00000 00000 00000 000 x 10^{0}	1. 00000 00000 00000 00000 00000 000 x 10^{0}	1. 00000 00000 00000 00000 00000 000 x 10^{0}
1	-2. 00000 00000 00000 00000 00000 000 x 10^{0}	-1. 00000 00000 00000 00000 00000 000 x 10^{1}	-1. 60000 00000 00000 00000 00000 000 x 10^{1}
2	-4. 00000 00000 00000 00000 00000 000 x 10^{0}	8. 00000 00000 00000 00000 00000 000 x 10^{0}	6. 40000 00000 00000 00000 00000 000 x 10^{1}
3	-2. 40000 00000 00000 00000 00000 000 x 10^{1}	-4. 80000 00000 00000 00000 00000 000 x 10^{1}	-1. 04000 00000 00000 00000 00000 000 x 10^{2}
4	-2. 00000 00000 00000 00000 00000 000 x 10^{2}	-5. 80000 00000 00000 00000 00000 000 x 10^{2}	-3. 28000 00000 00000 00000 00000 000 x 10^{2}
5	-2. 01600 00000 00000 00000 00000 000 x 10^{3}	-7. 48000 00000 00000 00000 00000 000 x 10^{3}	-4. 89600 00000 00000 00000 00000 000 x 10^{3}
6	-2. 31680 00000 00000 00000 00000 000 x 10^{4}	-1. 03568 00000 00000 00000 00000 000 x 10^{5}	-7. 28000 00000 00000 00000 00000 000 x 10^{4}
7	-2. 94144 00000 00000 00000 00000 000 x 10^{5}	-1. 52982 40000 00000 00000 00000 000 x 10^{6}	-1. 13612 80000 00000 00000 00000 000 x 10^{6}
8	-4. 04886 40000 00000 00000 00000 000 x 10^{6}	-2. 39283 52000 00000 00000 00000 000 x 10^{7}	-1. 85722 08000 00000 00000 00000 000 x 10^{7}
9	-5. 96958 72000 00000 00000 00000 000 x 10^{7}	-3. 93987 26400 00000 00000 00000 000 x 10^{8}	-3. 17245 05600 00000 00000 00000 000 x 10^{8}
10	-9. 35031 68000 00000 00000 00000 000 x 10^{8}	-6. 79920 53760 00000 00000 00000 000 x 10^{9}	-5. 65015 25760 00000 00000 00000 000 x 10^{9}
11	-1. 54693 27872 00000 00000 00000 000 x 10^{10}	-1. 22590 79884 80000 00000 00000 000 x 10^{11}	-1. 04728 20364 80000 00000 00000 000 x 10^{11}
12	-2. 69193 68371 20000 00000 00000 000 x 10^{11}	-2. 30392 03428 48000 00000 00000 000 x 10^{12}	-2. 01732 33895 68000 00000 00000 000 x 10^{12}
13	-4. 91201 56016 64000 00000 00000 000 x 10^{12}	-4. 50543 56797 82400 00000 00000 000 x 10^{13}	-4. 03372 18125 31200 00000 00000 000 x 10^{13}
14	-9. 37628 90723 32800 00000 00000 000 x 10^{13}	-9. 15592 81229 49120 00000 00000 000 x 10^{14}	-8. 36514 33929 06240 00000 00000 000 x 10^{14}
15	-1. 86885 76969 72800 00000 00000 000 x 10^{15}	-1. 93165 90899 22713 60000 00000 000 x 10^{16}	-1. 79793 93963 46265 60000 00000 000 x 10^{16}
16	-3. 88370 71338 67776 00000 00000 000 x 10^{16}	-4. 22741 50482 92408 32000 00000 000 x 10^{17}	-4. 00277 77477 65836 80000 00000 000 x 10^{17}
17	-8. 40420 68016 11857 92000 00000 000 x 10^{17}	-9. 59058 84493 80975 61600 00000 000 x 10^{18}	-9. 22605 31364 71498 75200 00000 000 x 10^{18}
18	-1. 89169 34886 99642 06080 00000 000 x 10^{19}	-2. 25415 45617 81600 41984 00000 000 x 10^{20}	-2. 20058 58918 34310 32832 00000 000 x 10^{20}
19	-4. 42462 17665 65281 05472 00000 000 x 10^{20}	-5. 48589 88501 96950 28633 60000 000 x 10^{21}	-5. 42916 44313 67332 99097 60800 000 x 10^{21}
20	-1. 07440 27756 35857 90894 08000 000 x 10^{22}	-1. 38165 27991 83060 69919 74400 000 x 10^{23}	-1. 38484 30328 17282 12963 32800 000 x 10^{23}
21	-2. 70603 51042 39472 98078 72000 000 x 10^{23}	-3. 59910 63521 10533 96414 05440 000 x 10^{24}	-3. 65033 35474 65427 44333 51680 000 x 10^{24}
22	-7. 06307 14522 84627 41507 27680 000 x 10^{24}	-9. 69136 19662 67827 05149 13280 000 x 10^{25}	-9. 93822 69721 12706 01209 77408 000 x 10^{25}
23	-1. 90884 86356 42899 25508 43187 200 x 10^{26}	-2. 69593 63553 29941 41437 42935 040 x 10^{27}	-2. 79316 96996 86573 81493 15215 360 x 10^{27}
24	-5. 33697 33102 89601 45846 41454 080 x 10^{27}	-7. 74284 03651 30866 09938 41119 232 x 10^{28}	-8. 09942 37604 10702 89308 06788 096 x 10^{28}
25	-1. 54239 78463 51307 58563 66488 781 x 10^{29}	-2. 29445 91630 54104 45539 96369 592 x 10^{30}	-2. 42173 23352 81385 51231 37515 684 x 10^{30}
26	-4. 60376 41702 78633 69811 98374 830 x 10^{30}	-7. 01080 26281 52372 76772 64822 010 x 10^{31}	-7. 46196 25743 21848 53308 91739 333 x 10^{31}
27	-1. 41804 17250 31727 51726 10206 309 x 10^{32}	-2. 20738 20760 34027 12384 02811 521 x 10^{33}	-2. 36793 61646 67898 62205 86112 125 x 10^{33}
28	-4. 50376 94527 22540 95973 68211 057 x 10^{33}	-7. 15688 43088 83317 05264 56626 571 x 10^{34}	-7. 73410 17795 78155 86706 42297 178 x 10^{34}
29	-1. 47378 96971 25289 26058 30488 482 x 10^{35}	-2. 38793 83703 43630 94475 80447 367 x 10^{36}	-2. 59839 90084 55357 53263 72962 166 x 10^{36}
30	-4. 96521 64280 81112 14342 78197 278 x 10^{36}	-8. 19396 72317 89302 91911 53902 723 x 10^{37}	-8. 97414 37133 40939 98093 29841 256 x 10^{37}
31	-1. 72094 08950 60214 53338 85764 683 x 10^{38}	-2. 88975 91120 63477 48480 58175 925 x 10^{39}	-3. 18427 23534 76594 72900 43246 414 x 10^{39}
32	-6. 13213 57385 70984 69034 47651 078 x 10^{39}	-1. 04678 09528 80914 92932 97202 597 x 10^{41}	-1. 16011 50478 78334 12209 56993 577 x 10^{41}
33	-2. 24481 12406 67547 79391 73805 946 x 10^{41}	-3. 89237 01919 74876 38441 55236 998 x 10^{42}	-4. 33725 58059 49575 09867 31546 774 x 10^{42}
34	-8. 43695 38955 83334 49409 59536 439 x 10^{42}	-1. 48484 64984 86378 34637 92912 871 x 10^{44}	-1. 66306 04740 10825 20485 42504 234 x 10^{44}
35	-3. 25353 84079 78630 75435 72353 408 x 10^{44}	-5. 80778 97647 62745 32334 30782 664 x 10^{45}	-6. 53646 37574 53146 48975 82917 538 x 10^{45}
36	-1. 28655 42403 03024 99411 24527 804 x 10^{46}	-2. 32789 27592 21978 16503 46432 946 x 10^{47}	-2. 63202 12722 45744 07511 67507 533 x 10^{47}
37	-5. 21374 94182 38823 50424 48239 120 x 10^{47}	-9. 55667 27556 83867 27111 41257 767 x 10^{48}	-1. 08523 75211 94378 82744 48132 443 x 10^{49}
38	-2. 16411 43365 49032 40103 03211 461 x 10^{49}	-4. 01623 40577 77871 93899 63445 474 x 10^{50}	-4. 57964 23345 86010 24148 98973 144 x 10^{50}
39	-9. 19572 63165 28012 99435 46621 835 x 10^{50}	-1. 72696 91957 80488 63154 53603 438 x 10^{52}	-1. 97700 10865 55540 07562 14630 475 x 10^{52}
40	-3. 99801 76984 58478 85839 30951 055 x 10^{52}	-7. 59444 06896 89895 50199 92081 660 x 10^{53}	-8. 72657 27525 64503 71852 92694 954 x 10^{53}
41	-1. 77763 30030 03953 13985 68352 041 x 10^{54}	-3. 41391 23547 10593 61242 09256 098 x 10^{55}	-3. 93685 37661 65573 34821 77509 223 x 10^{55}
42	-8. 07927 68518 20944 86792 92822 731 x 10^{55}	-1. 56805 46075 39565 68345 33212 958 x 10^{57}	-1. 81441 09847 33018 58730 45585 351 x 10^{57}
43	-3. 75178 66114 84874 93484 01114 947 x 10^{57}	-7. 35590 27477 51297 52543 24836 487 x 10^{58}	-8. 53928 15714 53621 25202 39539 069 x 10^{58}
44	-1. 77929 87191 74216 90990 68731 144 x 10^{59}	-3. 52287 37604 07422 17599 86641 306 x 10^{60}	-4. 10233 33480 91543 39763 79749 593 x 10^{60}
45	-8. 61433 48316 18318 76745 01538 475 x 10^{60}	-1. 72175 41174 38477 02490 31508 341 x 10^{62}	-2. 01092 15330 98022 79251 37733 026 x 10^{62}
46	-4. 25579 46361 88988 40652 73769 831 x 10^{62}	-8. 58402 18479 14235 85944 99103 971 x 10^{63}	-1. 00542 62179 42892 23922 90764 418 x 10^{64}
47	-2. 14464 78468 75634 72822 33920 275 x 10^{64}	-4. 36409 90995 97032 46814 62895 880 x 10^{65}	-5. 12552 10656 74151 60586 05945 406 x 10^{65}
48	-1. 10200 68188 84216 01455 22633 754 x 10^{66}	-2. 26165 57416 42607 33286 94221 006 x 10^{67}	-2. 66321 15861 13510 19355 32483 192 x 10^{67}
49	-5. 77175 57651 61523 65614 94220 444 x 10^{67}	-1. 19436 14723 88742 88435 17899 028 x 10^{69}	-1. 40995 51338 22096 70891 46864 535 x 10^{69}
50	-3. 08017 19432 47631 67846 14925 771 x 10^{69}	-6. 42505 42174 78515 31986 50090 213 x 10^{70}	-7. 60315 52960 37439 96066 53109 700 x 10^{70}
51	-1. 67432 05275 14734 41042 82490 310 x 10^{71}	-3. 51972 46750 67149 81233 74327 203 x 10^{72}	-4. 17477 40581 97506 34985 77375 030 x 10^{72}

$$\beta_2^{(N)} \sim -\frac{(N+4n_2+2m+1)!}{(n_2!)^2[(n_2+m)!]^2} \times \left[1+\frac{c^{(2)(1)}}{N+4n_2+2m+1} + \frac{c^{(2)(2)}}{(N+4n_2+2m+1)(N+4n_2+2m)}+\cdots\right]. \tag{229}$$

In Table IV, the fit between the numerical and asymptotic $\beta_2^{(N)}$'s is displayed for the same three states for orders 10–150 (by tens). The agreement is similar to that for the RSPT of the one-dimensional anharmonic oscillator:[24] for large N it is impressive.

The expansion (229) has some of the character of an asymptotic expansion in that at first the partial sums approach the exact result, but then as the number of terms increases the partial sums eventually diverge. The partial

TABLE IV. Accuracy of the asymptotic formula for $\beta_2^{(N)}$ to k terms,

$$\beta_2^{(N)} \sim -\frac{(N+4n_2+2m+1)!}{(n_2!)^2[(n_2+m)!]^2}\left[1+\frac{c^{[2](1)}}{N+4n_2+2m+1}+\frac{c^{[2](2)}}{(N+4n_2+2m+1)(N+4n_2+2m)}+\cdots+\frac{c^{[2](k)}}{(N+4n_2+2m+1)\cdots(N+4n_2+2m+2-k)}\right].$$

Boxed entries in the significant-figures columns are shown in bold.

N	$-\beta_2^{(N)}$(exact)[a]	$-\beta_2^{(N)}$(asympt. to $k=k_{best}$)[b]	k_{best}^{c}	k_{min}^{d}	Number of significant figures[e] in sum to k terms for k =										
					0	5	10	15	20	25	30	35	40	45	50
		Ground state: $n_2=0$, $m=0$													
10	1.80783 02000 00000 00000 00000 000 $\times 10^{7}$	1.81440 00000 00000 00000 00000 000 $\times 10^{7}$	1	3	0	**1**	0								
20	3.65163 71245 95240 29140 00000 000 $\times 10^{19}$	3.65181 12451 23148 80000 00000 000 $\times 10^{19}$	9	9	0	3	**3**	2							
30	6.64185 83025 05175 43644 14212 211 $\times 10^{33}$	6.64185 67341 40119 51127 36164 741 $\times 10^{33}$	15	14	0	4	5	**6**	5	3					
40	2.85870 36167 95211 42358 58706 384 $\times 10^{49}$	2.85870 36165 32667 95487 87068 898 $\times 10^{49}$	20	19	0	5	7	8	**10**	7	6	3			
50	1.36960 98468 21709 74345 22170 539 $\times 10^{66}$	1.36960 98468 21937 64957 80688 076 $\times 10^{66}$	25	25	0	5	8	10	10	**12**	10	9	7	4	
60	4.57887 70826 33415 42505 00263 865 $\times 10^{83}$	4.57887 70826 33417 88966 08031 516 $\times 10^{83}$	30	30	1	6	9	11	13	13	**15**	13	12	10	8
70	7.78904 18221 69343 93085 42809 826 $\times 10^{101}$	7.78904 16221 69343 93882 49608 962 $\times 10^{101}$	35	35	1	6	10	12	14	15	16	**18**	16	15	14
80	5.36929 57277 99859 95287 33544 732 $\times 10^{120}$	5.36929 57277 99859 95288 20414 138 $\times 10^{120}$	40	40	1	7	11	14	16	17	18	19	**20**	19	18
90	1.26315 59649 87504 79228 93873 012 $\times 10^{140}$	1.26315 59649 87504 79228 93902 279 $\times 10^{140}$	45	45	1	7	11	14	17	19	21	21	22	**23**	22
100	8.86769 22459 42392 25888 59953 573 $\times 10^{159}$	8.86769 22459 42392 25888 59953 849 $\times 10^{159}$	50	50	1	7	12	15	18	21	22	24	24	25	**26**
110	1.66792 36392 98188 02740 52859 789 $\times 10^{180}$	1.66792 36392 98188 02740 52859 790 $\times 10^{180}$	51	51	1	8	12	16	19	22	24	25	27	27	28
120	7.69396 26739 89238 59456 36348 094 $\times 10^{200}$	7.69396 26739 89238 59456 36348 094 $\times 10^{200}$	51	51	1	8	13	17	20	23	25	27	29	30	30
130	8.08449 83108 04571 30079 40173 389 $\times 10^{221}$	8.08449 83108 04571 30079 40173 390 $\times 10^{221}$	51	51	1	8	13	17	21	24	27	29	30	30	30
140	1.81755 22266 85751 87903 37981 498 $\times 10^{243}$	1.81755 22266 85751 87903 37981 498 $\times 10^{243}$	51	51	1	8	13	18	22	25	28	30	30	30	30
150	8.28512 52078 66554 03910 47333 007 $\times 10^{264}$	8.28512 52078 66554 03910 47333 008 $\times 10^{264}$	51	51	1	8	14	18	22	26	29	30	30	30	30
		Excited state: $n_2=1$, $m=0$													
10	3.23250 68706 00000 00000 00000 000 $\times 10^{10}$	-2.97380 16000 00000 00000 00000 000 $\times 10^{10}$	4	5	0	**1**	0								
20	2.37139 51306 64353 18768 28460 000 $\times 10^{24}$	2.37795 00505 17954 23232 00000 000 $\times 10^{24}$	5	6	0	**3**	1	0							
30	3.14920 34143 86974 19796 00692 752 $\times 10^{39}$	3.14930 03360 49735 04774 14300 210 $\times 10^{39}$	12	11	0	3	**3**	3	2	0					
40	4.98601 23372 61673 79697 98421 501 $\times 10^{55}$	4.98601 72147 12094 77815 03028 937 $\times 10^{55}$	18	17	0	3	4	5	**5**	4	3	0			
50	6.33916 49503 26059 31915 32049 022 $\times 10^{72}$	6.33916 49515 77497 21832 82665 459 $\times 10^{72}$	24	23	0	4	6	6	7	**8**	6	5	3	1	
60	4.63544 74996 34303 41334 53058 537 $\times 10^{90}$	4.63544 74997 58604 50158 08091 176 $\times 10^{90}$	29	28	0	5	7	8	9	9	**10**	9	8	6	4
70	1.51618 27058 20331 02030 62578 832 $\times 10^{109}$	1.51618 27058 20245 49131 12712 302 $\times 10^{109}$	35	34	0	5	7	9	10	11	12	**13**	12	11	9
80	1.83257 28247 25136 20913 17734 045 $\times 10^{128}$	1.83257 28247 25136 11398 45455 552 $\times 10^{128}$	40	39	0	5	8	10	12	13	14	14	**16**	14	13
90	7.05278 04064 63979 98969 48126 581 $\times 10^{147}$	7.05278 04064 63979 98983 94935 738 $\times 10^{147}$	45	44	0	6	9	11	13	15	16	17	17	**19**	17
100	7.67353 19779 42229 28064 17139 983 $\times 10^{167}$	7.67353 19779 42229 28064 35348 651 $\times 10^{167}$	50	49	0	6	9	12	14	16	18	19	19	20	**21**
110	2.14200 70197 90480 90232 50170 281 $\times 10^{188}$	2.14200 70197 90480 90232 50439 819 $\times 10^{188}$	51	51	0	6	10	13	15	17	19	20	21	22	22
120	1.41523 16756 71216 58447 27372 888 $\times 10^{209}$	1.41523 16756 71216 58447 27373 741 $\times 10^{209}$	51	51	0	7	10	13	16	18	20	22	23	24	25
130	2.06769 54720 42093 58405 38628 350 $\times 10^{230}$	2.06769 54720 42093 58405 38628 356 $\times 10^{230}$	51	51	0	7	10	14	17	19	22	24	25	26	27
140	6.30326 18392 06108 17159 58949 926 $\times 10^{251}$	6.30326 18392 06108 17159 58949 926 $\times 10^{251}$	51	51	0	7	11	14	18	20	23	25	27	28	29
150	3.81292 61315 81843 06671 95575 820 $\times 10^{273}$	3.81292 61315 81843 06671 95575 820 $\times 10^{273}$	51	51	0	7	11	15	18	21	24	26	28	30	30
		Excited state: $n_2=0$, $m=1$													
10	9.35031 68000 00000 00000 00000 000 $\times 10^{8}$	1.11767 04000 00000 00000 00000 000 $\times 10^{9}$	2	4	0	**1**	0								
20	1.07440 27756 35857 90894 08000 000 $\times 10^{22}$	1.07396 06557 43091 91680 00000 000 $\times 10^{22}$	8	7	0	2	**2**	1							
30	4.96521 64280 81112 14342 78197 278 $\times 10^{36}$	4.96520 42172 87689 89982 16581 626 $\times 10^{36}$	14	13	0	3	4	**4**	3	1					
40	3.99801 76984 58478 85839 30951 055 $\times 10^{52}$	3.99801 78619 07896 89409 93296 235 $\times 10^{52}$	19	19	0	4	5	6	**7**	6	4	2			
50	3.08017 19432 47631 67846 14925 771 $\times 10^{69}$	3.08017 19430 76802 71994 53898 548 $\times 10^{69}$	25	24	0	5	7	8	9	**10**	8	7	5	2	
60	1.51064 73927 65909 09148 07783 624 $\times 10^{87}$	1.51064 73927 65876 63319 01487 744 $\times 10^{87}$	30	29	0	5	8	9	11	11	**13**	11	10	8	6
70	3.54347 72322 61214 05011 24524 985 $\times 10^{105}$	3.54347 72322 61214 36283 70471 596 $\times 10^{105}$	35	34	0	6	8	11	12	13	14	**16**	14	13	12
80	3.22126 21010 05351 38105 57473 453 $\times 10^{124}$	3.22126 21010 05351 38207 78748 772 $\times 10^{124}$	40	39	0	6	9	12	14	15	16	17	**18**	17	16
90	9.66249 66725 03541 81258 59180 043 $\times 10^{143}$	9.66249 66725 03541 81259 28362 982 $\times 10^{143}$	45	44	0	6	10	13	15	17	18	19	19	**21**	19
100	8.42390 54522 94459 06273 21223 249 $\times 10^{163}$	8.42390 54522 94459 06273 21336 172 $\times 10^{163}$	50	50	0	7	10	13	16	18	20	21	22	22	**23**
110	1.92638 38811 73624 27229 46010 994 $\times 10^{184}$	1.92638 38811 73624 27229 46011 479 $\times 10^{184}$	51	51	0	7	11	14	17	19	21	23	24	25	25
120	1.06173 84185 01349 98205 76025 413 $\times 10^{205}$	1.06173 84185 01349 98205 76025 414 $\times 10^{205}$	51	51	0	7	11	15	18	21	23	25	26	27	27
130	1.31370 36327 74439 73620 80970 555 $\times 10^{226}$	1.31370 36327 74439 73620 80970 555 $\times 10^{226}$	51	51	0	7	12	15	19	22	24	26	28	29	30
140	3.43511 70363 70619 57753 36932 383 $\times 10^{247}$	3.43511 70363 70619 57753 36932 383 $\times 10^{247}$	51	51	0	7	12	16	19	22	25	27	29	30	30
150	1.80199 07698 85570 23304 01680 424 $\times 10^{269}$	1.80199 07698 85570 23304 01680 424 $\times 10^{269}$	51	51	0	8	12	16	20	23	26	29	30	30	30

TABLE IV. (*Continued*).

[a]Calculated by standard RSPT. Relative accuracy appears to be at least one part in 10^{29}.
[b]Calculated by the asymptotic formula, truncated at the value of k that gives a result closest to the exact value in the preceding column. This value of k is denoted by k_{best}.
[c]See b for definition of k_{best}. Generally, k_{best} increases with N. The "$k=51$" is not fundamentally significant in the sense that the maximum number of terms $c^{\{2\}(k)}$ available for this table was 51.
[d]The $k_{\min}$ is the value of k for which the term $c^{\{2\}(k)}/(N+4n_2+2m+1)\cdots(N+4n_2+2m+2-k)$ is smallest in magnitude, and which is a practical index for determining the truncation of the asymptotic formula.
[e]The number of significant figures in sum to k terms is operationally defined as the negative of the $\log_{10}$—truncated to an integer—of the magnitude of the relative error between the exact $\beta_2^{(N)}$ and the asymptotic formula. A box surrounds the entry on each line with the largest number of significant figures.

sum that comes closest to the exact result usually occurs when the last term is approximately the smallest. Compare the columns k_{best} and $k_{\min}$ in Table IV. The pattern of convergence followed by divergence is visible in the 11 rightmost columns of Table IV, in which are listed the approximate number of digits in the various partial sums that are the same as in the exact result. The best result is boxed.

The order at which the RSPT coefficients become asymptotic seems strongly dependent on n_2, more so than the corresponding n dependence for the anharmonic oscillator.[24] In particular, notice here that for the $(n_2=1, m=0)$ state, the best asymptotic value for $N=10$ does not even have the correct sign, while for the (0,0) and (0,1) states, for which n_2 is only 1 less, the errors in the best asymptotic values for the tenth-order coefficients are smaller than 2%. On the other hand, at the highest orders the accuracy obtained by using the asymptotic formula (229) is greater than the practical accuracy to which the RSPT calculation can be carried out.

IX. NUMERICAL CHARACTERIZATION OF THE β_1 SERIES

The asymptotics of the RSPT coefficients $\beta_1^{(N)}$ are more complicated than in the β_2 case because of the presence of small alternating-sign contributions, as in Eq. (197). First we list in Tables V–VIII the terms of the RSPT series, the induced exponentially small gap series $(\Delta\beta_1^{\{1\}})_{\text{ind}}$, and the induced doubly-exponentially-small imaginary series $(\Delta_i\beta_1^{\{2\}})_{\text{ind}}$, all through fifty-first order in $(2r)^{-1}$, for the ground state $(n_1=0, n_2=0, m=0)$ and for the three excited states for which n_1, n_2, and m are (1,0,0), (0,1,0), and (0,0,1). We use the notation $d^{\{1\}(N)}$ and $d^{\{2\}(N)}$ for the series coefficients for the two exponentially small quantities, according to

$$(\Delta\beta_1^{\{1\}})_{\text{ind}} = \mp 4\beta_1^{(0)} \frac{(2r)^{2\beta_2^{(0)}-1} e^{-r}}{n_2!(n_2+m)!} \times \sum_{N=0}^{\infty} d^{\{1\}(N)}(2r)^{-N}, \tag{230}$$

$$(\Delta_i\beta_1^{\{2\}})_{\text{ind}} = \pm \pi 4\beta_1^{(0)} \frac{(2r)^{4\beta_2^{(0)}-1} e^{-2r}}{[n_2!(n_2+m)!]^2} \times \sum_{N=0}^{\infty} d^{\{2\}(N)}(2r)^{-N} \quad (\pm \operatorname{Im} r \geq 0). \tag{231}$$

Notice that the coefficients (at least those with fewer than the maximum number of significant digits) appear to be integers, except in the (1,0,0) case for which multiplication of $d^{\{1\}(N)}$ and $d^{\{2\}(N)}$ by $4\beta_1^{(0)}$, which had been explicitly factored out in Eqs. (230) and (231) to make the leading coefficient of each power series equal to 1, is needed to restore the integer property of the coefficients. The coefficients are estimated to be accurate to the precision reported, with uncertainty only in the last digit. Notice that for the (0,1,0) state, only 27 digits have been reported for the coefficients $d^{\{1\}(N)}$ and $d^{\{2\}(N)}$, two fewer than the 29 reported for the other states. The lower accuracy comes from the lower accuracy of the $\Delta\beta_2$ quantities for $n_2=1$, as mentioned in Sec. VIII.

It is especially interesting to examine numerically the prediction of the asymptotics of the $\beta_1^{(N)}$ by the dispersion relation [Eqs. (196) and (197)], which in the notation of Eq. (231) becomes

$$\beta_1^{(N)} \sim 4\beta_1^{(0)} \frac{(N+4n_2+2m)!}{(n_2!)^2[(n_2+m)!]^2} \left[1 + \frac{d^{\{2\}(1)}}{N+4n_2+2m} + \frac{d^{\{2\}(2)}}{(N+4n_2+2m)(N+4n_2+2m-1)} + \cdots\right]$$
$$+ (-1)^{m+N-1} 16n^4 \frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(N-4n_2-2m-5)!$$
$$\times \left[1 + \frac{4n^2 - 12(\beta_2^{(0)})^2 + m^2 - 1 + 12n - 12\beta_2^{(0)}}{N-4n_2-2m-5} - \frac{4n^2[2\psi(N-4n_2-2m-5) - \psi(n_1+2n_2+2m+2) - \psi(n_1+2n_2+m+2)]}{N-4n_2-2m-5}\right.$$

TABLE V. Coefficients for the RSPT series, the induced $\Delta\beta_1^{[1]}$ series, and the induced $\Delta_i\beta_2^{[2]}$ series, as defined by Eqs. (24), (230), and (231) of the text, for the $(n_1=0, n_2=0, m=0)$ ground state of β_1.

Order N	Coefficient $\beta_1^{(N)}$	$d^{(1)(N)}$	$d^{(2)(N)}$
0	5.00000 00000 00000 00000 00000 000 x 10^{-1}	1.00000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}
1	-1.00000 00000 00000 00000 00000 000 x 10^{0}	-4.00000 00000 00000 00000 00000 000 x 10^{0}	-6.00000 00000 00000 00000 00000 000 x 10^{0}
2	3.00000 00000 00000 00000 00000 000 x 10^{0}	-1.30000 00000 00000 00000 00000 000 x 10^{1}	-8.00000 00000 00000 00000 00000 000 x 10^{0}
3	4.00000 00000 00000 00000 00000 000 x 10^{0}	2.40000 00000 00000 00000 00000 000 x 10^{1}	4.80000 00000 00000 00000 00000 000 x 10^{1}
4	-1.50000 00000 00000 00000 00000 000 x 10^{1}	7.80000 00000 00000 00000 00000 000 x 10^{1}	3.50000 00000 00000 00000 00000 000 x 10^{1}
5	2.00000 00000 00000 00000 00000 000 x 10^{1}	-2.41600 00000 00000 00000 00000 000 x 10^{3}	-2.80200 00000 00000 00000 00000 000 x 10^{3}
6	6.70000 00000 00000 00000 00000 000 x 10^{2}	-1.44210 00000 00000 00000 00000 000 x 10^{4}	-1.24280 00000 00000 00000 00000 000 x 10^{4}
7	2.08800 00000 00000 00000 00000 000 x 10^{3}	-6.96400 00000 00000 00000 00000 000 x 10^{4}	-6.46800 00000 00000 00000 00000 000 x 10^{4}
8	1.52370 00000 00000 00000 00000 000 x 10^{4}	-1.35187 40000 00000 00000 00000 000 x 10^{6}	-1.50376 60000 00000 00000 00000 000 x 10^{6}
9	2.69124 00000 00000 00000 00000 000 x 10^{5}	-1.78985 76000 00000 00000 00000 000 x 10^{7}	-1.92010 04000 00000 00000 00000 000 x 10^{7}
10	2.88203 40000 00000 00000 00000 000 x 10^{6}	-2.12840 24600 00000 00000 00000 000 x 10^{8}	-2.30908 57600 00000 00000 00000 000 x 10^{8}
11	3.29663 60000 00000 00000 00000 000 x 10^{7}	-3.01974 30720 00000 00000 00000 000 x 10^{9}	-3.36538 88000 00000 00000 00000 000 x 10^{9}
12	4.47459 56200 00000 00000 00000 000 x 10^{8}	-4.54483 26068 00000 00000 00000 000 x 10^{10}	-5.12049 92481 00000 00000 00000 000 x 10^{10}
13	6.32327 70640 00000 00000 00000 000 x 10^{9}	-7.09487 44979 20000 00000 00000 000 x 10^{11}	-8.07869 01361 00000 00000 00000 000 x 10^{11}
14	9.41615 84444 00000 00000 00000 000 x 10^{10}	-1.17305 06423 68100 00000 00000 000 x 10^{13}	-1.35028 57256 35600 00000 00000 000 x 10^{13}
15	1.49465 94569 76000 00000 00000 000 x 10^{12}	-2.04480 29691 93520 00000 00000 000 x 10^{14}	-2.37556 62095 05200 00000 00000 000 x 10^{14}
16	2.50896 21727 14900 00000 00000 000 x 10^{13}	-3.74331 40151 12722 00000 00000 000 x 10^{15}	-4.38467 93150 69466 00000 00000 000 x 10^{15}
17	4.44107 76959 07560 00000 00000 000 x 10^{14}	-7.19022 18098 94692 80000 00000 000 x 10^{16}	-8.48500 32208 31374 80000 00000 000 x 10^{16}
18	8.27630 22888 56874 00000 00000 000 x 10^{15}	-1.44695 39118 25111 86600 00000 000 x 10^{18}	-1.71897 91414 53706 41600 00000 000 x 10^{18}
19	1.62043 42820 08490 16000 00000 000 x 10^{17}	-3.04574 24704 37673 96480 00000 000 x 10^{19}	-3.64027 70588 19622 76800 00000 000 x 10^{19}
20	3.32665 42683 11276 86200 00000 000 x 10^{18}	-6.69600 56582 50457 56508 00000 000 x 10^{20}	-8.04706 76187 70086 51282 00000 000 x 10^{20}
21	7.14803 50018 55492 32880 00000 000 x 10^{19}	-1.53530 78046 69211 58653 44000 000 x 10^{22}	-1.85431 01328 54897 47353 80000 000 x 10^{22}
22	1.60477 13847 23674 76739 60000 000 x 10^{21}	-3.66628 58198 97639 97890 61000 000 x 10^{23}	-4.44824 07790 72045 28938 58400 000 x 10^{23}
23	3.75822 42734 76225 74061 28000 000 x 10^{22}	-9.10589 61922 53374 11879 54080 000 x 10^{24}	-1.10941 02254 27301 64289 46896 000 x 10^{25}
24	9.16687 40607 24638 96645 79400 000 x 10^{23}	-2.34923 05463 98923 88120 44786 000 x 10^{26}	-2.87312 29928 32114 21853 87076 400 x 10^{26}
25	2.32541 05776 70704 11091 43656 000 x 10^{25}	-6.28779 53475 23274 79711 73328 960 x 10^{27}	-7.71710 75070 86905 96202 39138 160 x 10^{27}
26	6.12658 95311 81374 81240 87256 400 x 10^{26}	-1.74394 00617 97450 20708 54868 574 x 10^{29}	-2.14732 66220 20407 06871 05123 738 x 10^{29}
27	1.67424 38963 83292 13100 20687 472 x 10^{28}	-5.00654 90356 19520 14511 37306 079 x 10^{30}	-6.18316 65965 47777 29663 63569 926 x 10^{30}
28	4.73988 78827 63629 42618 53595 122 x 10^{29}	-1.48613 62899 68605 85578 94408 670 x 10^{32}	-1.84053 19599 33359 41159 96180 297 x 10^{32}
29	1.38857 46039 83325 69450 67309 963 x 10^{31}	-4.55672 98159 02719 24283 57532 163 x 10^{33}	-5.65804 24291 63796 53078 73498 596 x 10^{33}
30	4.20484 95981 43437 52856 90821 189 x 10^{32}	-1.44180 81565 73968 70724 02003 666 x 10^{35}	-1.79462 10504 91853 93537 76137 803 x 10^{35}
31	1.31482 83626 14689 16879 39208 591 x 10^{34}	-4.70355 49835 76415 28224 07054 869 x 10^{36}	-5.86780 11770 06854 85250 09353 278 x 10^{36}
32	4.24136 03481 22180 14997 27011 495 x 10^{35}	-1.58065 01348 46874 87815 29386 805 x 10^{38}	-1.97608 96485 24209 62107 26071 045 x 10^{38}
33	1.41014 46206 91339 49621 17275 387 x 10^{37}	-5.46739 04626 04654 62131 21114 989 x 10^{39}	-6.84882 80023 28656 58282 40344 683 x 10^{39}
34	4.82802 38503 08125 29553 31706 145 x 10^{38}	-1.94501 04865 38007 62705 89026 561 x 10^{41}	-2.44102 29561 68495 33074 11857 879 x 10^{41}
35	1.70085 93393 95120 27806 01785 581 x 10^{40}	-7.11114 88069 46235 45580 81940 492 x 10^{42}	-8.94038 83980 72800 63585 02213 994 x 10^{42}
36	6.16061 45090 62291 67417 63524 285 x 10^{41}	-2.67010 49290 24547 30646 82501 896 x 10^{44}	-3.36254 79378 11179 82704 72966 162 x 10^{44}
37	2.29254 43917 84602 54356 91615 649 x 10^{43}	-1.02895 47233 99288 02882 42885 648 x 10^{46}	-1.29783 76181 84014 23550 13409 900 x 10^{46}
38	8.75883 13712 37131 11125 90672 419 x 10^{44}	-4.06692 79816 39936 66719 31097 761 x 10^{47}	-5.13733 64427 31482 44532 59877 707 x 10^{47}
39	3.43337 61289 94263 40892 50487 074 x 10^{46}	-1.64768 45572 54938 84277 56459 764 x 10^{49}	-2.08429 60111 77635 95585 28134 552 x 10^{49}
40	1.37996 71455 77679 10787 76135 778 x 10^{48}	-6.83859 07906 54300 79662 87561 655 x 10^{50}	-8.66232 76799 88636 03867 60700 370 x 10^{50}
41	5.68364 56777 76939 56715 93198 012 x 10^{49}	-2.90604 57004 74733 80153 60140 153 x 10^{52}	-3.68573 65915 36765 44188 24983 761 x 10^{52}
42	2.39743 27759 27379 99597 60225 684 x 10^{51}	-1.26371 98945 70728 36639 32144 929 x 10^{54}	-1.60472 18947 32593 53788 29146 432 x 10^{54}
43	1.03511 60128 81049 75473 64800 434 x 10^{53}	-5.62070 16397 30529 07839 69701 964 x 10^{55}	-7.14565 00217 41842 95198 37721 847 x 10^{55}
44	4.57221 74033 53607 00487 72182 285 x 10^{54}	-2.55570 06965 13417 47071 75188 468 x 10^{57}	-3.25267 21114 85612 13205 48935 330 x 10^{57}
45	2.06510 55699 12521 40804 36906 726 x 10^{56}	-1.18742 45487 22635 93155 27883 184 x 10^{59}	-1.51284 28667 38801 32058 17295 744 x 10^{59}
46	9.53293 04351 29736 97591 97094 776 x 10^{57}	-5.63487 11230 95230 98226 15587 151 x 10^{60}	-7.18636 22223 28394 26339 10695 832 x 10^{60}
47	4.49551 59480 84994 45992 12875 709 x 10^{59}	-2.72996 27008 91040 66955 52909 076 x 10^{62}	-3.48497 99601 97580 60174 00095 153 x 10^{62}
48	2.16475 98108 65986 41705 01864 034 x 10^{61}	-1.34972 28597 45531 09158 35676 142 x 10^{64}	-1.72460 22071 31291 37859 01445 327 x 10^{64}
49	1.06397 86918 94291 98777 54647 453 x 10^{63}	-6.80729 73896 42091 66017 06788 314 x 10^{65}	-8.70569 08740 69746 26721 82341 450 x 10^{65}
50	5.33546 42871 48682 10315 34475 375 x 10^{64}	-3.50090 95278 72955 47800 21045 029 x 10^{67}	-4.48103 14973 89817 73962 23980 551 x 10^{67}
51	2.72871 13571 54325 27727 07900 166 x 10^{66}	-1.83528 22801 78086 38938 40031 805 x 10^{69}	-2.35100 70046 58677 98591 85924 876 x 10^{69}

$$+\frac{A(n_1,n_2,m)+8\pi^2 n^4/3+B(n_1,n_2,m)[\psi(N-4n_2-2m-6)-\psi(1)]}{(N-4n_2-2m-5)(N-4n_2-2m-6)}$$

$$+\,32n^4\frac{[\psi(N-4n_2-2m-6)-\psi(1)]^2+[\psi^{(1)}(N-4n_2-2m-6)-\psi^{(1)}(1)]}{(N-4n_2-2m-5)(N-4n_2-2m-6)}+O(N^{-3}(\ln N)^3)\Bigg] , \qquad (232)$$

TABLE VI. Coefficients for the RSPT series, the induced $\Delta\beta_1^{[1]}$ series, and the induced $\Delta_i\beta_1^{[2]}$ series, as defined by Eqs. (24), (230), and (231) of the text, for the $(n_1=1, n_2=0, m=0)$ excited state of β_1.

Order N	$\beta_1^{(N)}$	Coefficient $d^{(1)(N)}$	$d^{(2)(N)}$
0	1. 50000 00000 00000 00000 00000 000 x 10^{0}	1. 00000 00000 00000 00000 00000 000 x 10^{0}	1. 00000 00000 00000 00000 00000 000 x 10^{0}
1	-7. 00000 00000 00000 00000 00000 000 x 10^{0}	-6. 66666 66666 66666 66666 66666 667 x 10^{0}	-8. 66666 66666 66666 66666 66666 667 x 10^{0}
2	4. 10000 00000 00000 00000 00000 000 x 10^{1}	-3. 16666 66666 66666 66666 66666 667 x 10^{1}	-2. 13333 33333 33333 33333 33333 333 x 10^{1}
3	-4. 40000 00000 00000 00000 00000 000 x 10^{1}	4. 93333 33333 33333 33333 33333 333 x 10^{2}	5. 62666 66666 66666 66666 66666 667 x 10^{2}
4	-1. 19300 00000 00000 00000 00000 000 x 10^{3}	1. 15000 00000 00000 00000 00000 000 x 10^{3}	2. 61666 66666 66666 66666 66666 667 x 10^{2}
5	6. 11600 00000 00000 00000 00000 000 x 10^{3}	-6. 23973 33333 33333 33333 33333 333 x 10^{4}	-6. 58340 00000 00000 00000 00000 000 x 10^{4}
6	7. 05620 00000 00000 00000 00000 000 x 10^{4}	1. 16248 33333 33333 33333 33333 333 x 10^{5}	2. 31964 00000 00000 00000 00000 000 x 10^{5}
7	-8. 29368 00000 00000 00000 00000 000 x 10^{5}	7. 72722 13333 33333 33333 33333 333 x 10^{6}	7. 62324 26666 66666 66666 66666 667 x 10^{6}
8	-3. 41667 70000 00000 00000 00000 000 x 10^{6}	-6. 18475 22000 00000 00000 00000 000 x 10^{7}	-7. 72888 00666 66666 66666 66666 667 x 10^{7}
9	1. 13068 88400 00000 00000 00000 000 x 10^{8}	-8. 42283 16000 00000 00000 00000 000 x 10^{8}	-7. 43142 97733 33333 33333 33333 333 x 10^{8}
10	-1. 79195 28200 00000 00000 00000 000 x 10^{8}	1. 46442 37396 66666 66666 66666 667 x 10^{10}	1. 63754 50149 33333 33333 33333 333 x 10^{10}
11	-1. 34513 82472 00000 00000 00000 000 x 10^{10}	3. 43071 41936 00000 00000 00000 000 x 10^{10}	7. 18175 56746 66666 66666 66666 667 x 10^{9}
12	1. 09344 37922 20000 00000 00000 000 x 10^{11}	-2. 73967 41295 98666 66666 66666 667 x 10^{12}	-2. 84917 31128 25000 00000 00000 000 x 10^{12}
13	1. 21222 07307 28000 00000 00000 000 x 10^{12}	1. 27609 49047 87733 33333 33333 333 x 10^{13}	1. 78532 34072 04600 00000 00000 000 x 10^{13}
14	-2. 34834 55342 78000 00000 00000 000 x 10^{13}	3. 50924 53122 81990 00000 00000 000 x 10^{14}	3. 29713 35833 86813 33333 33333 333 x 10^{14}
15	-6. 64147 48099 68000 00000 00000 000 x 10^{12}	-5. 21041 31435 67269 33333 33333 333 x 10^{15}	-5. 96872 95618 82021 33333 33333 333 x 10^{15}
16	3. 68198 03876 95443 00000 00000 000 x 10^{15}	-2. 53405 07211 42271 66666 66666 667 x 10^{16}	-1. 68740 75926 99814 86666 66666 667 x 10^{16}
17	-2. 42694 33864 25159 60000 00000 000 x 10^{16}	9. 88591 33706 46110 80000 00000 000 x 10^{17}	1. 03249 05058 03139 08400 00000 000 x 10^{18}
18	-3. 40561 99793 92368 74000 00000 000 x 10^{17}	-5. 91101 62495 79187 25800 00000 000 x 10^{18}	-8. 12990 29387 30036 64000 00000 000 x 10^{18}
19	7. 09501 97360 50132 44000 00000 000 x 10^{18}	-1. 66998 41800 96913 91504 00000 000 x 10^{20}	-1. 65251 97880 79554 23269 33333 333 x 10^{20}
20	1. 16915 00241 71507 44340 00000 000 x 10^{19}	1. 41744 91463 50752 99518 26666 667 x 10^{21}	1. 58760 39756 82137 42742 20000 000 x 10^{21}
21	-8. 81265 96450 72444 92872 00000 000 x 10^{20}	-5. 56501 87521 77884 73026 66666 666 x 10^{21}	-1. 18582 44364 69751 65837 48000 000 x 10^{22}
22	1. 20751 60057 96617 85615 00000 000 x 10^{22}	-7. 16663 11501 81188 25418 28466 667 x 10^{23}	-8. 03525 14474 24689 17412 33866 667 x 10^{23}
23	1. 97949 89310 65092 63420 91200 000 x 10^{23}	-5. 78042 75533 53166 32533 79840 000 x 10^{24}	-6. 74806 16793 35118 93178 77333 333 x 10^{24}
24	3. 26013 25212 39662 02953 56599 999 x 10^{23}	-1. 54293 83915 45296 33570 65315 067 x 10^{26}	-2. 03365 30320 00410 56577 75020 933 x 10^{26}
25	6. 15097 96937 35826 99326 82760 000 x 10^{25}	-6. 28071 67981 19877 21247 12644 960 x 10^{27}	-7. 64122 21966 67400 09200 60580 293 x 10^{27}
26	1. 92118 08535 14465 11744 90460 920 x 10^{27}	-1. 55442 04421 44982 18418 25633 240 x 10^{29}	-1. 89718 52844 56940 23490 18679 820 x 10^{29}
27	4. 15473 29342 15424 88507 72395 568 x 10^{28}	-4. 28157 92804 15504 43335 75287 735 x 10^{30}	-5. 32122 19424 87547 24371 08386 214 x 10^{30}
28	1. 22975 30198 68885 90077 25825 155 x 10^{30}	-1. 32939 23829 17679 54615 36481 879 x 10^{32}	-1. 64832 21478 16887 52799 75278 894 x 10^{32}
29	3. 76389 92476 17554 97550 20396 163 x 10^{31}	-4. 08341 21033 98877 37883 71430 426 x 10^{33}	-5. 06825 60499 48340 72030 31922 927 x 10^{33}
30	1. 12470 40077 84147 09191 26189 480 x 10^{33}	-1. 28888 58471 97819 83522 99974 850 x 10^{35}	-1. 60565 88891 13306 34501 41482 892 x 10^{35}
31	3. 52426 22803 36178 07278 53762 966 x 10^{34}	-4. 22967 71850 19734 28452 66515 917 x 10^{36}	-5. 28036 47481 68471 56190 98295 781 x 10^{36}
32	1. 14509 25465 07593 34240 09922 211 x 10^{36}	-1. 42715 05169 04092 29520 13118 295 x 10^{38}	-1. 78503 74027 81790 89105 75054 942 x 10^{38}
33	3. 81870 52287 55575 04208 17372 653 x 10^{37}	-4. 95079 02261 69961 98770 02705 393 x 10^{39}	-6. 20479 76531 90347 86246 40312 857 x 10^{39}
34	1. 31138 31610 02830 25514 44561 739 x 10^{39}	-1. 76685 55955 97570 54904 12681 767 x 10^{41}	-2. 21848 93047 47486 84579 77978 139 x 10^{41}
35	4. 63527 95548 81703 42107 57979 025 x 10^{40}	-6. 47936 62869 79387 92773 32935 212 x 10^{42}	-8. 14960 30888 19988 79134 49715 844 x 10^{42}
36	1. 68397 18149 95061 54938 41790 695 x 10^{42}	-2. 43968 53680 85297 45434 43318 711 x 10^{44}	-3. 07361 22533 12747 37997 19045 305 x 10^{44}
37	6. 28413 68274 68655 29873 69117 033 x 10^{43}	-9. 42659 54737 00890 76943 68986 191 x 10^{45}	-1. 18944 11294 93893 42292 68364 024 x 10^{46}
38	2. 40732 62624 95121 58317 30959 517 x 10^{45}	-3. 73524 32862 92268 32303 64578 464 x 10^{47}	-4. 72001 88009 45974 02065 18571 093 x 10^{47}
39	9. 46037 67189 73453 98270 12646 060 x 10^{46}	-1. 51692 02235 85775 30525 33352 513 x 10^{49}	-1. 91951 59080 15736 62417 05578 442 x 10^{49}
40	3. 81149 49519 09701 02495 76615 853 x 10^{48}	-6. 31013 44694 47637 47524 37046 491 x 10^{50}	-7. 99542 40832 01651 23761 28846 358 x 10^{50}
41	1. 57340 44239 91749 11825 05650 717 x 10^{50}	-2. 68725 67307 04044 83977 64280 558 x 10^{52}	-3. 40924 20085 10290 08938 00650 007 x 10^{52}
42	6. 65115 23979 40872 72589 32947 434 x 10^{51}	-1. 17097 17122 10135 02095 14213 719 x 10^{54}	-1. 48735 55373 75308 07083 86056 362 x 10^{54}
43	2. 87760 16315 26658 55137 53854 547 x 10^{53}	-5. 21834 33559 83625 90180 83838 383 x 10^{55}	-6. 63584 86522 20168 59775 35831 723 x 10^{55}
44	1. 27355 17426 99160 79925 99461 395 x 10^{55}	-2. 37716 19273 03823 97663 68418 574 x 10^{57}	-3. 02618 45821 84015 35826 92686 848 x 10^{57}
45	5. 76288 84684 97828 21323 99269 039 x 10^{56}	-1. 10643 14593 67734 27399 83948 857 x 10^{59}	-1. 40997 97023 30513 80341 05193 571 x 10^{59}
46	2. 66498 66877 42796 23929 86432 775 x 10^{58}	-5. 25941 35460 63484 80773 24744 773 x 10^{60}	-6. 70899 76276 90323 31483 78517 771 x 10^{60}
47	1. 25887 91199 86255 29617 78445 987 x 10^{60}	-2. 55218 69946 65667 82546 43291 314 x 10^{62}	-3. 25871 43206 69375 06791 54046 356 x 10^{62}
48	6. 07179 59383 97913 80942 15037 690 x 10^{61}	-1. 26378 20620 84775 64357 76979 738 x 10^{64}	-1. 61511 01709 81924 00820 30224 571 x 10^{64}
49	2. 98890 97959 38819 27707 38732 468 x 10^{63}	-6. 38330 46488 82303 07864 73303 599 x 10^{65}	-8. 16498 57475 89338 04235 55360 497 x 10^{65}
50	1. 50105 14192 52281 88217 50777 945 x 10^{65}	-3. 28751 66731 79286 06794 79285 017 x 10^{67}	-4. 20864 64045 76984 29032 05797 188 x 10^{67}
51	7. 68771 90349 10869 47644 32034 197 x 10^{66}	-1. 72576 20869 67645 27532 23739 782 x 10^{69}	-2. 21108 59288 93518 33482 72601 500 x 10^{69}

where the coefficients $A(n_1,n_2,m)$ and $B(n_1,n_2,m)$, which are independent of N, are given for the first few states in Table IX. The $\psi^{(1)}(z)$ denotes the digamma function,

$$\psi^{(1)}(z)=d\psi(z)/dz=d^2[\ln\Gamma(z)]/dz^2 . \tag{233}$$

In Table X we uncover numerically the alternating-sign contributions to the asymptotics by subtracting the terms in Eq. (233) that come from $(\Delta_i\beta_1^{[2]})_{\text{ind}}$ (those involving the coefficients $d^{(2)(k)}$). We truncate the partial sum after including the smallest term. Listed in Table X are the exact $\beta_1^{(N)}$, the k index of the last correction term included in the partial sum and the value of that term, the difference between the exact and asymptotic values—divided by

TABLE VII. Coefficients for the RSPT series, the induced $\Delta\beta_1^{(1)}$ series, and the induced $\Delta_t\beta_1^{(2)}$ series, as defined by Eqs. (24), (230), and (231) of the text, for the $(n_1=0, n_2=1, m=0)$ excited state of β_1.

Order	Coefficient		
N	$\beta_1^{(N)}$	$d^{(1)(N)}$	$d^{(2)(N)}$
0	5.00000 00000 00000 00000 00000 000 $\times 10^{-1}$	1.00000 00000 00000 00000 00000 0 $\times 10^{0}$	1.00000 00000 00000 00000 00000 0 $\times 10^{0}$
1	-3.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-1.60000 00000 00000 00000 00000 0 $\times 10^{1}$	-3.00000 00000 00000 00000 00000 0 $\times 10^{1}$
2	7.00000 00000 00000 00000 00000 000 $\times 10^{0}$	-1.10000 00000 00000 00000 00000 0 $\times 10^{1}$	2.36000 00000 00000 00000 00000 0 $\times 10^{2}$
3	7.60000 00000 00000 00000 00000 000 $\times 10^{1}$	3.60000 00000 00000 00000 00000 0 $\times 10^{1}$	-2.72000 00000 00000 00000 00000 0 $\times 10^{2}$
4	4.73000 00000 00000 00000 00000 000 $\times 10^{2}$	1.85900 00000 00000 00000 00000 0 $\times 10^{3}$	1.15700 00000 00000 00000 00000 0 $\times 10^{3}$
5	2.20400 00000 00000 00000 00000 000 $\times 10^{3}$	-8.10400 00000 00000 00000 00000 0 $\times 10^{3}$	-3.33660 00000 00000 00000 00000 0 $\times 10^{4}$
6	2.45420 00000 00000 00000 00000 000 $\times 10^{4}$	-7.32858 00000 00000 00000 00000 0 $\times 10^{5}$	-6.07552 00000 00000 00000 00000 0 $\times 10^{5}$
7	5.88216 00000 00000 00000 00000 000 $\times 10^{5}$	-1.53358 16000 00000 00000 00000 0 $\times 10^{7}$	-6.43637 60000 00000 00000 00000 0 $\times 10^{6}$
8	1.15534 45000 00000 00000 00000 000 $\times 10^{7}$	-2.63817 19300 00000 00000 00000 0 $\times 10^{8}$	-9.46010 89000 00000 00000 00000 0 $\times 10^{7}$
9	1.99186 09200 00000 00000 00000 000 $\times 10^{8}$	-5.27898 58240 00000 00000 00000 0 $\times 10^{9}$	-2.57506 07700 00000 00000 00000 0 $\times 10^{9}$
10	3.58753 16660 00000 00000 00000 000 $\times 10^{9}$	-1.22518 92719 40000 00000 00000 0 $\times 10^{11}$	-6.94628 38292 00000 00000 00000 0 $\times 10^{10}$
11	7.12503 04712 00000 00000 00000 000 $\times 10^{10}$	-2.92458 45919 28000 00000 00000 0 $\times 10^{12}$	-1.69282 38371 52000 00000 00000 0 $\times 10^{12}$
12	1.50188 07901 86000 00000 00000 000 $\times 10^{12}$	-7.00612 38516 15800 00000 00000 0 $\times 10^{13}$	-4.10705 37222 23800 00000 00000 0 $\times 10^{13}$
13	3.27019 82442 13600 00000 00000 000 $\times 10^{13}$	-1.71634 61686 62416 00000 00000 0 $\times 10^{15}$	-1.03799 71906 87804 00000 00000 0 $\times 10^{15}$
14	7.35183 87955 93560 00000 00000 000 $\times 10^{14}$	-4.33566 00299 36582 80000 00000 0 $\times 10^{16}$	-2.71321 51854 76465 60000 00000 0 $\times 10^{16}$
15	1.71157 82914 66660 80000 00000 000 $\times 10^{16}$	-1.12642 04094 27557 07200 00000 0 $\times 10^{18}$	-7.25861 96252 52186 40000 00000 0 $\times 10^{17}$
16	4.12157 16112 31827 65000 00000 000 $\times 10^{17}$	-3.00212 07586 55063 15410 00000 0 $\times 10^{19}$	-1.98571 92375 00830 26130 00000 0 $\times 10^{19}$
17	1.02434 70197 19986 60600 00000 000 $\times 10^{19}$	-8.20472 28370 77264 74512 00000 0 $\times 10^{20}$	-5.56286 69144 26918 07690 00000 0 $\times 10^{20}$
18	2.62424 97627 20094 94538 00000 000 $\times 10^{20}$	-2.29954 72976 55993 55852 90000 0 $\times 10^{22}$	-1.59637 90374 37729 53291 32000 0 $\times 10^{22}$
19	6.92538 54395 74197 44311 20000 000 $\times 10^{21}$	-6.60875 46363 32434 31188 24800 0 $\times 10^{23}$	-4.69193 48278 39251 52204 56000 0 $\times 10^{23}$
20	1.88159 56375 04565 96826 75000 000 $\times 10^{23}$	-1.94730 33237 03558 56981 86066 0 $\times 10^{25}$	-1.41226 02958 55028 55237 24914 0 $\times 10^{25}$
21	5.26069 16904 99237 79536 28880 000 $\times 10^{24}$	-5.88228 08612 96398 90851 60596 8 $\times 10^{26}$	-4.35344 24560 09007 63297 15101 2 $\times 10^{26}$
22	1.51293 29457 82333 19589 77795 600 $\times 10^{26}$	-1.82150 55926 13047 33772 85523 0 $\times 10^{28}$	-1.37439 96748 17561 34582 60723 5 $\times 10^{28}$
23	4.47414 01342 76342 64495 53986 720 $\times 10^{27}$	-5.78177 82459 83323 41812 01689 1 $\times 10^{29}$	-4.44376 84615 76293 49221 30142 0 $\times 10^{29}$
24	1.36012 57090 58448 64003 87781 443 $\times 10^{29}$	-1.88107 21862 51768 19988 56712 4 $\times 10^{31}$	-1.47140 89405 83249 42865 26866 8 $\times 10^{31}$
25	4.24912 38126 88853 45787 73952 599 $\times 10^{30}$	-6.27220 10831 94372 87878 32447 5 $\times 10^{32}$	-4.98921 95028 83656 84990 51092 9 $\times 10^{32}$
26	1.36376 99128 75067 39407 01023 402 $\times 10^{32}$	-2.14313 97789 29072 87061 18873 4 $\times 10^{34}$	-1.73224 48305 62366 72198 85388 2 $\times 10^{34}$
27	4.49541 85682 10455 46472 63013 143 $\times 10^{33}$	-7.50290 31849 57311 71342 16249 3 $\times 10^{35}$	-6.15756 99731 63269 51537 61930 2 $\times 10^{35}$
28	1.52140 71592 38878 96045 67931 230 $\times 10^{35}$	-2.69076 14480 47055 87220 26024 5 $\times 10^{37}$	-2.24060 22086 96186 78737 78186 3 $\times 10^{37}$
29	5.28467 15512 36667 88595 75075 701 $\times 10^{36}$	-9.88310 79544 33969 04507 72181 1 $\times 10^{38}$	-8.34437 94041 44198 83888 04852 0 $\times 10^{38}$
30	1.88334 79843 92160 98539 04706 216 $\times 10^{38}$	-3.71687 22699 60920 88735 20085 7 $\times 10^{40}$	-3.17982 74915 14242 22242 27842 8 $\times 10^{40}$
31	6.88364 51840 29576 27236 56430 660 $\times 10^{39}$	-1.43090 21471 40646 68397 44812 4 $\times 10^{42}$	-1.23962 09173 29935 85986 91713 5 $\times 10^{42}$
32	2.57935 21900 02766 31409 31923 341 $\times 10^{41}$	-5.63720 30878 95206 87404 96219 8 $\times 10^{43}$	-4.94238 35747 05747 99400 68339 3 $\times 10^{43}$
33	9.90446 48234 20972 19338 80297 117 $\times 10^{42}$	-2.27198 06644 33492 85026 06632 1 $\times 10^{45}$	-2.01476 80336 03267 59953 27464 7 $\times 10^{45}$
34	3.89583 00598 59278 99861 66241 170 $\times 10^{44}$	-9.36467 56365 68936 33564 11383 7 $\times 10^{46}$	-8.39513 27726 98622 27360 48169 3 $\times 10^{46}$
35	1.56904 71125 19523 88830 98567 601 $\times 10^{46}$	-3.94624 22600 40202 03825 69350 8 $\times 10^{48}$	-3.57447 58295 46803 80449 80418 6 $\times 10^{48}$
36	6.46780 04383 22177 60983 23330 043 $\times 10^{47}$	-1.69953 68815 05508 44788 49297 2 $\times 10^{50}$	-1.55469 30023 77696 61790 98848 9 $\times 10^{50}$
37	2.72759 58567 26769 65576 05805 592 $\times 10^{49}$	-7.47798 70543 94860 03838 19688 5 $\times 10^{51}$	-6.90538 06752 21001 36018 40912 1 $\times 10^{51}$
38	1.17632 09503 68074 33933 05565 329 $\times 10^{51}$	-3.36044 69139 49031 58016 25038 4 $\times 10^{53}$	-3.13114 76417 84381 12689 93059 2 $\times 10^{53}$
39	5.18580 22925 69076 99152 89133 741 $\times 10^{52}$	-1.54176 77215 37580 87487 55089 8 $\times 10^{55}$	-1.44895 36974 60787 21752 55337 6 $\times 10^{55}$
40	2.33601 29632 88540 34686 03844 720 $\times 10^{54}$	-7.21943 04199 76172 71275 61786 6 $\times 10^{56}$	-6.84074 12754 02706 37451 18826 4 $\times 10^{56}$
41	1.07481 07355 18888 10286 39238 594 $\times 10^{56}$	-3.44907 93995 45493 55225 13672 0 $\times 10^{58}$	-3.29392 18626 44321 64684 19958 2 $\times 10^{58}$
42	5.04914 98739 45764 19114 11397 049 $\times 10^{57}$	-1.68064 52537 51663 22973 95316 2 $\times 10^{60}$	-1.61714 97003 01863 59069 86553 9 $\times 10^{60}$
43	2.42086 25611 74634 93479 28437 857 $\times 10^{59}$	-8.34988 16823 33922 62150 65013 9 $\times 10^{61}$	-8.09247 19511 97967 51152 59699 3 $\times 10^{61}$
44	1.18420 76673 22064 89336 55536 184 $\times 10^{61}$	-4.22841 41006 42764 41662 88191 1 $\times 10^{63}$	-4.12644 10065 18375 08391 53343 4 $\times 10^{63}$
45	5.90793 85637 45149 24753 04073 134 $\times 10^{62}$	-2.18188 58441 45653 68791 98808 3 $\times 10^{65}$	-2.14341 03255 98137 49274 17318 9 $\times 10^{65}$
46	3.00499 12592 94226 08574 01435 798 $\times 10^{64}$	-1.14686 22369 21255 27935 70489 3 $\times 10^{67}$	-1.13382 10736 83294 68910 78415 7 $\times 10^{67}$
47	1.55776 74229 43548 10705 53484 823 $\times 10^{66}$	-6.13883 06655 24239 74139 48667 7 $\times 10^{68}$	-6.10618 77092 76137 44056 96316 6 $\times 10^{68}$
48	8.22756 64307 51413 82854 65427 712 $\times 10^{67}$	-3.34525 15267 84437 60764 35124 6 $\times 10^{70}$	-3.34704 65424 72815 14960 39210 2 $\times 10^{70}$
49	4.42599 46484 79762 08813 37494 638 $\times 10^{69}$	-1.85531 33466 22017 11678 58337 7 $\times 10^{72}$	-1.86681 62659 81557 41120 72547 9 $\times 10^{72}$
50	2.42430 03916 44025 05264 53488 183 $\times 10^{71}$	-1.04696 18292 31769 77372 32974 1 $\times 10^{74}$	-1.05919 17211 63757 51686 52725 0 $\times 10^{74}$
51	1.35165 95277 13310 09839 94743 745 $\times 10^{73}$	-6.00969 28536 88763 00572 36191 0 $\times 10^{75}$	-6.11178 96856 09539 41313 76803 3 $\times 10^{75}$

the leading asymptotic term (called the relative asymptotic error in the table), and the relative asymptotic error after taking account of one, two, and three terms from the alternating-sign asymptotic formula. These quantities are listed for various orders, up to order 150.

Notice that for the ground state the residual remaining after subtraction of the same-sign terms is alternating in sign after order $N=32$, and that it has relative magnitude 10^{-10} at order 150—which is small compared to unity, but large compared with the corresponding relative residual for $\beta_2^{(N)}$, which at order 110 is already less than 10^{-30}. The first alternating-sign asymptotic contribution significantly overcompensates, but by the third alternating-sign contribution the relative error has dropped by a factor of 10^{-3} at $N=150$ (see Table X).

For the excited states, the threshold for alternation is

TABLE VIII. Coefficients for the RSPT series, the induced $\Delta\beta_1^{(1)}$ series, and the induced $\Delta_t\beta_1^{(2)}$ series, as defined by Eqs. (24), (230), and (231) of the text, for the $(n_1=0, n_2=0, m=1)$ excited state of β_1.

Order N	Coefficient $\beta_1^{(N)}$	$d^{(1)(N)}$	$d^{(2)(N)}$
0	1.00000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}
1	-6.00000 00000 00000 00000 00000 000 x 10^{0}	-9.00000 00000 00000 00000 00000 000 x 10^{0}	-1.50000 00000 00000 00000 00000 000 x 10^{1}
2	2.00000 00000 00000 00000 00000 000 x 10^{1}	-3.60000 00000 00000 00000 00000 000 x 10^{1}	1.40000 00000 00000 00000 00000 000 x 10^{1}
3	7.20000 00000 00000 00000 00000 000 x 10^{1}	1.68000 00000 00000 00000 00000 000 x 10^{2}	3.72000 00000 00000 00000 00000 000 x 10^{2}
4	-2.96000 00000 00000 00000 00000 000 x 10^{2}	2.88400 00000 00000 00000 00000 000 x 10^{3}	1.96800 00000 00000 00000 00000 000 x 10^{3}
5	-2.97600 00000 00000 00000 00000 000 x 10^{3}	-1.67160 00000 00000 00000 00000 000 x 10^{4}	-3.41520 00000 00000 00000 00000 000 x 10^{4}
6	2.46400 00000 00000 00000 00000 000 x 10^{4}	-4.65200 00000 00000 00000 00000 000 x 10^{5}	-3.87488 00000 00000 00000 00000 000 x 10^{5}
7	3.71712 00000 00000 00000 00000 000 x 10^{5}	-8.39280 00000 00000 00000 00000 000 x 10^{5}	1.66396 80000 00000 00000 00000 000 x 10^{6}
8	-2.25760 00000 00000 00000 00000 000 x 10^{5}	2.18013 12000 00000 00000 00000 000 x 10^{7}	2.41559 52000 00000 00000 00000 000 x 10^{7}
9	-1.27848 96000 00000 00000 00000 000 x 10^{7}	-4.17311 71200 00000 00000 00000 000 x 10^{8}	-6.01960 36800 00000 00000 00000 000 x 10^{8}
10	3.37753 98400 00000 00000 00000 000 x 10^{8}	-1.20459 12192 00000 00000 00000 000 x 10^{10}	-1.07949 72000 00000 00000 00000 000 x 10^{10}
11	6.29207 80800 00000 00000 00000 000 x 10^{9}	-1.11054 41817 60000 00000 00000 000 x 10^{11}	-6.17923 47840 00000 00000 00000 000 x 10^{10}
12	4.46035 53024 00000 00000 00000 000 x 10^{10}	-1.49466 42764 16000 00000 00000 000 x 10^{12}	-1.24621 59482 88000 00000 00000 000 x 10^{12}
13	7.15418 32089 60000 00000 00000 000 x 10^{11}	-4.48421 16789 69600 00000 00000 000 x 10^{13}	-4.45028 21904 00000 00000 00000 000 x 10^{13}
14	2.03911 95740 16000 00000 00000 000 x 10^{13}	-9.83228 35735 52640 00000 00000 000 x 10^{14}	-9.00756 33791 33440 00000 00000 000 x 10^{14}
15	3.91597 65915 64800 00000 00000 000 x 10^{14}	-1.85692 24673 25772 80000 00000 000 x 10^{16}	-1.67195 75006 63654 40000 00000 000 x 10^{16}
16	6.96322 20405 08928 00000 00000 000 x 10^{15}	-4.01464 36322 76270 08000 00000 000 x 10^{17}	-3.80769 86293 01468 16000 00000 000 x 10^{17}
17	1.46605 53194 98629 12000 00000 000 x 10^{17}	-9.46012 45723 67989 24800 00000 000 x 10^{18}	-9.17003 67331 94049 02400 00000 000 x 10^{18}
18	3.29272 11924 03306 49600 00000 000 x 10^{18}	-2.23320 58433 09975 36768 00000 000 x 10^{20}	-2.17689 35595 90026 08640 00000 000 x 10^{20}
19	7.40730 32159 32305 40800 00000 000 x 10^{19}	-5.40352 14885 93695 77267 20000 000 x 10^{21}	-5.33572 67800 95879 02668 80000 000 x 10^{21}
20	1.72561 16432 82305 15916 80000 000 x 10^{21}	-1.36437 79028 23278 43743 74400 000 x 10^{23}	-1.36710 90561 57953 16219 90400 000 x 10^{23}
21	4.20880 66125 03693 22352 64000 000 x 10^{22}	-3.56771 47632 05346 92466 89280 000 x 10^{24}	-3.61694 68087 31243 86955 67360 000 x 10^{24}
22	1.06438 80878 57307 70655 64160 000 x 10^{24}	-9.62363 70434 66291 72383 66208 000 x 10^{25}	-9.86029 61822 99713 08328 55840 000 x 10^{25}
23	2.78393 13703 71200 11050 02496 000 x 10^{25}	-2.68089 98759 50788 22605 89199 360 x 10^{27}	-2.77518 47502 25593 04511 45687 040 x 10^{27}
24	7.53852 00041 68339 87337 86316 800 x 10^{26}	-7.71195 72340 42472 84314 97265 152 x 10^{28}	-8.06032 89809 48260 83524 83905 536 x 10^{28}
25	2.11198 76904 88910 99508 67046 400 x 10^{28}	-2.28861 33721 35542 53994 10402 755 x 10^{30}	-2.41344 41537 00352 81655 60085 176 x 10^{30}
26	6.11464 65872 55323 40683 39523 584 x 10^{29}	-7.00170 66012 65845 26038 53523 976 x 10^{31}	-7.44555 57545 58028 51011 01329 211 x 10^{31}
27	1.82797 96604 62615 88022 55010 857 x 10^{31}	-2.20700 93799 04238 39769 51855 376 x 10^{33}	-2.36537 72213 61303 19132 05487 849 x 10^{33}
28	5.63852 03255 91947 05247 64528 640 x 10^{32}	-7.16299 43060 34201 28929 77653 586 x 10^{34}	-7.73360 48344 22401 45356 56815 643 x 10^{34}
29	1.79312 47384 82091 52262 65275 347 x 10^{34}	-2.39217 16874 59205 51969 91700 407 x 10^{36}	-2.60061 25445 47291 12371 87170 248 x 10^{36}
30	5.87451 48992 96768 23194 89954 723 x 10^{35}	-8.21525 55000 34653 27540 43155 874 x 10^{37}	-8.98920 26054 14045 09471 12333 781 x 10^{37}
31	1.98119 32373 63998 58121 55427 092 x 10^{37}	-2.89940 92932 46504 76441 02995 823 x 10^{39}	-3.19198 92003 63830 27048 95663 515 x 10^{39}
32	6.87325 20735 84420 35294 02226 527 x 10^{38}	-1.05097 34607 02630 44992 05085 627 x 10^{41}	-1.16370 61845 89977 27611 21056 789 x 10^{41}
33	2.45118 34082 97553 95324 88815 077 x 10^{40}	-3.91028 47723 82726 92217 39085 949 x 10^{42}	-4.35330 85697 95494 62054 68953 708 x 10^{42}
34	8.97998 82196 75969 55623 82117 975 x 10^{41}	-1.49247 59671 91028 47855 01526 589 x 10^{44}	-1.67012 29776 37649 12978 13267 411 x 10^{44}
35	3.37739 10182 51818 55680 08871 467 x 10^{43}	-5.84042 04860 89666 09999 73313 066 x 10^{45}	-6.56743 30633 07798 27704 63949 694 x 10^{45}
36	1.30323 41503 40617 71793 17227 595 x 10^{45}	-2.34197 33079 60815 58421 88893 972 x 10^{47}	-2.64565 52721 49439 17631 61585 426 x 10^{47}
37	5.15631 55948 30872 56299 21925 933 x 10^{46}	-9.61815 74995 36974 88794 25465 360 x 10^{48}	-1.09129 06998 01908 92295 09961 828 x 10^{49}
38	2.09065 82562 58745 50515 57167 087 x 10^{48}	-4.04345 64385 16972 65290 03940 175 x 10^{50}	-4.60684 37915 84883 54396 05309 551 x 10^{50}
39	8.68187 52142 23307 11183 62797 430 x 10^{49}	-1.73920 60891 88114 13144 90475 746 x 10^{52}	-1.98936 99758 47439 27652 31344 784 x 10^{52}
40	3.69063 26675 18006 00208 60429 351 x 10^{51}	-7.65033 79882 36403 00791 15754 417 x 10^{53}	-8.78368 46027 07649 53056 63673 097 x 10^{53}
41	1.60518 01749 19566 75006 47462 211 x 10^{53}	-3.43987 47287 25057 07624 64147 698 x 10^{55}	-3.96363 59968 50718 39338 07890 750 x 10^{55}
42	7.13953 55081 81224 56795 12009 987 x 10^{54}	-1.58032 05317 54483 47365 57341 989 x 10^{57}	-1.82717 40290 18809 47226 51926 710 x 10^{57}
43	3.24589 95781 17038 85425 61729 472 x 10^{56}	-7.41486 32510 73020 13385 05689 433 x 10^{58}	-8.60111 47974 09253 37993 68754 721 x 10^{58}
44	1.50772 70549 53703 73005 42506 269 x 10^{58}	-3.55171 28658 38617 24523 02337 713 x 10^{60}	-4.13279 53435 36142 71584 33200 534 x 10^{60}
45	7.15227 04422 62387 82302 78905 417 x 10^{59}	-1.73610 83866 30573 56724 54188 635 x 10^{62}	-2.02618 40080 46676 34647 15810 363 x 10^{62}
46	3.46351 27027 92517 52568 83207 133 x 10^{61}	-8.65672 46881 41991 49853 13887 812 x 10^{63}	-1.01320 38574 82571 76908 11616 640 x 10^{64}
47	1.71145 75733 99702 90564 51859 238 x 10^{63}	-4.40156 74704 32062 42241 23152 691 x 10^{65}	-5.16583 23267 77131 18550 99552 836 x 10^{65}
48	8.62627 34972 23210 78390 48989 304 x 10^{64}	-2.28130 19298 15868 74203 94559 384 x 10^{67}	-2.68446 06615 27810 01250 47682 301 x 10^{67}
49	4.43328 20579 38699 70577 93143 863 x 10^{66}	-1.20484 08918 78608 36066 66226 948 x 10^{69}	-1.42134 58961 00771 32425 47090 578 x 10^{69}
50	2.32228 57781 67440 81308 76905 700 x 10^{68}	-6.48191 04733 54002 05926 80356 188 x 10^{70}	-7.66524 46235 73762 00834 94081 407 x 10^{70}
51	1.23948 91484 14093 91664 14728 722 x 10^{70}	-3.55109 59039 00731 77995 57258 289 x 10^{72}	-4.20918 33669 92515 24030 37021 756 x 10^{72}

pushed higher to $N=38$ for (1,0,0), $N=67$ for (0,0,1), and $N=112$ for (0,1,0). For (1,0,0) the alternating-sign contribution is moderately larger than for the ground state—a consequence of the increased value of n_1. For (0,0,1) and (0,1,0), the alternating-sign contribution is significantly smaller, which is a consequence of the dependence on n_2 and m that bring it down from the same-sign contribution by a factor of N^{-8n_2-4m-5}. Thus, for (0,1,0) the alternating-sign contribution is $\sim -10^{-25}$ versus $\sim -10^{-10}$ for the ground state.

Comparison of Table X with Table IV reveals clearly that the $\beta_1^{(N)}$ becomes asymptotic much more slowly than the $\beta_2^{(N)}$.

TABLE IX. Coefficients $A(n_1,n_2,m)$, $B(n_1,n_2,m)$, $C(n_1,n_2,m)$, and $D(n_1,n_2,m)$ for the alternating-sign contributions to the asymptotics of $\beta_1^{(N)}$, as in Eq. (232), and to the asymptotics of $E^{(N)}$, as in Eq. (236).

n_1	n_2	m	$A(n_1,n_2,m)$	$B(n_1,n_2,m)$	$C(n_1,n_2,m)$	$D(n_1,n_2,m)$
0	0	0	83	-120	243	-184
1	0	0	2983	-2656	6179	-3680
0	1	0	7459/9	-4960/3	22039/9	-7264/3
0	0	1	2060	-6848/3	13492/3	-9536/3

X. NUMERICAL CHARACTERIZATION OF THE ENERGY SERIES

The asymptotics of the RSPT coefficients $E^{(N)}$ for the energy are similar to those for the $\beta_1^{(N)}$: again there is an alternating-sign contribution down several powers of N from the dominant same-sign contribution [cf. Eq. (199)]. First we list in Tables XI–XIV the terms of the RSPT series, the exponentially small gap series $\Delta E^{\{1\}}$, and the doubly-exponentially-small imaginary series $\Delta_i E^{\{2\}}$, all through fifty-first order in $(2R/n)^{-1}$, for the ground state $(n_1=n_2=m=0)$ and for the three $n=2$ excited states for which n_1, n_2, and m are (1,0,0), and (0,1,0) and (0,0,1). We use the notation $C^{\{1\}(N)}$ and $C^{\{2\}(N)}$ for the series coefficients for the two exponentially small quantities, according to [cf. Eqs. (176) and (179)]

$$\Delta E^{\{1\}}=\pm\frac{(2R/n)^{2\beta_2^{(0)}}e^{-R/n-n}}{n^3 n_2!(n_2+m)!}\sum_{N=0}^{\infty}C^{\{1\}(N)}(2R/n)^{-N}, \tag{234}$$

$$\Delta_i E^{\{2\}}=\mp\pi\frac{(2R/n)^{4\beta_2^{(0)}}e^{-2R/n-2n}}{n^3[n_2!(n_2+m)!]^2}\times\sum_{N=0}^{\infty}C^{\{2\}(N)}(2R/n)^{-N}\quad(\pm\mathrm{Im}R\geq 0)\,. \tag{235}$$

As for β_1 and β_2, the coefficients are estimated to be accurate to the precision reported [29 digits for $(n_1,n_2,m)=(0,0,0)$, (1,0,0), and (0,0,1), and 27 digits for (0,1,0)]. We call the reader's attention to the sign pattern, which settles down quickly to uniform minus signs for the ground state and two of the excited states, but which is quite irregular until after twenty-seventh order for the (1,0,0) state.

The asymptotics of the $E^{(N)}$ have two contributions, as did the $\beta_1^{(N)}$. In the notation of Eq. (235), Eq. (199) becomes

$$\begin{aligned}E^{(N)}\sim&-\frac{e^{-2n}(N+4n_2+2m+1)!}{n^3(n_2!)^2[(n_2+m)!]^2}\left[1+\frac{C^{\{2\}(1)}}{N+4n_2+2m+1}+\frac{C^{\{2\}(2)}}{(N+4n_2+2m+1)(N+4n_2+2m)}+\cdots\right]\\&+(-1)^{m+N-1}e^{2n}16n\frac{(n_1+2n_2+2m+1)!(n_1+2n_2+m+1)!}{n_1!(n_1+m)!}(N-4n_2-2m-5)!\\&\times\left[1+\frac{12n^2-12(\beta_2^{(0)})^2+m^2-1+12n-12\beta_2^{(0)}-4n\beta_2^{(0)}}{N-4n_2-2m-5}\right.\\&-\frac{4n^2[2\psi(N-4n_2-2m-5)-\psi(n_1+2n_2+2m+2)-\psi(n_1+2n_2+m+2)]}{N-4n_2-2m-5}\\&+\frac{C(n_1,n_2,m)+8\pi^2n^4/3+D(n_1,n_2,m)[\psi(N-4n_2-2m-6)-\psi(1)]}{(N-4n_2-2m-5)(N-4n_2-2m-6)}\\&\left.+32n^4\frac{[\psi(N-4n_2-2m-6)-\psi(1)]^2+[\psi^{(1)}(N-4n_2-2m-6)-\psi^{(1)}(1)]}{(N-4n_2-2m-5)(N-4n_2-2m-6)}+O(N^{-3}(\ln N)^3)\right],\end{aligned} \tag{236}$$

where the coefficients $C(n_1,n_2,m)$ and $D(n_1,n_2,m)$ are independent of N. The first few are listed in Table IX.

In Table XV we uncover numerically the alternating-sign contributions to the asymptotics by subtracting the terms in Eq. (236) that come from $\Delta_i E^{\{2\}}$ (those involving the coefficients $C^{\{2\}(k)}$). We truncate the partial sum after including the smallest term. Listed in Table XV are the exact $E^{(N)}$, the k index of the last correction term included in the partial sum and the value of that term, the difference between the exact and asymptotic values—

TABLE X. Asymptotic analysis of the RSPT $\beta_1^{(N)}$. The dominant, same-sign subseries in the asymptotic formula (232) of the text is truncated with the inclusion of the smallest term, whose index has been indicated by $k_{\min}$. The relative asymptotic error refers to the difference between the exact coefficient $\beta_1^{(N)}$ and the asymptotic formula to the indicated number of terms, divided by the leading asymptotic term, which is $(4n_1+2m+2)(N+4n_2+2m)!/(n_2!)^2[(n_2+m)!]^2$. For sufficiently large N, the relative asymptotic error, after accounting for the same-sign subseries, is alternating in sign. The effect of the alternating-sign subseries is seen through the inclusion of up to three terms.

		same-sign subseries			alternating-sign subseries		
					relative asymptotic error after inclusion of terms through order (in N^{-1})		
N	$\beta_1^{(N)}$(exact)	$k_{\min}$	smallest term	relative asymptotic error	0	1	2
Ground state: $n_1=0$, $n_2=0$, $m=0$							
30	4.20484 95981 43437 52856 90821 189 $\times 10^{32}$	14	1.1×10^{-6}	-3.6×10^{-7}	1.0×10^{-7}	-2.0×10^{-7}	-1.6×10^{-7}
31	1.31482 83626 14689 16879 39208 591 $\times 10^{34}$	14	5.8×10^{-7}	-2.1×10^{-7}	-6.1×10^{-7}	-3.6×10^{-7}	-3.9×10^{-7}
32	4.24136 03481 22180 14997 27011 495 $\times 10^{35}$	15	3.2×10^{-7}	-2.3×10^{-7}	1.0×10^{-7}	-1.0×10^{-7}	-7.1×10^{-8}
33	1.41014 46206 91339 49621 17275 387 $\times 10^{37}$	15	1.8×10^{-7}	7.0×10^{-9}	-2.7×10^{-7}	-1.0×10^{-7}	-1.3×10^{-7}
34	4.82802 38503 08125 29553 31706 145 $\times 10^{38}$	16	9.5×10^{-8}	-1.5×10^{-7}	9.4×10^{-8}	-5.0×10^{-8}	-2.8×10^{-8}
35	1.70085 93393 95120 27806 01785 581 $\times 10^{40}$	16	5.2×10^{-8}	6.3×10^{-8}	-1.4×10^{-7}	-2.1×10^{-8}	-4.0×10^{-8}
36	6.16061 45090 62291 67417 63524 285 $\times 10^{41}$	17	2.8×10^{-8}	-1.0×10^{-7}	7.7×10^{-8}	-2.6×10^{-8}	-9.8×10^{-9}
37	2.29254 43917 84602 54356 91615 649 $\times 10^{43}$	17	1.5×10^{-8}	6.7×10^{-8}	-8.6×10^{-8}	1.6×10^{-9}	-1.2×10^{-8}
38	8.75883 13712 37131 11125 90672 419 $\times 10^{44}$	18	8.0×10^{-9}	-7.4×10^{-8}	5.9×10^{-8}	-1.5×10^{-8}	-3.3×10^{-9}
39	3.43337 61289 94263 40892 50487 074 $\times 10^{46}$	18	4.3×10^{-9}	5.9×10^{-8}	-5.7×10^{-8}	6.5×10^{-9}	-3.6×10^{-9}
40	1.37996 71455 77679 10787 76135 778 $\times 10^{48}$	19	2.3×10^{-9}	-5.6×10^{-8}	4.5×10^{-8}	-9.7×10^{-9}	-1.0×10^{-9}
45	2.06510 55699 12521 40804 36906 726 $\times 10^{56}$	22	9.6×10^{-11}	3.1×10^{-8}	-2.3×10^{-8}	4.2×10^{-9}	-4.9×10^{-11}
60	1.49440 30280 94080 16957 06185 790 $\times 10^{82}$	29	5.6×10^{-15}	-7.9×10^{-9}	4.3×10^{-9}	-6.9×10^{-10}	2.9×10^{-11}
75	4.55831 63582 14424 59695 34188 535 $\times 10^{109}$	37	2.7×10^{-19}	2.7×10^{-9}	-1.2×10^{-9}	1.7×10^{-10}	-8.2×10^{-12}
90	2.77057 11141 95650 94203 64577 899 $\times 10^{138}$	44	1.2×10^{-23}	-1.1×10^{-9}	4.1×10^{-10}	-5.2×10^{-11}	2.6×10^{-12}
105	2.03771 32634 96922 30359 18117 521 $\times 10^{168}$	51	5.0×10^{-28}	5.2×10^{-10}	-1.7×10^{-10}	1.9×10^{-11}	-9.5×10^{-13}
120	1.27029 42073 70747 46762 41761 449 $\times 10^{199}$	51	6.0×10^{-32}	-2.7×10^{-10}	7.9×10^{-11}	-8.2×10^{-12}	3.9×10^{-13}
135	5.13952 02223 01706 16760 56611 113 $\times 10^{230}$	51	2.9×10^{-35}	1.5×10^{-10}	-4.0×10^{-11}	3.8×10^{-12}	-1.7×10^{-13}
150	1.09657 73249 78189 64805 40729 875 $\times 10^{263}$	51	3.8×10^{-38}	-9.1×10^{-11}	2.2×10^{-11}	-1.9×10^{-12}	8.4×10^{-14}
Excited state: $n_1=1$, $n_2=0$, $m=0$							
35	4.63527 95548 81703 42107 57979 025 $\times 10^{40}$	21	1.0×10^{-7}	6.0×10^{-6}	1.6×10^{-6}	8.7×10^{-6}	8.5×10^{-6}
36	1.68397 18149 95061 54938 41790 695 $\times 10^{42}$	21	4.2×10^{-8}	1.3×10^{-5}	1.7×10^{-5}	1.1×10^{-5}	1.1×10^{-5}
37	6.28413 68274 68655 29873 69117 033 $\times 10^{43}$	21	1.8×10^{-8}	-3.3×10^{-6}	-6.6×10^{-6}	-1.4×10^{-6}	-1.8×10^{-6}
38	2.40732 62624 95121 58317 30959 517 $\times 10^{45}$	21	8.1×10^{-9}	-8.9×10^{-7}	1.9×10^{-6}	-2.5×10^{-6}	-2.0×10^{-6}
39	9.46037 67189 73453 98270 12646 060 $\times 10^{46}$	21	3.7×10^{-9}	6.9×10^{-7}	-1.8×10^{-6}	2.1×10^{-6}	1.5×10^{-6}
40	3.81149 49519 09701 02495 76615 853 $\times 10^{48}$	21	1.8×10^{-9}	-1.7×10^{-7}	2.0×10^{-6}	-1.3×10^{-6}	-8.3×10^{-7}
41	1.57340 44239 91749 11825 05650 717 $\times 10^{50}$	21	8.6×10^{-10}	9.1×10^{-8}	-1.8×10^{-6}	1.1×10^{-6}	5.9×10^{-7}
42	6.65115 23979 40872 72589 32947 434 $\times 10^{51}$	21	4.3×10^{-10}	-1.2×10^{-7}	1.6×10^{-6}	-9.6×10^{-7}	-5.0×10^{-7}
43	2.87760 16315 26658 55137 53854 547 $\times 10^{53}$	21	2.2×10^{-10}	1.3×10^{-7}	-1.4×10^{-6}	8.4×10^{-7}	4.1×10^{-7}
44	1.27355 17426 99160 79925 99461 395 $\times 10^{55}$	21	1.2×10^{-10}	-1.2×10^{-7}	1.2×10^{-6}	-7.3×10^{-7}	-3.3×10^{-7}
45	5.76288 84684 97828 21323 99269 039 $\times 10^{56}$	21	6.2×10^{-11}	1.1×10^{-7}	-1.1×10^{-6}	6.4×10^{-7}	2.7×10^{-7}
60	4.25469 21649 34195 83172 33508 800 $\times 10^{82}$	29	5.0×10^{-15}	-4.7×10^{-8}	2.1×10^{-7}	-1.1×10^{-7}	-1.4×10^{-8}
75	1.31285 33314 91568 17177 38410 795 $\times 10^{110}$	37	2.5×10^{-19}	2.1×10^{-8}	-6.2×10^{-8}	2.8×10^{-8}	4.4×10^{-10}
90	8.03918 89765 54943 53588 04877 827 $\times 10^{138}$	44	1.1×10^{-23}	-1.0×10^{-8}	2.2×10^{-8}	-9.1×10^{-9}	3.4×10^{-10}
105	5.94338 14608 72294 73269 41028 217 $\times 10^{168}$	51	4.7×10^{-28}	5.3×10^{-9}	-9.4×10^{-9}	3.5×10^{-9}	-2.3×10^{-10}
120	3.71916 15533 21328 05918 28739 902 $\times 10^{199}$	51	5.7×10^{-32}	-3.0×10^{-9}	4.5×10^{-9}	-1.5×10^{-9}	1.2×10^{-10}
135	1.50912 32797 30865 49194 88339 840 $\times 10^{231}$	51	2.7×10^{-35}	1.8×10^{-9}	-2.3×10^{-9}	7.3×10^{-10}	-6.3×10^{-11}
150	3.22727 61757 73613 99640 39047 709 $\times 10^{263}$	51	3.6×10^{-38}	-1.1×10^{-9}	1.3×10^{-9}	-3.8×10^{-10}	3.4×10^{-11}
Excited state: $n_1=0$, $n_2=1$, $m=0$							
110	3.84066 68154 66344 53494 67272 941 $\times 10^{186}$	51	4.8×10^{-24}	-2.1×10^{-23}	-4.3×10^{-24}	-2.3×10^{-23}	-1.4×10^{-23}
111	4.42831 79529 24774 51625 18522 473 $\times 10^{188}$	51	2.7×10^{-24}	-5.2×10^{-24}	-2.0×10^{-23}	-3.5×10^{-24}	-1.2×10^{-23}
112	5.15003 51797 28241 91850 55330 994 $\times 10^{190}$	51	1.5×10^{-24}	-1.0×10^{-23}	3.4×10^{-24}	-1.1×10^{-23}	-4.3×10^{-24}
113	6.04072 59073 33858 38876 59420 723 $\times 10^{192}$	51	8.4×10^{-25}	1.8×10^{-25}	-1.2×10^{-23}	1.4×10^{-24}	-5.0×10^{-24}
114	7.14569 41846 99620 35747 03243 307 $\times 10^{194}$	51	4.8×10^{-25}	-5.4×10^{-24}	5.2×10^{-24}	-6.4×10^{-24}	-8.1×10^{-25}
115	8.52403 88989 87193 37750 23460 236 $\times 10^{196}$	51	2.7×10^{-25}	1.8×10^{-24}	-7.7×10^{-24}	2.6×10^{-24}	-2.3×10^{-24}
116	1.02532 59914 08535 71897 61735 152 $\times 10^{199}$	51	1.6×10^{-25}	-3.4×10^{-24}	5.0×10^{-24}	-4.1×10^{-24}	2.6×10^{-25}
117	1.24355 32652 55245 94115 13581 471 $\times 10^{201}$	51	9.0×10^{-26}	2.0×10^{-24}	-5.5×10^{-24}	2.5×10^{-24}	-1.3×10^{-24}
118	1.52062 98594 46173 47627 08109 775 $\times 10^{203}$	51	5.3×10^{-26}	-2.4×10^{-24}	4.3×10^{-24}	-2.8×10^{-24}	5.1×10^{-25}

TABLE X. (*Continued*).

		same-sign subseries			alternating-sign subseries		
					relative asymptotic error after inclusion of terms through order (in N^{-1})		
N	$\beta_1^{(N)}$(exact)	k_{min}	smallest term	relative asymptotic error	0	1	2
119	1. 87460 86416 42265 94460 30816 980 x 10^{205}	51	3.1×10^{-26}	1.8×10^{-24}	-4.2×10^{-24}	2.2×10^{-24}	-8.1×10^{-25}
120	2. 32968 62305 67245 00079 98391 415 x 10^{207}	51	1.8×10^{-26}	-1.9×10^{-24}	3.5×10^{-24}	-2.1×10^{-24}	5.0×10^{-25}
125	7. 77622 45330 15126 32981 58236 992 x 10^{217}	51	1.4×10^{-27}	1.1×10^{-24}	-2.1×10^{-24}	1.1×10^{-24}	-3.2×10^{-25}
130	3. 14585 46826 64292 16242 59039 798 x 10^{228}	51	1.2×10^{-28}	-6.6×10^{-25}	1.2×10^{-24}	-6.3×10^{-25}	1.7×10^{-25}
135	1. 53154 39326 78469 42414 90862 477 x 10^{239}	51	1.2×10^{-29}	4.2×10^{-25}	-7.2×10^{-25}	3.7×10^{-25}	-9.7×10^{-26}
140	8. 91417 76528 46513 18858 83709 809 x 10^{249}	51	1.3×10^{-30}	-2.7×10^{-25}	4.4×10^{-25}	-2.2×10^{-25}	5.6×10^{-26}
145	6. 16495 21436 76917 94321 95285 938 x 10^{260}	51	1.5×10^{-31}	1.7×10^{-25}	-2.7×10^{-25}	1.3×10^{-25}	-3.3×10^{-26}
150	5. 03716 89616 45249 73328 18252 223 x 10^{271}	51	2.0×10^{-32}	-1.1×10^{-25}	1.7×10^{-25}	-7.9×10^{-26}	2.0×10^{-26}
	Excited state: $n_1=0$, $n_2=0$, $m=1$						
65	1. 13885 00590 21654 30449 69843 011 x 10^{95}	31	3.3×10^{-14}	-4.2×10^{-14}	7.3×10^{-15}	-6.0×10^{-14}	-3.0×10^{-14}
66	7. 77531 43019 45827 29475 89791 639 x 10^{96}	32	1.7×10^{-14}	-1.0×10^{-15}	-4.4×10^{-14}	1.4×10^{-14}	-1.2×10^{-14}
67	5. 38584 79493 22852 74308 15564 229 x 10^{98}	32	9.4×10^{-15}	-1.7×10^{-14}	2.0×10^{-14}	-2.9×10^{-14}	-7.3×10^{-15}
68	3. 78430 66855 26025 29819 08827 997 x 10^{100}	33	5.0×10^{-15}	3.7×10^{-15}	-2.9×10^{-14}	1.4×10^{-14}	-4.9×10^{-15}
69	2. 69667 40945 68716 52063 62962 081 x 10^{102}	33	2.7×10^{-15}	-8.6×10^{-15}	2.0×10^{-14}	-1.7×10^{-14}	-9.4×10^{-15}
70	1. 94848 30612 01337 28345 91680 476 x 10^{104}	34	1.4×10^{-15}	4.3×10^{-15}	-2.1×10^{-14}	1.2×10^{-14}	-2.5×10^{-15}
71	1. 42728 01030 14265 96995 99307 339 x 10^{106}	34	7.6×10^{-16}	-5.5×10^{-15}	1.6×10^{-14}	-1.2×10^{-14}	6.5×10^{-16}
72	1. 05970 92346 33030 19251 82579 320 x 10^{108}	35	4.0×10^{-16}	3.9×10^{-15}	-1.5×10^{-14}	9.0×10^{-15}	-1.5×10^{-15}
73	7. 97355 05617 87022 18242 21594 741 x 10^{109}	35	2.2×10^{-16}	-4.0×10^{-15}	1.3×10^{-14}	-8.3×10^{-15}	9.0×10^{-16}
74	6. 07895 46016 11356 16506 76649 181 x 10^{111}	36	1.1×10^{-16}	3.3×10^{-15}	-1.2×10^{-14}	6.9×10^{-15}	-1.1×10^{-15}
75	4. 69509 80519 05535 03298 01084 668 x 10^{113}	36	6.1×10^{-17}	-3.1×10^{-15}	1.0×10^{-14}	-6.1×10^{-15}	8.2×10^{-16}
90	4. 17505 47693 53232 78059 13419 611 x 10^{142}	44	4.1×10^{-21}	7.0×10^{-16}	-1.7×10^{-15}	9.1×10^{-16}	-1.5×10^{-16}
105	4. 22596 42190 25580 41268 06350 781 x 10^{172}	51	2.4×10^{-25}	-2.0×10^{-16}	3.9×10^{-16}	-1.8×10^{-16}	3.1×10^{-17}
120	3. 46896 63375 28781 08724 93612 405 x 10^{203}	51	3.6×10^{-29}	6.5×10^{-17}	-1.1×10^{-16}	4.6×10^{-17}	-7.6×10^{-18}
135	1. 78742 61945 40356 87670 07584 213 x 10^{235}	51	2.0×10^{-32}	-2.4×10^{-17}	3.5×10^{-17}	-1.3×10^{-17}	2.2×10^{-18}
150	4. 73149 48064 78678 81088 48155 313 x 10^{267}	51	3.0×10^{-35}	1.0×10^{-17}	-1.3×10^{-17}	4.5×10^{-18}	-7.0×10^{-19}

divided by the leading asymptotic term (called the relative asymptotic error in the table), and the relative asymptotic error after taking account of one, two, and three terms from the alternating-sign asymptotic formula. These quantities are listed for various orders, up to order 150.

Notice that for the ground state the residual remaining after subtraction of the same-sign terms is alternating in sign after order $N=25$, and that it has relative magnitude 7×10^{-11} at order 150—which is small compared to unity, but large compared with the corresponding relative residual for $\beta_2^{(N)}$, which at order 110 is already less than 10^{-30}. The first alternating-sign asymptotic contribution significantly overcompensates, but by the third alternating-sign contribution the relative error has dropped by a factor of 10^{-4} at $N=150$ (see Table XV).

For the excited states, the threshold for alternation is pushed higher to $N=39$ for (1,0,0), $N=50$ for (0,0,1), and $N=93$ for (0,1,0). For (1,0,0) the alternating-sign contribution is significantly larger than for the ground state—a consequence of the increased value of n_1. For (0,0,1) and (0,1,0), the alternating-sign contribution is significantly smaller, which is a consequence of the dependence on n_2 and m that brings it down from the same-sign contribution by a factor of N^{-8n_2-4m-6}. Thus, for (0,1,0) the alternating-sign contribution is $\sim5\times10^{-24}$, versus $\sim7\times10^{-11}$ for the ground state.

Comparison of Table XV with Tables IV and X reveals clearly that like the $\beta_1^{(N)}$, the $E^{(N)}$ become asymptotic much more slowly than the $\beta_2^{(N)}$.

It is of some interest to turn to an observation made in Ref. 13, that the "Neville table" for the ground-state $E^{(N)}$ seems to converge in a zigzag fashion,[12] and that much better convergence is obtained by treating the even and odd terms separately. An aim of that study was to confirm the asymptotic behavior, $E^{(N)}\sim -e^{-2n}(N+1)!$. The Neville table for the quantities a_N is the matrix, defined recursively with $a_N^0=a_N$,

$$a_N^k=[Na_N^{k-1}-(N-k)a_{N-1}^{k-1}]/k \;. \tag{237}$$

If a_N is given asymptotically by the expression

$$a_N\sim 1+A/N+B/[N(N-1)] +C/[N(N-1)(N-2)]+\cdots \;, \tag{238}$$

then the difference between each entry and unity, a_N^k-1, approaches 0 as N^{-k-1}. If, however, a_N has additional terms, say of the form

$$(-1)^N D/[N(N-1)(N-2)(N-3)(N-4)(N-5)] \;,$$

as is the case for $E^{(N)}$ for the ground state, then the entry a_N^k has an alternating-sign contribution proportional to N^{k-6}. That is, the difference with unity has an alternating-sign contribution that *grows* with k. This is the explanation of alternation phenomenon observed in Ref. 13. If the alternating-sign contribution could be eliminated, then the Neville table should converge more

TABLE XI. Coefficients for the RSPT series, the $\Delta E^{(1)}$ series, and the $\Delta_l E^{(2)}$ series, as defined by Eqs. (166), (234), and (235) of the text, for the ($n_1=0$, $n_2=0$, $m=0$) ground state of H_2^+.

Order	Coefficient		
N	$E^{(N)}$	$C^{(1)(N)}$	$C^{(2)(N)}$
0	-5. 00000 00000 00000 00000 00000 000 $\times 10^{-1}$	1. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	1. 00000 00000 00000 00000 00000 000 $\times 10^{0}$
1	-2. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	1. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	2. 00000 00000 00000 00000 00000 000 $\times 10^{0}$
2	0. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	-1. 25000 00000 00000 00000 00000 000 $\times 10^{1}$	-1. 80000 00000 00000 00000 00000 000 $\times 10^{1}$
3	0. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	-2. 18333 33333 33333 33333 33333 333 $\times 10^{1}$	-6. 46666 66666 66666 66666 66666 667 $\times 10^{1}$
4	-3. 60000 00000 00000 00000 00000 000 $\times 10^{1}$	-1. 63458 33333 33333 33333 33333 333 $\times 10^{2}$	-1. 40333 33333 33333 33333 33333 333 $\times 10^{2}$
5	0. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	-1. 21165 83333 33333 33333 33333 333 $\times 10^{3}$	-1. 52440 00000 00000 00000 00000 000 $\times 10^{3}$
6	-4. 80000 00000 00000 00000 00000 000 $\times 10^{2}$	-7. 24887 36111 11111 11111 11111 111 $\times 10^{3}$	-1. 24825 77777 77777 77777 77777 778 $\times 10^{4}$
7	-6. 81600 00000 00000 00000 00000 000 $\times 10^{3}$	-1. 01012 48313 49206 34920 63492 063 $\times 10^{5}$	-1. 24665 30793 65079 36507 93650 794 $\times 10^{5}$
8	-3. 10200 00000 00000 00000 00000 000 $\times 10^{4}$	-9. 36248 50969 74206 34920 63492 063 $\times 10^{5}$	-1. 32387 27047 61904 76190 47619 048 $\times 10^{6}$
9	-4. 53888 00000 00000 00000 00000 000 $\times 10^{5}$	-1. 03330 47428 96549 82363 31569 665 $\times 10^{7}$	-1. 48066 78106 52557 31922 39858 907 $\times 10^{7}$
10	-5. 42457 60000 00000 00000 00000 000 $\times 10^{6}$	-1. 39652 81569 23856 37125 22045 855 $\times 10^{8}$	-1. 90613 92758 70194 00352 73368 607 $\times 10^{8}$
11	-5. 95039 68000 00000 00000 00000 000 $\times 10^{7}$	-1. 78848 65467 99068 53755 81208 915 $\times 10^{9}$	-2. 52087 44293 93246 75324 67532 468 $\times 10^{9}$
12	-8. 38205 20800 00000 00000 00000 000 $\times 10^{8}$	-2. 56750 96449 21180 08687 23611 779 $\times 10^{10}$	-3. 59704 02597 82538 82742 77163 166 $\times 10^{10}$
13	-1. 18278 18240 00000 00000 00000 000 $\times 10^{10}$	-3. 93101 33620 54025 84926 48683 621 $\times 10^{11}$	-5. 49379 21993 59230 00127 44457 189 $\times 10^{11}$
14	-1. 78418 03616 00000 00000 00000 000 $\times 10^{11}$	-6. 30860 30120 96369 94706 69711 865 $\times 10^{12}$	-8. 84328 05607 80952 19263 98116 874 $\times 10^{12}$
15	-2. 89561 86272 64000 00000 00000 000 $\times 10^{12}$	-1. 07905 21375 52958 94081 47697 134 $\times 10^{14}$	-1. 51035 49002 20563 37248 24107 893 $\times 10^{14}$
16	-4. 94927 77000 42800 00000 00000 000 $\times 10^{13}$	-1. 94504 09431 65771 57196 65044 203 $\times 10^{15}$	-2. 72136 22449 18935 43643 79387 025 $\times 10^{15}$
17	-8. 95386 41889 94560 00000 00000 000 $\times 10^{14}$	-3. 69190 69424 98668 33380 88003 127 $\times 10^{16}$	-5. 16228 40287 16972 74018 42068 987 $\times 10^{16}$
18	-1. 70775 91118 31129 60000 00000 000 $\times 10^{16}$	-7. 36691 08866 93962 34950 04035 051 $\times 10^{17}$	-1. 02917 32010 86507 40966 31176 246 $\times 10^{18}$
19	-3. 42401 84054 44785 60000 00000 000 $\times 10^{17}$	-1. 54150 20632 41004 58513 97150 697 $\times 10^{19}$	-2. 15160 26728 99255 60149 59473 763 $\times 10^{19}$
20	-7. 20352 71847 96734 02400 00000 000 $\times 10^{18}$	-3. 37647 18615 98035 45095 74336 884 $\times 10^{20}$	-4. 70830 56141 97598 24827 92116 495 $\times 10^{20}$
21	-1. 58663 37018 30904 41984 00000 000 $\times 10^{20}$	-7. 72759 80864 27204 89987 64471 393 $\times 10^{21}$	-1. 07651 94098 84186 93990 97946 024 $\times 10^{22}$
22	-3. 65198 45724 20448 69676 80000 000 $\times 10^{21}$	-1. 84481 55054 45899 90504 36842 115 $\times 10^{23}$	-2. 56744 52149 71371 40328 15826 700 $\times 10^{23}$
23	-8. 76818 18011 54661 46806 40000 000 $\times 10^{22}$	-4. 58661 97503 05278 22926 67251 432 $\times 10^{24}$	-6. 37699 28377 52626 56173 21947 749 $\times 10^{24}$
24	-2. 19237 89692 87299 63470 43120 000 $\times 10^{24}$	-1. 18581 57747 76732 14364 04939 318 $\times 10^{26}$	-1. 64709 96320 07583 72117 51034 632 $\times 10^{26}$
25	-5. 69988 90347 32373 98500 94080 000 $\times 10^{25}$	-3. 18355 83644 61635 78147 16798 644 $\times 10^{27}$	-4. 41778 93549 93934 37636 08871 324 $\times 10^{27}$
26	-1. 53868 45406 24901 90391 24834 560 $\times 10^{27}$	-8. 86359 51548 82034 55518 28981 017 $\times 10^{28}$	-1. 22885 62062 29670 07480 29362 914 $\times 10^{29}$
27	-4. 30701 59428 07344 63159 84849 344 $\times 10^{28}$	-2. 55604 56435 44030 79195 81850 995 $\times 10^{30}$	-3. 54055 42239 64881 51860 39522 499 $\times 10^{30}$
28	-1. 24856 46387 44255 27154 90329 645 $\times 10^{30}$	-7. 62581 42566 49438 26356 68133 888 $\times 10^{31}$	-1. 05538 73385 15058 26984 64609 363 $\times 10^{32}$
29	-3. 74403 87313 41340 10875 15630 039 $\times 10^{31}$	-2. 35118 32175 44112 98058 07830 405 $\times 10^{33}$	-3. 25123 45534 80517 31436 45408 326 $\times 10^{33}$
30	-1. 16009 28518 92770 55962 92709 845 $\times 10^{33}$	-7. 48383 74003 70202 63362 29847 182 $\times 10^{34}$	-1. 03403 30618 00998 71361 63200 561 $\times 10^{35}$
31	-3. 71037 69005 48712 87703 51920 613 $\times 10^{34}$	-2. 45684 57197 25637 52075 09725 748 $\times 10^{36}$	-3. 39194 73866 39399 86362 25343 054 $\times 10^{36}$
32	-1. 22376 73764 98047 98279 36551 621 $\times 10^{36}$	-8. 31096 43578 93358 83865 73372 462 $\times 10^{37}$	-1. 14655 69540 07235 99096 60792 257 $\times 10^{38}$
33	-4. 15850 46386 52791 79250 06421 463 $\times 10^{37}$	-2. 89447 16053 73106 19866 75975 367 $\times 10^{39}$	-3. 99023 68870 75134 01710 49666 266 $\times 10^{39}$
34	-1. 45466 05269 16266 44223 27876 155 $\times 10^{39}$	-1. 03699 81564 05009 79484 75183 657 $\times 10^{41}$	-1. 42857 74193 90117 87840 82240 525 $\times 10^{41}$
35	-5. 23380 98909 58899 15495 95876 552 $\times 10^{40}$	-3. 81892 67651 11900 66517 64777 557 $\times 10^{42}$	-5. 25744 62109 52309 55992 57531 415 $\times 10^{42}$
36	-1. 93541 35686 18694 56546 97666 524 $\times 10^{42}$	-1. 44458 10606 36116 14398 05282 839 $\times 10^{44}$	-1. 98743 80445 14512 84289 85592 760 $\times 10^{44}$
37	-7. 35041 52418 21237 84191 62047 088 $\times 10^{43}$	-5. 60889 61415 57971 74124 95354 039 $\times 10^{45}$	-7. 71183 32271 33780 24422 34967 571 $\times 10^{45}$
38	-2. 86505 73217 61526 57741 39553 536 $\times 10^{45}$	-2. 23388 80962 10866 74370 87630 041 $\times 10^{47}$	-3. 06958 62026 56960 89416 43834 872 $\times 10^{47}$
39	-1. 14538 73358 92800 41315 04907 402 $\times 10^{47}$	-9. 12054 35207 82225 47645 27322 087 $\times 10^{48}$	-1. 25252 61489 84422 94865 32767 287 $\times 10^{49}$
40	-4. 69352 18341 43224 86001 66161 484 $\times 10^{48}$	-3. 81501 09910 40204 37163 01749 417 $\times 10^{50}$	-5. 23622 58322 48921 38716 29520 814 $\times 10^{50}$
41	-1. 97021 71451 55716 54651 93292 483 $\times 10^{50}$	-1. 63394 92914 80080 03879 36472 874 $\times 10^{52}$	-2. 24143 56144 80234 39000 70866 983 $\times 10^{52}$
42	-8. 46745 17579 34230 37130 94628 568 $\times 10^{51}$	-7. 16164 61078 88398 19543 79712 967 $\times 10^{53}$	-9. 81914 64503 04750 45017 14147 510 $\times 10^{53}$
43	-3. 72374 19906 83640 20995 29606 338 $\times 10^{53}$	-3. 21064 65125 22034 10147 66875 402 $\times 10^{55}$	-4. 39981 49010 52360 91191 82712 265 $\times 10^{55}$
44	-1. 67483 04120 56231 51325 53616 379 $\times 10^{55}$	-1. 47150 46629 92978 43009 77197 609 $\times 10^{57}$	-2. 01554 24510 55075 37912 12031 149 $\times 10^{57}$
45	-7. 70037 25595 40304 33979 57208 022 $\times 10^{56}$	-6. 89149 31471 87806 72268 13012 454 $\times 10^{58}$	-9. 43494 05210 86612 28038 44183 269 $\times 10^{58}$
46	-3. 61740 69023 44197 63149 03727 041 $\times 10^{58}$	-3. 29647 34909 93636 44250 90128 325 $\times 10^{60}$	-4. 51105 03260 68594 13184 53084 808 $\times 10^{60}$
47	-1. 73552 47980 40244 27895 64957 019 $\times 10^{60}$	-1. 60983 10532 42913 94475 07304 622 $\times 10^{62}$	-2. 20199 90640 66198 93151 05453 051 $\times 10^{62}$
48	-8. 50009 57733 00430 30156 86665 842 $\times 10^{61}$	-8. 02275 02931 69226 37180 63385 367 $\times 10^{63}$	-1. 09692 00611 48850 99681 67460 533 $\times 10^{64}$
49	-4. 24810 45332 68548 46607 67018 480 $\times 10^{63}$	-4. 07852 65026 06111 74618 73019 639 $\times 10^{65}$	-5. 57411 32964 57813 71075 94343 361 $\times 10^{65}$
50	-2. 16556 55778 20181 55845 44248 962 $\times 10^{65}$	-2. 11422 94904 67728 48102 87477 156 $\times 10^{67}$	-2. 88835 80523 22927 76072 66918 834 $\times 10^{67}$
51	-1. 12560 24353 67844 96777 46394 055 $\times 10^{67}$	-1. 11714 04828 30431 70236 36058 355 $\times 10^{69}$	-1. 52559 23473 13970 04827 93441 687 $\times 10^{69}$

normally. In Table XVI we have calculated the Neville table for the quantity $-1-E^{(N)}e^2/(N+1)!$ with up to three alternating-sign contributions removed, as indicated by Eq. (236) and by Table XV. The value before any processing differs from 0 by ~ 0.012 for N between 145 and 150. The subtraction of the alternating-sign terms shows up only in the twelfth decimal place. As the Neville iteration is carried out, the entries without removal of the alternating-sign contribution reach -0.00002 for $k=2$, but then grow to ± 0.024 at $k=4$. The sign alternation is clearly evident. As the leading, $1/N$, and $1/N^2$ alternating-sign terms are incorporated, the growing, alternating-sign behavior is pushed to higher values of k, and the approach of the entries to zero is closer. The best

TABLE XII. Coefficients for the RSPT series, the $\Delta E^{(1)}$ series, and the $\Delta_i E^{(2)}$ series, as defined by Eqs. (166), (234), and (235) of the text, for the $(n_1,n_2,m)=(1,0,0)$ excited state of H_2^+.

Order N	Coefficient $E^{(N)}$	$C^{(1)(N)}$	$C^{(2)(N)}$
0	-1. 25000 00000 00000 00000 00000 000 $\times 10^{-1}$	1. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	1. 00000 00000 00000 00000 00000 000 $\times 10^{0}$
1	-1. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	1. 20000 00000 00000 00000 00000 000 $\times 10^{1}$	2. 40000 00000 00000 00000 00000 000 $\times 10^{1}$
2	3. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	-1. 70000 00000 00000 00000 00000 000 $\times 10^{1}$	1. 22000 00000 00000 00000 00000 000 $\times 10^{2}$
3	-6. 00000 00000 00000 00000 00000 000 $\times 10^{0}$	-2. 69333 33333 33333 33333 33333 333 $\times 10^{2}$	-8. 66666 66666 66666 66666 66666 667 $\times 10^{2}$
4	-7. 80000 00000 00000 00000 00000 000 $\times 10^{1}$	9. 10000 00000 00000 00000 00000 000 $\times 10^{2}$	-4. 47500 00000 00000 00000 00000 000 $\times 10^{3}$
5	1. 22400 00000 00000 00000 00000 000 $\times 10^{3}$	-7. 45733 33333 33333 33333 33333 333 $\times 10^{3}$	3. 19546 66666 66666 66666 66666 667 $\times 10^{4}$
6	-8. 81400 00000 00000 00000 00000 000 $\times 10^{3}$	5. 87785 55555 55555 55555 55555 556 $\times 10^{4}$	-1. 28683 77777 77777 77777 77777 778 $\times 10^{5}$
7	-5. 28000 00000 00000 00000 00000 000 $\times 10^{2}$	-7. 06415 42857 14285 71428 57142 857 $\times 10^{5}$	-9. 87438 85714 28571 42857 14285 714 $\times 10^{5}$
8	8. 27436 00000 00000 00000 00000 000 $\times 10^{5}$	-3. 53690 35873 01587 30158 73015 873 $\times 10^{6}$	9. 95790 05396 82539 68253 96825 397 $\times 10^{6}$
9	-9. 61396 80000 00000 00000 00000 000 $\times 10^{6}$	1. 88686 32944 62081 12874 77954 145 $\times 10^{8}$	-8. 46073 03731 92239 85890 65255 732 $\times 10^{7}$
10	9. 90721 80000 00000 00000 00000 000 $\times 10^{6}$	-3. 15201 17618 01058 20105 82010 582 $\times 10^{9}$	-2. 39704 42908 35978 83597 88359 788 $\times 10^{8}$
11	1. 27262 10240 00000 00000 00000 000 $\times 10^{9}$	1. 28815 59385 49584 73625 14029 181 $\times 10^{10}$	-3. 21851 07104 84143 01747 63508 097 $\times 10^{9}$
12	-1. 99901 00364 00000 00000 00000 000 $\times 10^{10}$	3. 81023 29566 40769 17321 36176 581 $\times 10^{11}$	4. 33491 10283 20819 83859 76163 754 $\times 10^{10}$
13	8. 53720 25136 00000 00000 00000 000 $\times 10^{10}$	-1. 02389 55657 81621 55671 48900 482 $\times 10^{13}$	-1. 18715 17415 68802 85146 95181 362 $\times 10^{12}$
14	2. 15315 34951 24000 00000 00000 000 $\times 10^{12}$	9. 35632 83452 95452 46611 11962 699 $\times 10^{13}$	-2. 39992 56892 79449 59790 35661 575 $\times 10^{13}$
15	-5. 08411 86927 84000 00000 00000 000 $\times 10^{13}$	3. 85854 62758 17243 37551 53331 873 $\times 10^{14}$	5. 13239 50387 76683 74741 22976 769 $\times 10^{14}$
16	4. 36975 77689 27280 00000 00000 000 $\times 10^{14}$	-3. 02931 91770 33217 82359 46064 517 $\times 10^{16}$	-9. 76182 13860 45106 44710 13994 823 $\times 10^{15}$
17	2. 27309 65366 68000 00000 00000 000 $\times 10^{15}$	4. 48498 24456 60625 75432 48386 523 $\times 10^{17}$	-2. 88337 84590 36878 21022 37981 727 $\times 10^{16}$
18	-1. 29108 99772 26249 42000 00000 000 $\times 10^{17}$	-2. 45880 27158 17418 87215 87083 116 $\times 10^{18}$	1. 49556 21500 83097 01324 88019 635 $\times 10^{18}$
19	1. 84814 58775 64340 67200 00000 000 $\times 10^{18}$	-6. 79303 43668 58330 24709 04376 503 $\times 10^{19}$	-5. 34675 75848 58079 53131 26858 617 $\times 10^{19}$
20	-8. 33084 55869 39679 03600 00000 000 $\times 10^{18}$	1. 64252 01268 70773 53086 99674 202 $\times 10^{21}$	1. 54633 15097 94322 94457 05069 356 $\times 10^{20}$
21	-2. 40972 22867 09166 75664 00000 000 $\times 10^{20}$	-2. 30112 63946 06663 17965 20081 224 $\times 10^{22}$	-2. 21360 52023 96051 22924 27711 883 $\times 10^{21}$
22	6. 09101 69950 00482 14223 60000 000 $\times 10^{21}$	-3. 61230 75819 53202 55256 21975 926 $\times 10^{22}$	-2. 50584 90664 58102 43373 17750 518 $\times 10^{23}$
23	-7. 51468 51164 92636 15363 51999 999 $\times 10^{22}$	3. 11833 11862 12830 99609 67381 608 $\times 10^{24}$	-1. 27088 63506 42950 81661 03911 680 $\times 10^{23}$
24	4. 45799 85403 42591 05397 19999 958 $\times 10^{22}$	-1. 26184 17602 52519 49054 53520 383 $\times 10^{26}$	-7. 86996 73272 15504 21484 38953 706 $\times 10^{25}$
25	1. 08630 12941 49210 00574 99680 001 $\times 10^{25}$	1. 59628 06441 87831 60637 72599 200 $\times 10^{26}$	-1. 77906 31207 18445 75737 46227 773 $\times 10^{27}$
26	-3. 32113 46075 60316 24709 48791 604 $\times 10^{26}$	-2. 11549 86193 83311 04688 88562 507 $\times 10^{28}$	-3. 41218 37700 54843 32830 92946 730 $\times 10^{28}$
27	1. 72292 23997 49134 89775 87364 494 $\times 10^{27}$	-8. 42246 28381 03414 45635 40509 730 $\times 10^{29}$	-1. 28293 06078 42347 05692 44169 678 $\times 10^{30}$
28	-4. 47414 20271 47563 05334 34104 099 $\times 10^{28}$	-1. 30087 98641 10446 15623 68850 491 $\times 10^{31}$	-3. 23806 09854 04302 80546 18391 779 $\times 10^{31}$
29	-1. 65861 15772 76205 08915 50927 847 $\times 10^{30}$	-5. 76696 90788 60371 45436 01386 740 $\times 10^{32}$	-9. 75845 26387 98611 17263 25821 676 $\times 10^{32}$
30	-2. 37954 29016 54278 26085 66449 166 $\times 10^{31}$	-1. 63152 67399 37452 08595 28386 649 $\times 10^{34}$	-3. 05362 99087 36676 43129 29934 883 $\times 10^{34}$
31	-1. 24203 33874 78179 98081 22666 394 $\times 10^{33}$	-5. 13239 85663 09207 13998 97200 639 $\times 10^{35}$	-9. 50983 21985 28737 47424 02797 366 $\times 10^{35}$
32	-3. 54702 67825 83947 44775 29012 452 $\times 10^{34}$	-1. 74041 46349 26595 87684 77324 874 $\times 10^{37}$	-3. 13135 11053 71890 51165 18470 806 $\times 10^{37}$
33	-1. 19516 26701 97816 94921 46572 314 $\times 10^{36}$	-5. 82804 60599 29608 17651 08755 412 $\times 10^{38}$	-1. 05487 39712 70658 60728 28247 671 $\times 10^{39}$
34	-4. 20663 29269 84478 44058 81886 028 $\times 10^{37}$	-2. 04721 13913 99884 96056 03412 083 $\times 10^{40}$	-3. 66268 39010 04406 38687 52165 380 $\times 10^{40}$
35	-1. 47781 93269 22509 49398 00218 784 $\times 10^{39}$	-7. 37127 62923 91937 06836 07554 473 $\times 10^{41}$	-1. 31039 00757 92959 77590 48194 142 $\times 10^{42}$
36	-5. 42131 69465 84306 30428 52084 376 $\times 10^{40}$	-2. 72736 36101 25607 79065 29713 533 $\times 10^{43}$	-4. 81861 79188 01250 01683 92780 839 $\times 10^{43}$
37	-2. 03461 96166 09154 99124 05276 702 $\times 10^{42}$	-1. 03759 29809 16116 20193 70873 781 $\times 10^{45}$	-1. 82134 02107 12747 30857 16204 662 $\times 10^{45}$
38	-7. 84562 80622 84487 21909 84822 569 $\times 10^{43}$	-4. 05122 30560 32525 69842 30735 332 $\times 10^{46}$	-7. 06944 68583 01165 03503 25827 492 $\times 10^{46}$
39	-3. 10431 97519 61902 94805 38840 486 $\times 10^{45}$	-1. 62295 45793 49161 02695 75880 397 $\times 10^{48}$	-2. 81590 12538 76096 09805 21502 918 $\times 10^{48}$
40	-1. 25968 87575 41054 10432 57093 241 $\times 10^{47}$	-6. 66601 12631 84854 79432 97128 839 $\times 10^{49}$	-1. 15025 19028 17681 37812 77845 181 $\times 10^{50}$
41	-5. 23747 50130 94393 89530 20851 158 $\times 10^{48}$	-2. 80547 29821 42826 69650 76335 332 $\times 10^{51}$	-4. 81558 78661 67003 15007 25500 657 $\times 10^{51}$
42	-2. 23079 43468 42744 90353 52610 975 $\times 10^{50}$	-1. 20910 84668 99724 79837 60817 927 $\times 10^{53}$	-2. 06496 74807 37093 29418 99378 545 $\times 10^{53}$
43	-9. 72417 45894 88816 20660 32201 663 $\times 10^{51}$	-5. 33344 61157 47437 50139 25217 718 $\times 10^{54}$	-9. 06461 11197 43912 67668 82211 735 $\times 10^{54}$
44	-4. 33750 12238 23479 90153 12750 852 $\times 10^{53}$	-2. 40656 13515 99441 81091 85731 154 $\times 10^{56}$	-4. 07107 88631 34689 63643 31718 159 $\times 10^{56}$
45	-1. 97804 24293 56898 01864 26922 166 $\times 10^{55}$	-1. 11023 50140 03369 15709 91292 612 $\times 10^{58}$	-1. 86972 93001 39003 25397 19637 015 $\times 10^{58}$
46	-9. 22105 32631 10449 88955 27997 887 $\times 10^{56}$	-5. 23417 74637 67647 53852 96920 033 $\times 10^{59}$	-8. 77671 53968 46893 92419 35444 155 $\times 10^{59}$
47	-4. 39063 14994 42184 66619 03868 999 $\times 10^{58}$	-2. 52055 30064 96779 32327 15978 697 $\times 10^{61}$	-4. 20892 76739 67323 48257 10893 164 $\times 10^{61}$
48	-2. 13508 23157 37712 97855 05133 847 $\times 10^{60}$	-1. 23926 39677 92349 83731 44021 570 $\times 10^{63}$	-2. 06106 71076 13584 18954 23307 887 $\times 10^{63}$
49	-1. 05957 13537 85055 12879 30535 346 $\times 10^{62}$	-6. 21820 66425 33572 78929 57093 596 $\times 10^{64}$	-1. 03017 64447 06438 25290 30053 796 $\times 10^{65}$
50	-5. 36552 30971 89024 45500 82759 098 $\times 10^{63}$	-3. 18290 60555 79916 74828 40595 168 $\times 10^{66}$	-5. 25342 34104 40529 75013 18298 572 $\times 10^{66}$
51	-2. 77062 58304 65887 09708 47673 808 $\times 10^{65}$	-1. 66136 75110 70091 61856 23152 256 $\times 10^{68}$	-2. 73222 08689 54459 04897 04853 559 $\times 10^{68}$

example is for $N=150$ and $k=3$, for which the entry with three alternating-sign terms accounted for is 0.000 000 4, and which is an improvement of three orders of magnitude over the corresponding entry with no alternating-sign correction terms.

XI. NUMERICAL SOLUTION FOR β_2 AND SUMMATION OF THE EXPANSIONS

In this section we compare values of β_2 obtained by numerical solution of the eigenvalue equation with values

TABLE XIII. Coefficients for the RSPT series, the $\Delta E^{[1]}$ series, and the $\Delta_i E^{[2]}$ series, as defined by Eqs. (166), (234), and (235) of the text, for the $(n_1,n_2,m)=(0,1,0)$ excited state of H_2^+.

Order N	Coefficient $E^{(N)}$	Coefficient $C^{(1)(N)}$	Coefficient $C^{(2)(N)}$
0	-1.25000 00000 00000 00000 00000 000 × 10^{-1}	1.00000 00000 00000 00000 00000 0 × 10^{0}	1.00000 00000 00000 00000 00000 0 × 10^{0}
1	-1.00000 00000 00000 00000 00000 000 × 10^{0}	-4.00000 00000 00000 00000 00000 0 × 10^{0}	-8.00000 00000 00000 00000 00000 0 × 10^{0}
2	-3.00000 00000 00000 00000 00000 000 × 10^{0}	-6.30000 00000 00000 00000 00000 0 × 10^{1}	-7.40000 00000 00000 00000 00000 0 × 10^{1}
3	-6.00000 00000 00000 00000 00000 000 × 10^{0}	-2.77333 33333 33333 33333 33333 3 × 10^{2}	-1.62666 66666 66666 66666 66666 7 × 10^{2}
4	-9.00000 00000 00000 00000 00000 000 × 10^{1}	-1.96766 66666 66666 66666 66666 7 × 10^{3}	3.88333 33333 33333 33333 33333 3 × 10^{2}
5	-1.22400 00000 00000 00000 00000 000 × 10^{3}	-3.08176 00000 00000 00000 00000 0 × 10^{4}	-6.59786 66666 66666 66666 66666 7 × 10^{3}
6	-1.19220 00000 00000 00000 00000 000 × 10^{4}	-4.57557 37777 77777 77777 77777 8 × 10^{5}	-3.18823 51111 11111 11111 11111 1 × 10^{5}
7	-1.48464 00000 00000 00000 00000 000 × 10^{5}	-7.45529 11365 07936 50793 65079 4 × 10^{6}	-6.61211 50730 15873 01587 30158 7 × 10^{6}
8	-2.45434 80000 00000 00000 00000 000 × 10^{6}	-1.39686 45440 95238 09523 80952 4 × 10^{8}	-1.21726 02948 25396 82539 68254 0 × 10^{8}
9	-4.04557 92000 00000 00000 00000 000 × 10^{7}	-2.65014 09796 83950 61728 39506 2 × 10^{9}	-2.31846 76383 35097 00176 36684 3 × 10^{9}
10	-6.76111 89000 00000 00000 00000 000 × 10^{8}	-5.10616 90774 20007 05467 37213 4 × 10^{10}	-4.66622 71320 45954 14462 08112 9 × 10^{10}
11	-1.23090 34464 00000 00000 00000 000 × 10^{10}	-1.04247 12453 03395 32467 53246 8 × 10^{12}	-9.84809 97179 51261 69632 83629 9 × 10^{11}
12	-2.38412 99211 60000 00000 00000 000 × 10^{11}	-2.23016 29650 85629 37865 42675 4 × 10^{13}	-2.14980 07877 36538 29768 58532 4 × 10^{13}
13	-4.78926 88827 36000 00000 00000 000 × 10^{12}	-4.91944 72964 29282 58912 11669 0 × 10^{14}	-4.83496 01163 42960 68018 23690 7 × 10^{14}
14	-1.00299 60764 62920 00000 00000 000 × 10^{14}	-1.12225 28675 25768 45165 53217 5 × 10^{16}	-1.12401 35072 47601 94486 12528 0 × 10^{16}
15	-2.19391 40584 10784 00000 00000 000 × 10^{15}	-2.65295 91858 70059 08542 19598 3 × 10^{17}	-2.70125 37563 66712 47262 57043 4 × 10^{17}
16	-4.98913 38393 59109 60000 00000 000 × 10^{16}	-6.48199 61850 23826 22729 67446 6 × 10^{18}	-6.69779 85890 44998 34046 32374 8 × 10^{18}
17	-1.17721 33789 78895 71200 00000 000 × 10^{18}	-1.63494 60327 61396 18599 43983 0 × 10^{20}	-1.71247 09879 02293 66130 38586 9 × 10^{20}
18	-2.88058 43388 66001 82580 00000 000 × 10^{19}	-4.25659 28284 19743 45424 73387 8 × 10^{21}	-4.51439 22010 11258 82664 38086 1 × 10^{21}
19	-7.30209 82248 39883 55520 00000 000 × 10^{20}	-1.14334 33867 13204 03393 45887 2 × 10^{23}	-1.22655 00201 58564 38832 39288 5 × 10^{23}
20	-1.91564 48562 67545 21945 00000 000 × 10^{22}	-3.16673 73813 03954 79804 08780 5 × 10^{24}	-3.43325 19223 39610 05699 60825 4 × 10^{24}
21	-5.19690 13809 24973 96791 21600 000 × 10^{23}	-9.04044 65735 66963 94912 61340 3 × 10^{25}	-9.89740 68575 41075 34003 79363 9 × 10^{25}
22	-1.45686 05280 77824 53021 96252 000 × 10^{25}	-2.65909 74088 83205 00554 27661 4 × 10^{27}	-2.93755 78773 17364 95086 14964 8 × 10^{27}
23	-4.21719 12580 22755 91176 19011 200 × 10^{26}	-8.05487 65908 80379 25062 66439 5 × 10^{28}	-8.97310 57626 32034 42631 39732 5 × 10^{28}
24	-1.25967 94654 24442 36755 85922 504 × 10^{28}	-2.51173 13301 48609 92987 62592 6 × 10^{30}	-2.81984 43774 15905 44331 56212 8 × 10^{30}
25	-3.88002 45958 54034 72757 66618 730 × 10^{29}	-8.05898 08749 29748 77315 30964 6 × 10^{31}	-9.11294 89928 60760 81697 89730 6 × 10^{31}
26	-1.23156 18914 48207 79510 27323 520 × 10^{31}	-2.65934 77299 91991 69947 04818 7 × 10^{33}	-3.02733 18655 21228 75404 05841 9 × 10^{33}
27	-4.02566 98806 20394 69138 44635 383 × 10^{32}	-9.02084 17726 16145 42317 13540 3 × 10^{34}	-1.03332 27815 45672 51025 31966 2 × 10^{35}
28	-1.35424 24210 16489 21939 79592 644 × 10^{34}	-3.14397 93313 12732 90917 29422 5 × 10^{36}	-3.62232 76612 73675 84487 97258 2 × 10^{36}
29	-4.68544 75442 38667 24995 06874 748 × 10^{35}	-1.12526 07148 86044 84077 11133 1 × 10^{38}	-1.30350 01473 24107 21489 06879 0 × 10^{38}
30	-1.66619 91081 12221 44530 75990 316 × 10^{37}	-4.13376 48554 81829 50663 67925 6 × 10^{39}	-4.81280 97930 09928 29278 75091 9 × 10^{39}
31	-6.08631 04372 84698 90199 00511 196 × 10^{38}	-1.55788 53861 85628 91404 25986 4 × 10^{41}	-1.82239 14592 68996 77682 45153 6 × 10^{41}
32	-2.28228 12507 85834 12798 16822 652 × 10^{40}	-6.02006 93400 94138 15860 47590 2 × 10^{42}	-7.07344 66737 29949 37561 84717 2 × 10^{42}
33	-8.78042 25977 17389 15037 56947 826 × 10^{41}	-2.38410 42750 50020 18495 10149 6 × 10^{44}	-2.81293 24755 22493 31360 81692 0 × 10^{44}
34	-3.46372 59781 60770 70431 46364 763 × 10^{43}	-9.67145 13086 63695 32105 62437 6 × 10^{45}	-1.14556 85717 78145 62829 08794 2 × 10^{46}
35	-1.40026 99808 77340 28790 33201 661 × 10^{45}	-4.01688 83158 69910 15916 67148 4 × 10^{47}	-4.77545 13746 07933 01640 60098 4 × 10^{47}
36	-5.79810 75784 61483 13779 28371 024 × 10^{46}	-1.70731 38981 54727 92312 48876 2 × 10^{49}	-2.03676 63980 95327 10302 79579 2 × 10^{49}
37	-2.45776 83467 34762 55880 08187 252 × 10^{48}	-7.42269 27067 44164 25656 63287 9 × 10^{50}	-8.88398 42234 76867 67453 97625 6 × 10^{50}
38	-1.06600 08819 26512 34909 70387 860 × 10^{50}	-3.29942 67297 25793 16904 29985 3 × 10^{52}	-3.96118 52062 63918 08076 63542 6 × 10^{52}
39	-4.72852 35175 23039 41684 75576 411 × 10^{51}	-1.49883 69874 28103 85887 03408 0 × 10^{54}	-1.80471 79835 05179 76991 45339 9 × 10^{54}
40	-2.14408 42507 99885 67706 80474 753 × 10^{53}	-6.95544 43277 62059 42755 27395 3 × 10^{55}	-8.39810 83786 08792 46629 11403 1 × 10^{55}
41	-9.93369 12013 03364 97060 47121 705 × 10^{54}	-3.29587 86844 69093 03980 22832 9 × 10^{57}	-3.98995 29490 85868 17879 20812 8 × 10^{57}
42	-4.70049 09765 31913 16033 29034 337 × 10^{56}	-1.59411 73680 19089 84037 10866 1 × 10^{59}	-1.93463 75203 34546 40507 16008 5 × 10^{59}
43	-2.27068 85253 36619 89256 94923 984 × 10^{58}	-7.86691 49377 51629 50970 48554 9 × 10^{60}	-9.57003 21977 08557 92413 42140 9 × 10^{60}
44	-1.11938 16860 65051 88188 31837 106 × 10^{60}	-3.95969 18532 28589 44223 55991 9 × 10^{62}	-4.82781 43119 36926 66208 37658 9 × 10^{62}
45	-5.62905 98312 32797 88997 01881 543 × 10^{61}	-2.03204 80899 73028 22339 94284 3 × 10^{64}	-2.48288 92737 25694 54558 34330 0 × 10^{64}
46	-2.88647 15078 74552 54081 55714 251 × 10^{63}	-1.06284 55007 01580 81728 63182 1 × 10^{66}	-1.30132 20428 94060 82772 51424 9 × 10^{66}
47	-1.50874 14896 77968 88842 09398 943 × 10^{65}	-5.66399 19589 73289 66761 01483 5 × 10^{67}	-6.94845 83468 13190 87646 67923 7 × 10^{67}
48	-8.03574 94933 05403 97340 21811 168 × 10^{66}	-3.07431 88224 77668 01154 28549 8 × 10^{69}	-3.77857 82063 30328 50661 93961 0 × 10^{69}
49	-4.35968 37949 97962 43339 35268 334 × 10^{68}	-1.69906 86683 08437 42409 10465 5 × 10^{71}	-2.09203 52686 24217 27613 67235 4 × 10^{71}
50	-2.40856 65421 69654 47050 34554 238 × 10^{70}	-9.55817 58313 17034 50810 29931 8 × 10^{72}	-1.17890 47292 28163 21278 91491 0 × 10^{73}
51	-1.35456 58158 53828 79035 71962 601 × 10^{72}	-5.47156 58928 71467 87770 00035 0 × 10^{74}	-6.75974 05784 98781 49704 68065 1 × 10^{74}

obtained by summation of the asymptotic series.

As mentioned in the Introduction, proved in Ref. 6, and discussed in Sec. III I, the Borel sum of the RSPT series is the eigenvalue of the η equation [(11) or (16)] considered on a semi-infinite interval—that is, the ξ equation for the proton-antiproton-electron analog of H_2^+, analytically continued to negative $r'=e^{\pm\pi i}r$. We illustrate this fact by numerically solving Eq. (11) and comparing the results with the Borel sum of the RSPT. Also, as mentioned in the Introduction and elaborated in Sec. III I, the imaginary second-exponential-order series cancels (in that order) the imaginary part of the Borel sum. This too is illustrated numerically.

To solve the η equation [Eq. (11)] numerically is straightforward. There are two cases: the physical problem, for which the boundary conditions are

TABLE XIV. Coefficients for the RSPT series, the $\Delta E^{[1]}$ series, and the $\Delta_i E^{[2]}$ series, as defined by Eqs. (166), (234), and (235) of the text, for the $(n_1, n_2, m) = (0,0,1)$ excited state of H_2^+.

Order	Coefficient		
N	$E^{(N)}$	$C^{(1)(N)}$	$C^{(2)(N)}$
0	-1.25000 00000 00000 00000 00000 000 x 10^{-1}	1.00000 00000 00000 00000 00000 000 x 10^{0}	1.00000 00000 00000 00000 00000 000 x 10^{0}
1	-1.00000 00000 00000 00000 00000 000 x 10^{0}	6.00000 00000 00000 00000 00000 000 x 10^{0}	1.20000 00000 00000 00000 00000 000 x 10^{1}
2	0.00000 00000 00000 00000 00000 000 x 10^{0}	-4.00000 00000 00000 00000 00000 000 x 10^{1}	-2.00000 00000 00000 00000 00000 000 x 10^{1}
3	6.00000 00000 00000 00000 00000 000 x 10^{0}	-3.13333 33333 33333 33333 33333 333 x 10^{2}	-9.30666 66666 66666 66666 66666 667 x 10^{2}
4	-7.80000 00000 00000 00000 00000 000 x 10^{1}	-6.36000 00000 00000 00000 00000 000 x 10^{2}	-3.88800 00000 00000 00000 00000 000 x 10^{3}
5	0.00000 00000 00000 00000 00000 000 x 10^{0}	-9.74346 66666 66666 66666 66666 667 x 10^{3}	4.25173 33333 33333 33333 33333 333 x 10^{3}
6	2.40000 00000 00000 00000 00000 000 x 10^{3}	-6.63105 77777 77777 77777 77777 778 x 10^{4}	-8.92423 11111 11111 11111 11111 111 x 10^{4}
7	-3.38880 00000 00000 00000 00000 000 x 10^{4}	-8.72937 90476 19047 61904 76190 476 x 10^{5}	-2.38107 58095 23809 52380 95238 095 x 10^{6}
8	-2.01552 00000 00000 00000 00000 000 x 10^{5}	-2.06407 56317 46031 74603 17460 317 x 10^{7}	-2.39404 25092 06349 20634 92063 492 x 10^{7}
9	1.83590 40000 00000 00000 00000 000 x 10^{6}	-1.64124 98162 68077 60141 09347 443 x 10^{8}	-2.93346 08305 89065 25573 19223 986 x 10^{8}
10	-2.84832 00000 00000 00000 00000 000 x 10^{7}	-2.09346 28756 24973 54497 35449 735 x 10^{9}	-4.63594 52763 15767 19576 71957 672 x 10^{9}
11	-5.03357 18400 00000 00000 00000 000 x 10^{8}	-5.70273 72832 45704 02437 06910 374 x 10^{10}	-7.85280 39569 21771 36443 80311 047 x 10^{10}
12	-3.22391 80800 00000 00000 00000 000 x 10^{8}	-7.52912 16606 84289 66917 85580 674 x 10^{11}	-1.25763 36191 02109 51846 50740 206 x 10^{12}
13	-6.05107 89120 00000 00000 00000 000 x 10^{10}	-1.10073 27081 05853 68409 36840 937 x 10^{13}	-2.07249 94023 45520 68612 86861 287 x 10^{13}
14	-1.55779 98520 32000 00000 00000 000 x 10^{12}	-2.56776 25455 98525 52148 33373 564 x 10^{14}	-3.96915 29593 73711 61752 43921 276 x 10^{14}
15	-1.55274 77514 24000 00000 00000 000 x 10^{13}	-4.67624 56349 41309 76112 04660 517 x 10^{15}	-7.63729 81098 86979 04298 51802 127 x 10^{15}
16	-3.55602 36364 87680 00000 00000 000 x 10^{14}	-8.69833 64731 46741 38952 49319 757 x 10^{16}	-1.48433 14650 21301 54467 04211 250 x 10^{17}
17	-8.45853 72059 68896 00000 00000 000 x 10^{15}	-1.94649 25960 50903 22910 74877 754 x 10^{18}	-3.14046 57783 86843 13845 77898 246 x 10^{18}
18	-1.55030 34534 60357 12000 00000 000 x 10^{17}	-4.23441 34580 44079 75888 46140 692 x 10^{19}	-6.88146 50168 65476 54439 58189 105 x 10^{19}
19	-3.47435 07633 56000 25600 00000 000 x 10^{18}	-9.47952 69136 31857 74985 45926 974 x 10^{20}	-1.55217 89615 30295 12284 42711 434 x 10^{21}
20	-8.26403 64221 95610 41920 00000 000 x 10^{19}	-2.27912 53793 21052 23534 50175 530 x 10^{22}	-3.68030 04405 46240 72734 18513 140 x 10^{22}
21	-1.93593 62616 33120 65740 80000 000 x 10^{21}	-5.62936 66395 36119 66727 47596 637 x 10^{23}	-9.06656 89837 58496 80487 69325 947 x 10^{23}
22	-4.83196 36650 94828 52352 00000 000 x 10^{22}	-1.44079 90980 28800 94926 31215 775 x 10^{25}	-2.31486 05013 69089 36122 67602 133 x 10^{25}
23	-1.25672 41823 94826 59550 00320 000 x 10^{24}	-3.84388 95512 42687 36148 29820 525 x 10^{26}	-6.14236 84542 90483 96293 16621 596 x 10^{26}
24	-3.37013 29576 46065 01404 26240 000 x 10^{25}	-1.06135 67327 59470 75379 34351 339 x 10^{28}	-1.68936 34595 43544 26784 87746 187 x 10^{28}
25	-9.39290 75638 92952 64919 65030 400 x 10^{26}	-3.03376 12021 30512 42240 06684 588 x 10^{29}	-4.81024 54768 03946 65503 88209 722 x 10^{29}
26	-2.71132 00561 65065 36836 23198 720 x 10^{28}	-8.97386 87029 24775 14417 97191 318 x 10^{30}	-1.41714 07609 16723 79689 97157 605 x 10^{31}
27	-8.09128 32612 42646 01222 90729 779 x 10^{29}	-2.74271 70573 43868 58021 36429 000 x 10^{32}	-4.31482 59411 72027 81563 48012 436 x 10^{32}
28	-2.49548 99420 83753 11255 23605 488 x 10^{31}	-8.65417 13474 22334 60100 18384 543 x 10^{33}	-1.35645 10024 47194 41857 90235 353 x 10^{34}
29	-7.94489 17212 85325 72940 45133 642 x 10^{32}	-2.81665 70663 08002 65701 39940 827 x 10^{35}	-4.39899 31536 84522 79913 57202 101 x 10^{35}
30	-2.60850 98915 74160 48759 40746 084 x 10^{34}	-9.44739 79326 16179 43050 82872 490 x 10^{36}	-1.47037 16906 69530 38102 56997 560 x 10^{37}
31	-8.82462 45508 00721 88099 02514 514 x 10^{35}	-3.26287 92722 86534 06252 05338 037 x 10^{38}	-5.06130 97420 74784 39918 58599 659 x 10^{38}
32	-3.07346 14862 62045 86105 09599 824 x 10^{37}	-1.15945 86093 45338 37345 86528 258 x 10^{40}	-1.79272 88486 36957 26310 14564 378 x 10^{40}
33	-1.10112 73649 30558 82575 59892 250 x 10^{39}	-4.23588 81092 84463 58024 43893 831 x 10^{41}	-6.52906 45911 03117 41294 04729 508 x 10^{41}
34	-4.05503 45195 29661 16680 23721 088 x 10^{40}	-1.58984 29830 77319 32496 31244 358 x 10^{43}	-2.44318 29183 87407 82755 20664 104 x 10^{43}
35	-1.53385 27913 91403 90547 20192 044 x 10^{42}	-6.12610 64551 10198 67769 01162 691 x 10^{44}	-9.38702 74388 65808 27712 41738 516 x 10^{44}
36	-5.95532 36273 01744 53409 88975 043 x 10^{43}	-2.42186 08439 48805 73956 79783 253 x 10^{46}	-3.70066 17534 38737 75273 38728 610 x 10^{46}
37	-2.37178 07899 28912 95636 13997 205 x 10^{45}	-9.81691 53742 78235 87270 35546 216 x 10^{47}	-1.49601 18442 71354 98293 15059 027 x 10^{48}
38	-9.68321 71094 63935 57357 24092 937 x 10^{46}	-4.07756 90855 82929 08603 15521 049 x 10^{49}	-6.19772 73227 03502 30614 23742 777 x 10^{49}
39	-4.05025 00974 05692 38867 98013 331 x 10^{48}	-1.73451 81709 06197 01771 38845 635 x 10^{51}	-2.62978 82798 73247 56954 59236 777 x 10^{51}
40	-1.73465 86175 36075 37666 46651 630 x 10^{50}	-7.55212 90343 61711 80522 56109 454 x 10^{52}	-1.14224 71213 20255 94148 37941 051 x 10^{53}
41	-7.60291 70182 24680 08150 85650 852 x 10^{51}	-3.36391 53585 79469 67683 86916 436 x 10^{54}	-5.07599 00458 59755 30397 78225 672 x 10^{54}
42	-3.40843 47604 02489 55538 60620 653 x 10^{53}	-1.53210 18169 00582 50921 85434 809 x 10^{56}	-2.30665 71954 95785 04387 82845 898 x 10^{56}
43	-1.56214 88856 74643 09257 31923 393 x 10^{55}	-7.13161 76542 23869 05167 95196 474 x 10^{57}	-1.07136 23139 48168 46122 10361 335 x 10^{58}
44	-7.31603 73911 17733 54980 96019 876 x 10^{56}	-3.39114 13767 52748 22306 21643 045 x 10^{59}	-5.08368 67259 82297 59093 05435 433 x 10^{59}
45	-3.49959 20366 93598 91668 17769 328 x 10^{58}	-1.64652 69780 08236 65118 91084 320 x 10^{61}	-2.46329 58768 55334 29456 33945 448 x 10^{61}
46	-1.70905 86893 95210 74016 63064 942 x 10^{60}	-8.15966 39046 03939 03795 80043 150 x 10^{62}	-1.21832 67347 46780 24063 44817 110 x 10^{63}
47	-8.51750 20559 09728 74946 57078 558 x 10^{61}	-4.12552 04419 46326 19565 13532 794 x 10^{64}	-6.14811 05845 66131 44197 51279 325 x 10^{64}
48	-4.33020 10973 72823 98193 60749 684 x 10^{63}	-2.12724 58801 31380 60942 97115 307 x 10^{66}	-3.16430 59699 84058 53906 59799 837 x 10^{66}
49	-2.24479 16414 87821 85905 65104 858 x 10^{65}	-1.11821 41806 45854 03997 46226 448 x 10^{68}	-1.66038 53659 20864 96222 15559 216 x 10^{68}
50	-1.18618 97135 90882 24223 81705 143 x 10^{67}	-5.99021 82780 86620 26463 55509 093 x 10^{69}	-8.87920 00375 59267 12556 46813 721 x 10^{69}
51	-6.38684 60774 93345 40838 33238 854 x 10^{68}	-3.26902 63820 18303 29932 40091 959 x 10^{71}	-4.83748 94548 79326 00323 72842 538 x 10^{71}

$\Phi_2(\eta) \sim \eta^{m/2+1/2}$ at $\eta = 0$, and $\Phi_2(\eta) \sim (2-\eta)^{m/2+1/2}$ at $\eta = 2$; and the semi-infinite problem for which the boundary condition at $\eta = 2$ is replaced by $\Phi_2(\eta) \sim e^{-r\eta/2}$ as $\eta \to \infty$. In both cases the wave function near the origin can be expanded in a convergent power series in η. For the physical case, the power series can be summed at the midpoint of the physical interval, $\eta = 1$, and the eigenvalue β_2 determined to make either Φ_2 or $d\Phi_2/d\eta$ vanish for odd or even states, respectively. For the unphysical case, $e^{r\eta/2}\Phi_2$ for large η can be expanded in a divergent series in powers of η^{-1}. This series can be summed to sufficient accuracy for the ground state for $|\eta|$ near 4, and then integrated numerically by a fourth-order Runge-Kutta algorithm[25] to a value of η for which the

TABLE XV. Asymptotic analysis of the RSPT $E^{(N)}$. The dominant, same-sign subseries in the asymptotic formula (236) of the text is truncated with the inclusion of the smallest term, whose index has been indicated by $k_{\min}$. The relative asymptotic error refers to the difference between the exact coefficient $E^{(N)}$ and the asymptotic formula to the indicated number of terms, divided by the leading asymptotic term, which is $-e^{-2n}(N+4n_2+2m+1)!/(n_2!)^2[(n_2+m)!]^2$. For sufficiently large N, the relative asymptotic error, after accounting for the same-sign subseries, is alternating in sign. The effect of the alternating-sign subseries is seen through the inclusion of up to three terms.

		same-sign subseries			alternating-sign subseries		
					relative asymptotic error after inclusion of terms through order (in N^{-1})		
N	$E^{(N)}$(exact)	$k_{\min}$	smallest term	relative asymptotic error	0	1	2
		Ground state: $n_1=0$, $n_2=0$, $m=0$					
20	$-7.20352\,71847\,96734\,02400\,00000\,000\times 10^{18}$	9	1.4×10^{-4}	-3.0×10^{-5}	-5.2×10^{-5}	-4.3×10^{-5}	-3.8×10^{-5}
21	$-1.58663\,37018\,30904\,41984\,00000\,000\times 10^{20}$	10	8.1×10^{-5}	1.1×10^{-5}	2.7×10^{-5}	2.1×10^{-5}	1.8×10^{-5}
22	$-3.65198\,45724\,20448\,69676\,80000\,000\times 10^{21}$	10	4.6×10^{-5}	-9.5×10^{-6}	-2.2×10^{-5}	-1.7×10^{-5}	-1.5×10^{-5}
23	$-8.76818\,18011\,54661\,46806\,40000\,000\times 10^{22}$	11	2.5×10^{-5}	-2.9×10^{-7}	8.7×10^{-6}	5.0×10^{-6}	3.9×10^{-6}
24	$-2.19237\,89692\,87299\,63470\,43120\,000\times 10^{24}$	11	1.4×10^{-5}	-1.9×10^{-6}	-8.7×10^{-6}	-5.9×10^{-6}	-5.1×10^{-6}
25	$-5.69988\,90347\,32373\,98500\,94080\,000\times 10^{25}$	12	7.8×10^{-6}	-1.8×10^{-6}	3.5×10^{-6}	1.2×10^{-6}	7.7×10^{-7}
26	$-1.53868\,45406\,24901\,90391\,24834\,560\times 10^{27}$	12	4.3×10^{-6}	3.6×10^{-7}	-3.7×10^{-6}	-2.0×10^{-6}	-1.7×10^{-6}
27	$-4.30701\,59428\,07344\,63159\,84849\,344\times 10^{28}$	13	2.4×10^{-6}	-1.5×10^{-6}	1.7×10^{-6}	3.5×10^{-7}	1.4×10^{-7}
28	$-1.24856\,46387\,44255\,27154\,90329\,645\times 10^{30}$	13	1.3×10^{-6}	8.2×10^{-7}	-1.7×10^{-6}	-6.7×10^{-7}	-5.3×10^{-7}
29	$-3.74403\,87313\,41340\,10875\,15630\,039\times 10^{31}$	14	7.0×10^{-7}	-1.1×10^{-6}	9.5×10^{-7}	1.1×10^{-7}	1.4×10^{-8}
30	$-1.16009\,28518\,92770\,55962\,92709\,845\times 10^{33}$	14	3.8×10^{-7}	7.6×10^{-7}	-8.9×10^{-7}	-2.2×10^{-7}	-1.6×10^{-7}
45	$-7.70037\,25595\,40304\,33979\,57208\,022\times 10^{56}$	22	2.9×10^{-11}	-8.6×10^{-8}	4.4×10^{-8}	-1.5×10^{-9}	-4.9×10^{-10}
60	$-7.05864\,08371\,50714\,38838\,94260\,882\times 10^{82}$	30	1.7×10^{-15}	1.6×10^{-8}	-6.2×10^{-9}	3.5×10^{-10}	3.2×10^{-11}
75	$-2.61042\,76701\,03107\,25304\,91597\,603\times 10^{110}$	37	8.3×10^{-20}	-4.2×10^{-9}	1.4×10^{-9}	-8.6×10^{-11}	-3.2×10^{-12}
90	$-1.86576\,07764\,04173\,29829\,65438\,924\times 10^{139}$	45	3.8×10^{-24}	1.4×10^{-9}	-4.1×10^{-10}	2.5×10^{-11}	3.8×10^{-13}
105	$-1.57799\,46924\,10063\,42268\,12311\,752\times 10^{169}$	51	1.7×10^{-28}	-5.7×10^{-10}	1.4×10^{-10}	-8.7×10^{-12}	-3.4×10^{-14}
120	$-1.11215\,08837\,06133\,49504\,42764\,523\times 10^{200}$	51	2.3×10^{-32}	2.6×10^{-10}	-5.8×10^{-11}	3.4×10^{-12}	-8.7×10^{-15}
135	$-5.01981\,18745\,10824\,25602\,25491\,753\times 10^{231}$	51	1.2×10^{-35}	-1.3×10^{-10}	2.6×10^{-11}	-1.5×10^{-12}	9.6×10^{-15}
150	$-1.18207\,97343\,39949\,69605\,83966\,744\times 10^{264}$	51	1.7×10^{-38}	6.8×10^{-11}	-1.3×10^{-11}	7.0×10^{-13}	-6.3×10^{-15}
		Excited state: $n_1=1$, $n_2=0$, $m=0$					
35	$-1.47781\,93269\,22509\,49398\,00218\,784\times 10^{39}$	23	2.1×10^{-9}	-5.5×10^{-3}	-3.3×10^{-3}	-4.8×10^{-3}	-6.8×10^{-3}
36	$-5.42131\,69465\,84306\,30428\,52084\,376\times 10^{40}$	23	8.0×10^{-10}	1.1×10^{-3}	-7.4×10^{-4}	5.4×10^{-4}	2.0×10^{-3}
37	$-2.03461\,96166\,09154\,99124\,05276\,702\times 10^{42}$	23	3.2×10^{-10}	-9.2×10^{-6}	1.5×10^{-3}	4.3×10^{-4}	-7.4×10^{-4}
38	$-7.84562\,80622\,84487\,21909\,84822\,569\times 10^{43}$	23	1.3×10^{-10}	-2.6×10^{-5}	-1.3×10^{-3}	-3.9×10^{-4}	5.3×10^{-4}
39	$-3.10431\,97519\,61902\,94805\,38840\,486\times 10^{45}$	23	5.5×10^{-11}	-5.5×10^{-5}	1.1×10^{-3}	2.4×10^{-4}	-4.7×10^{-4}
40	$-1.25968\,87575\,41054\,10432\,57093\,241\times 10^{47}$	23	2.4×10^{-11}	8.5×10^{-5}	-8.6×10^{-4}	-1.6×10^{-4}	4.0×10^{-4}
41	$-5.23747\,50130\,94393\,89530\,20851\,158\times 10^{48}$	23	1.1×10^{-11}	-8.7×10^{-5}	7.2×10^{-4}	1.2×10^{-4}	-3.3×10^{-4}
42	$-2.23079\,43468\,42744\,90353\,52610\,975\times 10^{50}$	23	5.1×10^{-12}	8.2×10^{-5}	-6.1×10^{-4}	-9.5×10^{-5}	2.6×10^{-4}
43	$-9.72417\,45894\,88816\,20660\,32201\,663\times 10^{51}$	23	2.4×10^{-12}	-7.6×10^{-5}	5.2×10^{-4}	7.4×10^{-5}	-2.1×10^{-4}
44	$-4.33750\,12238\,23479\,90153\,12750\,852\times 10^{53}$	23	1.2×10^{-12}	7.2×10^{-5}	-4.5×10^{-4}	-5.8×10^{-5}	1.7×10^{-4}
45	$-1.97804\,24293\,56898\,01864\,26922\,166\times 10^{55}$	23	6.0×10^{-13}	-6.7×10^{-5}	3.9×10^{-4}	4.5×10^{-5}	-1.4×10^{-4}
60	$-1.65302\,36911\,22050\,21932\,71446\,744\times 10^{81}$	23	1.3×10^{-16}	2.1×10^{-5}	-5.5×10^{-5}	7.5×10^{-7}	1.0×10^{-5}
75	$-5.76286\,57185\,48714\,72612\,15623\,042\times 10^{108}$	38	2.0×10^{-20}	-7.0×10^{-6}	1.2×10^{-5}	-9.5×10^{-7}	-1.3×10^{-6}
90	$-3.95393\,93851\,27749\,03143\,18218\,325\times 10^{137}$	45	7.6×10^{-25}	2.7×10^{-6}	-3.7×10^{-6}	4.0×10^{-7}	2.5×10^{-7}
105	$-3.24525\,84385\,46167\,21188\,41955\,517\times 10^{167}$	51	3.0×10^{-29}	-1.2×10^{-6}	1.3×10^{-6}	-1.6×10^{-7}	-5.9×10^{-8}
120	$-2.23532\,44929\,47468\,07900\,46507\,163\times 10^{198}$	51	4.0×10^{-33}	5.6×10^{-7}	-5.4×10^{-7}	7.2×10^{-8}	1.6×10^{-8}
135	$-9.90814\,88516\,78231\,94553\,22580\,787\times 10^{229}$	51	2.1×10^{-36}	-2.9×10^{-7}	2.5×10^{-7}	-3.4×10^{-8}	-5.2×10^{-9}
150	$-2.29920\,86344\,61569\,20265\,54610\,723\times 10^{262}$	51	3.0×10^{-39}	1.6×10^{-7}	-1.2×10^{-7}	1.7×10^{-8}	1.8×10^{-9}
		Excited state: $n_1=0$, $n_2=1$, $m=0$					
90	$-2.14579\,08730\,97608\,03804\,76312\,533\times 10^{145}$	44	7.2×10^{-20}	-2.4×10^{-20}	-3.9×10^{-20}	-2.3×10^{-20}	-2.9×10^{-20}
91	$-2.06235\,64052\,64978\,98704\,71054\,615\times 10^{147}$	45	3.9×10^{-20}	3.0×10^{-22}	1.3×10^{-20}	-4.4×10^{-22}	4.8×10^{-21}
92	$-2.00275\,88289\,87262\,10407\,16448\,251\times 10^{149}$	45	2.1×10^{-20}	-4.9×10^{-21}	-1.6×10^{-20}	-4.4×10^{-21}	-8.8×10^{-21}
93	$-1.96488\,19052\,26077\,10849\,82754\,451\times 10^{151}$	46	1.1×10^{-20}	-1.7×10^{-21}	7.9×10^{-21}	-2.1×10^{-21}	1.6×10^{-21}
94	$-1.94734\,22525\,53073\,90685\,34596\,759\times 10^{153}$	46	6.0×10^{-21}	1.4×10^{-22}	-8.2×10^{-21}	4.1×10^{-22}	-2.8×10^{-21}
95	$-1.94940\,56487\,88341\,35709\,98583\,644\times 10^{155}$	47	3.2×10^{-21}	-1.9×10^{-21}	5.3×10^{-21}	-2.0×10^{-21}	6.5×10^{-22}
96	$-1.97093\,89906\,90687\,68548\,88768\,219\times 10^{157}$	47	1.7×10^{-21}	1.2×10^{-21}	-4.9×10^{-21}	1.3×10^{-21}	-9.7×10^{-22}
97	$-2.01239\,36508\,51118\,68518\,27733\,602\times 10^{159}$	48	9.1×10^{-22}	-1.6×10^{-21}	3.7×10^{-21}	-1.6×10^{-21}	3.3×10^{-22}
98	$-2.07481\,83306\,90000\,98785\,56764\,834\times 10^{161}$	48	4.8×10^{-22}	1.3×10^{-21}	-3.3×10^{-21}	1.3×10^{-21}	-4.0×10^{-22}
99	$-2.15990\,16249\,32295\,06419\,32336\,636\times 10^{163}$	49	2.6×10^{-22}	-1.2×10^{-21}	2.7×10^{-21}	-1.2×10^{-21}	2.0×10^{-22}
100	$-2.27004\,65857\,57870\,57892\,29967\,158\times 10^{165}$	49	1.4×10^{-22}	1.1×10^{-21}	-2.4×10^{-21}	1.0×10^{-21}	-2.1×10^{-22}

TABLE XV. (*Continued*).

		same-sign subseries			alternating-sign subseries		
				relative	relative asymptotic error after inclusion of terms through order (in N^{-1})		
N	$E^{(N)}$(exact)	k_{min}	smallest term	asymptotic error	0	1	2
105	$-3.34887\ 31765\ 21245\ 83788\ 50242\ 260 \times 10^{175}$	51	5.9×10^{-24}	-5.9×10^{-22}	1.1×10^{-21}	-5.1×10^{-22}	6.8×10^{-23}
110	$-6.19247\ 66051\ 35553\ 60449\ 62734\ 926 \times 10^{185}$	51	2.9×10^{-25}	3.1×10^{-22}	-5.7×10^{-22}	2.5×10^{-22}	-3.7×10^{-23}
115	$-1.42134\ 73900\ 14061\ 05461\ 23906\ 579 \times 10^{196}$	51	1.7×10^{-26}	-1.7×10^{-22}	3.0×10^{-22}	-1.2×10^{-22}	1.8×10^{-23}
120	$-4.01350\ 46348\ 84955\ 00256\ 59932\ 505 \times 10^{206}$	51	1.2×10^{-27}	9.8×10^{-23}	-1.6×10^{-22}	6.4×10^{-23}	-9.5×10^{-24}
125	$-1.38280\ 24776\ 68477\ 37271\ 74455\ 133 \times 10^{217}$	51	9.4×10^{-29}	-5.7×10^{-23}	8.7×10^{-23}	-3.4×10^{-23}	5.0×10^{-24}
130	$-5.76908\ 79997\ 60099\ 90273\ 22398\ 986 \times 10^{227}$	51	8.3×10^{-30}	3.4×10^{-23}	-4.9×10^{-23}	1.9×10^{-23}	-2.7×10^{-24}
135	$-2.89404\ 47723\ 41030\ 70694\ 09814\ 842 \times 10^{238}$	51	8.3×10^{-31}	-2.0×10^{-23}	2.8×10^{-23}	-1.0×10^{-23}	1.5×10^{-24}
140	$-1.73425\ 01258\ 17999\ 54002\ 35382\ 259 \times 10^{249}$	51	9.1×10^{-32}	1.2×10^{-23}	-1.6×10^{-23}	6.0×10^{-24}	-8.6×10^{-25}
145	$-1.23389\ 62504\ 95032\ 24434\ 05554\ 295 \times 10^{260}$	51	1.1×10^{-32}	-7.7×10^{-24}	9.8×10^{-24}	-3.5×10^{-24}	5.0×10^{-25}
150	$-1.03641\ 42160\ 91805\ 70362\ 06542\ 761 \times 10^{271}$	51	1.5×10^{-33}	4.9×10^{-24}	-6.0×10^{-24}	2.1×10^{-24}	-2.9×10^{-25}
	Excited state: $n_1=0$, $n_2=0$, $m=1$						
45	$-3.49959\ 20366\ 93598\ 91668\ 17769\ 328 \times 10^{58}$	22	7.5×10^{-10}	-2.7×10^{-10}	-6.6×10^{-10}	-2.4×10^{-10}	-1.7×10^{-10}
46	$-1.70905\ 86893\ 95210\ 74016\ 63064\ 942 \times 10^{60}$	23	4.1×10^{-10}	-5.7×10^{-12}	3.0×10^{-10}	-2.9×10^{-11}	-7.6×10^{-11}
47	$-8.51750\ 20559\ 09728\ 74946\ 57078\ 558 \times 10^{61}$	23	2.2×10^{-10}	-6.1×10^{-11}	-3.1×10^{-10}	-4.4×10^{-11}	-1.3×10^{-11}
48	$-4.33020\ 10973\ 72823\ 98193\ 60749\ 684 \times 10^{63}$	24	1.2×10^{-10}	-1.8×10^{-11}	1.8×10^{-10}	-3.1×10^{-11}	-5.1×10^{-11}
49	$-2.24479\ 16414\ 87821\ 85905\ 65104\ 858 \times 10^{65}$	24	6.4×10^{-11}	-3.6×10^{-12}	-1.6×10^{-10}	5.4×10^{-12}	1.8×10^{-11}
50	$-1.18618\ 97135\ 90882\ 24223\ 81705\ 143 \times 10^{67}$	25	3.4×10^{-11}	-1.7×10^{-11}	1.1×10^{-10}	-2.4×10^{-11}	-3.2×10^{-11}
51	$-6.38684\ 60774\ 93345\ 40838\ 33238\ 854 \times 10^{68}$	25	1.8×10^{-11}	9.3×10^{-12}	-9.6×10^{-11}	1.4×10^{-11}	1.8×10^{-11}
52	$-3.50285\ 91147\ 92997\ 96351\ 76467\ 618 \times 10^{70}$	26	9.9×10^{-12}	-1.4×10^{-11}	7.2×10^{-11}	-1.7×10^{-11}	-1.9×10^{-11}
53	$-1.95622\ 12316\ 73804\ 17530\ 76068\ 320 \times 10^{72}$	26	5.3×10^{-12}	1.0×10^{-11}	-6.1×10^{-11}	1.2×10^{-11}	1.3×10^{-11}
54	$-1.11207\ 12695\ 26913\ 49760\ 71599\ 369 \times 10^{74}$	27	2.8×10^{-12}	-1.1×10^{-11}	4.8×10^{-11}	-1.2×10^{-11}	-1.2×10^{-11}
55	$-6.43326\ 98100\ 20438\ 74103\ 15384\ 765 \times 10^{75}$	27	1.5×10^{-12}	8.6×10^{-12}	-4.0×10^{-11}	9.3×10^{-12}	8.5×10^{-12}
60	$-5.36148\ 52495\ 03114\ 46697\ 41902\ 328 \times 10^{84}$	30	6.4×10^{-14}	-4.4×10^{-12}	1.5×10^{-11}	-4.0×10^{-12}	-2.7×10^{-12}
75	$-2.97729\ 96882\ 91636\ 90670\ 94542\ 361 \times 10^{112}$	37	4.4×10^{-18}	6.1×10^{-13}	-1.4×10^{-12}	3.7×10^{-13}	1.2×10^{-13}
90	$-2.98060\ 26338\ 04127\ 24387\ 81243\ 041 \times 10^{141}$	45	2.6×10^{-22}	-1.1×10^{-13}	2.0×10^{-13}	-5.2×10^{-14}	-8.1×10^{-15}
105	$-3.36203\ 13361\ 38534\ 15647\ 21639\ 506 \times 10^{171}$	51	1.5×10^{-26}	2.7×10^{-14}	-3.8×10^{-14}	9.5×10^{-15}	7.4×10^{-16}
120	$-3.04696\ 22545\ 61093\ 87351\ 71675\ 528 \times 10^{202}$	51	2.4×10^{-30}	-7.7×10^{-15}	9.2×10^{-15}	-2.2×10^{-15}	-7.0×10^{-17}
135	$-1.71925\ 10469\ 39378\ 61467\ 12246\ 696 \times 10^{234}$	51	1.5×10^{-33}	2.5×10^{-15}	-2.6×10^{-15}	5.9×10^{-16}	2.3×10^{-18}
150	$-4.94850\ 17433\ 83943\ 65938\ 49553\ 170 \times 10^{266}$	51	2.3×10^{-36}	-9.1×10^{-16}	8.5×10^{-16}	-1.8×10^{-16}	2.6×10^{-18}

series at the origin converges. The value of β_2 is determined by matching logarithmic derivatives. The integration path is kept away from $\eta=2$, at which the potential is singular, by keeping η in the lower half-plane. As a consequence, $\beta_2(r)$ for $r>0$ is continuous with $\mathrm{Im}\,r>0$. The numerical values of β_2 so obtained are listed in Table XVII.

To calculate the Borel sum is also straightforward.[26] For unimportant reasons of convenience, the values reported here were not calculated directly by the Borel method, but instead by the sequential Padé approximant method of Reinhardt,[27] which for the related problem of the LoSurdo-Stark effect in hydrogen[26,27] is known from numerical studies to give the same results as the Borel method. (The idea of this method is to generate the power-series expansion at some point away from the origin via Padé approximants of the series at the origin. At a point near the real axis in the right half-plane, β_2 is an analytic function of r, and the power series at that point converges on the nearby real axis. The procedure is most easily implemented in a continued-fraction representation of the RSPT series in which the even and odd approximants are the $[N/N]$ and $[N/N+1]$ Padé approximants,[26,28] We were able to calculate up to 70 continued-fraction coefficients for the function and its first 70 derivatives— using the RSPT coefficients through order 140—before completely losing numerical significance.) The numerical results are illustrated in Table XVII for the ground state at three internuclear distances. The values obtained by summing the RSPT series agree within the accuracy of the calculations with the values obtained by solving the differential equation numerically on the semi-infinite interval.

Summation of the imaginary second-exponential-order series for $\Delta_i\beta_2^{[2]}$ [Eq. (228)] and the real first-exponential-order series [Eq. (227)] is also reported in Table XVII. The sequential Padé-Padé method again was used, since these series are even more divergent than the RSPT series. Since only 51 power-series coefficients are available for these two series, Table I, the accuracy of the approximants for the higher derivatives is not as great as for the RSPT series. For $r=12$ and 10, the imaginary series cancels quite well the imaginary part of the Borel sum. For $r=6$, the cancellation is not so marked: clearly, higher-exponential-order series are not so small in the $r=6$ case and are needed to cancel the imaginary part of the Borel sum.

It should be noted that for each of the exponentially

TABLE XVI. Neville table for $-E^{(N)}/[e^{-2}(N+1)!]-1$ with up to three alternating-sign correction terms, for the ground state.

N	kth Neville iterate for k =				
	0	1	2	3	4
	with no alternating-sign correction term				
145	0.01282 68094 126	0.0009 887	−0.0000 199	−0.0003 504	−0.0253 500
146	0.01274 56323 515	0.0009 750	−0.0000 124	0.0003 444	0.0250 107
147	0.01266 54677 424	0.0009 614	−0.0000 190	−0.0003 365	−0.0246 785
148	0.01258 62975 623	0.0009 483	−0.0000 119	0.0003 308	0.0243 527
149	0.01250 81030 018	0.0009 353	−0.0000 182	−0.0003 233	−0.0240 335
150	0.01243 08668 759	0.0009 227	−0.0000 115	0.0003 179	0.0237 204
	with first alternating-sign correction term				
145	0.01282 68095 127	0.0009 887	−0.0000 156	0.0000 697	0.0050 078
146	0.01274 56322 555	0.0009 749	−0.0000 166	−0.0000 669	−0.0049 134
147	0.01266 54678 345	0.0009 615	−0.0000 149	0.0000 662	0.0048 212
148	0.01258 62974 739	0.0009 483	−0.0000 159	−0.0000 635	−0.0047 316
149	0.01250 81030 867	0.0009 353	−0.0000 143	0.0000 629	0.0046 440
150	0.01243 08667 944	0.0009 227	−0.0000 153	−0.0000 604	−0.0045 589
	with two alternating-sign correction terms				
145	0.01282 68094 954	0.0009 887	−0.0000 163	−0.0000 032	−0.0002 738
146	0.01274 56322 719	0.0009 749	−0.0000 159	0.0000 042	0.0002 678
147	0.01266 54678 188	0.0009 615	−0.0000 156	−0.0000 031	−0.0002 621
148	0.01258 62974 889	0.0009 483	−0.0000 152	0.0000 039	0.0002 564
149	0.01250 81030 724	0.0009 353	−0.0000 150	−0.0000 029	−0.0002 510
150	0.01243 08668 081	0.0009 227	−0.0000 146	0.0000 037	0.0002 456
	with three alternating-sign correction terms				
145	0.01282 68094 963	0.0009 887	−0.0000 163	0.0000 006	0.0000 021
146	0.01274 56322 711	0.0009 749	−0.0000 159	0.0000 005	−0.0000 022
147	0.01266 54678 196	0.0009 615	−0.0000 156	0.0000 005	0.0000 021
148	0.01258 62974 881	0.0009 483	−0.0000 153	0.0000 005	−0.0000 022
149	0.01250 81030 731	0.0009 353	−0.0000 150	0.0000 005	0.0000 021
150	0.01243 08668 074	0.0009 227	−0.0000 147	0.0000 004	−0.0000 022

small terms, the sum of each real power-series factor is itself also complex. However, here we have only listed the contribution that comes from the real part of the sum of each power-series factor, since the imaginary part would be expected to be canceled by higher-exponential-order series.

The sum of the first-exponential-order series can be either added or subtracted to the sum of the RSPT, leading to the symmetric or antisymmetric members of the double-well pair. Moreover, for quantitative accuracy, it is also necessary to include the real second-exponential-order series, for which we have given two terms in Eqs. (227) and (110), and which comes in only with one sign. The agreement of the sum of the asymptotic series with the numerical eigenvalues for the physical double-well pair is nicely illustrated for $r=12$ and 10, as well as the deteriorating convergence at $r=6$. At this shortest distance, the two-term truncation of the real second-exponential-order series is inadequate, and higher exponential-order contributions are also significant both for the accuracy of the real part and to cancel the imaginary part.

XII. SUMMARY

As set out in the Introduction, we have developed the quasisemiclassical method to solve the H_2^+ eigenvalue problem by asymptotic expansion. The bulk of the calculation has focused on the separation constants β_1 and β_2, which arise from separation in prolate spheroidal coordinates (Sec. II A). The transformation from separation constants to energy $E(R)$ is relatively elementary (Sec. V).

The development of asymptotic expansions for β_1 (Sec. IV) and β_2 (Sec. III) depends first on solving the separated Schrödinger equation near the boundary points, which are also singular points, in terms of Whittaker confluent hypergeometric functions. These solutions are extended away from the boundary points, by expanding the natural variable in a series in the reciprocal internuclear distance. The Schrödinger equation is thereby turned into a Riccati equation that is solved by expansion. A crucial role is played by the b index of the Whittaker function. If taken equal to the unperturbed separation constant, then RSPT is the result of solving the Riccati equation, but the wave function satisfies only the boundary condition at $\eta=0$. If

TABLE XVII. Comparison of values of β_2 obtained by summation of the asymptotic expansion and by numerical solution of the eigenvalue equation (11) with (physical) boundary conditions at $\eta=0$ and $\eta=2$, and with (nonphysical) boundary conditions at $\eta=0$ and $\eta=\infty$, for the ground state.

Computational Method	$\beta_2(r)$		
r=12			
Numerical solution, boundary conditions at 0 and $\infty - i\epsilon$	0.45620 55605 36	+ i 0.51348	x10^{-7}
Sequential Padé-Padé [35/35] for RSPT series	0.45620 55605 36	+ i 0.51347	x10^{-7}
Sequential Padé-Padé [25/26] for $\Delta\beta_2^{(1)}$	-0.00012 17975 46		
Sequential Padé-Padé [25/26] for $i\Delta_i\beta_2^{(2)}$		- i 0.51348	x10^{-7}
Two-term formula (110) for $\Delta_r\beta_2^{(2)}$	0.00000 01152 38		
RSPT + $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.45608 38782 28		
Sym. num. solution, boundary conditions at 0 and 2	0.45608 38789 89		
RSPT − $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.45632 74733 20		
Antisym. num. solution, boundary conditions at 0 and 2	0.45632 74743 50		
r=10			
Numerical solution, boundary conditions at 0 and $\infty - i\epsilon$	0.44675 97795 93	+ i 0.18165 34	x10^{-5}
Sequential Padé-Padé [35/35] for RSPT series	0.44675 97795 92	+ i 0.18165 34	x10^{-5}
Sequential Padé-Padé [25/26] for $\Delta\beta_2^{(1)}$	-0.00071 57275 4		
Sequential Padé-Padé [25/26] for $i\Delta_i\beta_2^{(2)}$		- i 0.18166	x10^{-5}
Two-term formula (110) for $\Delta_r\beta_2^{(2)}$	0.00000 37943		
RSPT + $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.44604 78463		
Sym. num. solution, boundary conditions at 0 and 2	0.44604 78627 33		
RSPT − $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.44747 93014		
Antisym. num. solution, boundary conditions at 0 and 2	0.44747 93660 55		
r=6			
Numerical solution, boundary conditions at 0 and $\infty - i\epsilon$	0.40438 98390 4	+ i 0.13374 2866	x10^{-2}
Sequential Padé-Padé [35/35] for RSPT series	0.40438 984	+ i 0.13374 3	x10^{-2}
Sequential Padé-Padé [25/26] for $\Delta\beta_2^{(1)}$	-0.01825 5		
Sequential Padé-Padé [25/26] for $i\Delta_i\beta_2^{(2)}$		- i 0.13508 0	x10^{-2}
Two-term formula (110) for $\Delta_r\beta_2^{(2)}$	0.00211 94		
RSPT + $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.38825 4	- i 0.00133 7	x10^{-2}
Sym. num. solution, boundary conditions at 0 and 2	0.38805 89412 28		
RSPT − $\Delta\beta_2^{(1)}$ + $i\Delta_i\beta_2^{(2)}$ + $\Delta_r\beta_2^{(2)}$	0.42476 5	- i 0.00133 7	x10^{-2}
Antisym. num. solution, boundary conditions at 0 and 2	0.42504 99757 82		

the boundary condition at $\eta=2$ is also to be satisfied, then the b index gains a sequence of exponentially small series, which in turn imply exponentially small contributions to the separation constant.

The explicit complexness of the expansions, starting in second exponential order, is a consequence of the explicit complexness of the asymptotic expansions for the Whittaker function. That a real function should have a complex asymptotic expansion is not as paradoxical as it might seem (Sec. III F): the asymptotic expansion for the Whittaker function is summable through the Borel summability of its associated power series. The real axis is a cut of the Borel sum. Thus the Borel sum of the RSPT series is complex and discontinuous on the real axis, but the explicit second-exponential-order series has the effect of canceling the implicit imaginary part and making the sum of the entire expansion (including all exponential orders) real and continuous.

The explicit imaginary series is directly related to the discontinuity on the positive real axis (Sec. III I) of the

Borel sum of RSPT for the separation constants, which in turn determines the asymptotics of the RSPT coefficients via a dispersion relation (Sec. VI). In the course of deriving the imaginary second-exponential-order expansion, the relation to the square of the first-exponential-order expansion is obtained, which is the exact version (Secs. III G and V C) of the approximate relation discovered by Brézin and Zinn-Justin.[12] There is also a second imaginary series (Sec. IV) associated with the discontinuity of β_1 on the negative r axis that leads both to alternating-sign and logarithmic contributions to the asymptotics of the RSPT coefficients (Sec. VI). These contributions had in fact implicitly been discovered in an earlier Bender-Wu analysis of the asymptotics of the RSPT for H_2^+.[13]

Extensive numerical illustration has been provided for both the values (Tables I–III, V–VIII, and XI–XIV) and the asymptotic behavior (Tables IV, X, XV, and XVI) of the coefficients of the various series. In particular, the relation between the imaginary series and the RSPT asymptotics is verified in practice (Tables IV, X, XV, and XVI). The higher the quantum numbers n_1 and n_2 the more slowly the RSPT approaches asymptotic behavior. The alternating-sign contributions to both $\beta_1^{(N)}$ and to $E^{(N)}$ have been explicitly demonstrated (Tables X, XV, and XVI).

The RSPT series for β_2 has been summed and shown (Table XVII) to agree numerically with the numerical solution of the differential equation for β_2 on a semi-infinite domain, the analytic continuation to negative r' or the closely related $\beta_1'(r')$ for the electron moving in the field of a proton and an antiproton. For instance, at $r=10$ the sum of the RSPT series for β_2 is $0.446\,759\,779\,592+i\,0.181\,653\,4\times10^{-5}$, while direct numerical integration of the differential equation gives $0.446\,759\,779\,593+i\,0.181\,653\,4\times10^{-5}$. For the physical β_2, the sum of all the β_2 subseries together agrees well with the numerically solved values for β_2 for large r (≥ 10), but still more terms and subseries are needed for smaller r ($r=6$ being the example given in Table XVII).

Such a richly complex asymptotic expansion for such a simple problem was not anticipated.

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[1]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Academic, New York, 1965).

[2]R. J. Damburg and R. Kh, Propin, J. Phys. B 1, 681 (1968).

[3]J. D. Morgan and B. Simon, Int. J. Quantum Chem. 17, 1143 (1980).

[4]E. M. Harrell, Commun. Math. Phys. 75, 239 (1980).

[5]R. J. Damburg, R. Kh. Propin, S. Graffi, V. Grecchi, E. M. Harrell II, J. Čížek, J. Paldus, and H. J. Silverstone, Phys. Rev. Lett. 52, 1112 (1984).

[6]S. Graffi, V. Grecchi, E. Harrell, and H. J. Silverstone, Ann. Phys. (N.Y.) (to be published). See this reference, as well as Refs. 2 and 3, for an extensive bibliography and for references to earlier work.

[7]H. J. Silverstone, S. Nakai, and J. G. Harris, Phys. Rev. A 32, 1341 (1985).

[8]J. Zinn-Justin, Nucl. Phys. B192, 125 (1981).

[9]J. Zinn-Justin, Nucl. Phys. B218, 333 (1983).

[10]J. Zinn-Justin, J. Math. Phys. 25, 549 (1984).

[11]C. G. J. Jacobi, *Gesammelte Werke*, Vol. 8, *Vorlesungen über Dynamik* (Reimer, Berlin, 1884).

[12]E. Brézin and J. Zinn-Justin, J. Phys. (Paris) Lett. 40, L-511 (1979).

[13]J. Čížek, M. R. Clay, and J. Paldus, Phys. Rev. A 22, 793 (1980).

[14]R. Damburg and R. Propin, Int. J. Quantum Chem. 21, 191 (1981).

[15]E. Schrödinger, Ann. Phys. (Leipzig) 80, 437 (1926).

[16]H. J. Silverstone, Phys. Rev. A 18, 1853 (1978).

[17]R. E. Langer, Phys. Rev. 51, 669 (1937).

[18]T. M. Cherry, Trans. Am. Math. Soc. 68, 224 (1950).

[19]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun, Natl. Bur. Stand. (U.S.) Appl. Math. Ser. No. 55 (U.S. GPO, Washington, D.C., 1964).

[20]H. Buchholtz, *The Confluent Hypergeometric Function* (Springer, New York, 1969).

[21]R. B. Dingle, *Asymptotic Expansions: Their Derivation and Interpretation* (Academic, New York, 1973).

[22]Logarithmic terms in the small-R energy expansion have been known for some time. See, for instance, W. Byers-Brown and E. Steiner, J. Chem. Phys. 44, 3934 (1966), and M. Klaus, J. Phys. A 16, 2709 (1983).

[23]B. Simon, Int. J. Quantum. Chem. 21, 3 (1982).

[24]H. J. Silverstone, J. G. Harris, J. Čížek, and J. Paldus, Phys. Rev. A 32, 1965 (1985).

[25]See, e.g., G. Birkhoff and G.-C. Rota, *Ordinary Differential Equations*, 3rd ed. (Wiley, New York, 1978).

[26]V. Franceschini, V. Grecchi, and H. J. Silverstone, Phys. Rev. A 32, 1338 (1985).

[27]W. P. Reinhardt, Int. J. Quantum. Chem. 21, 133 (1982).

[28]G. Graffi, V. Grecchi, and G. Turchetti, Nuovo Cimento B 4, 313 (1971).

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POTENTIALS PRODUCING MAXIMALLY SHARP RESONANCES

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ABSTRACT. We consider quantum-mechanical potentials consisting of a fixed background plus an additional piece constrained only by having finite height and being supported in a given finite region in dimension $d \leqslant 3$. We characterize the potentials in this class that produce the sharpest resonances. In the one-dimensional or spherically symmetric specialization, a quite detailed description is possible. The maximally sharp resonances that we find are, roughly speaking, caused by barrier confinement of a metastable state, although in some situations they call for interactions in the interior of the confining barrier as well.

I. Introduction. One of the standard topics of quantum mechanics is the tunneling effect. A large potential barrier blocks a particle imperfectly, and the effect of the penetration can show up in scattering as a sharp resonance. In the time-independent analysis of the Schrödinger equation, resonances make their appearance in the guise of nonreal eigenvalues defined with an outgoing-wave condition or complex scaling. Up to physical constants, ε, which will denote (minus) the imaginary part of this eigenvalue, measures the width of the resonance in units of energy, and a sharp resonance is one with small ε. The real part, E, roughly locates the physical energy at which the resonance is observed. The quantity ε may also be inversely proportional to the lifetime of a metastable state, according to the indeterminacy principle. We shall consider relatively compact potentials V supported in finite regions in one or three dimensions, which are exterior-dilatation analytic in the sense described by Simon and by Graffi and Yajima **[14, 6]**. They also seem to fall within the scope of other recent generalizations of the complex scaling method **[3, 4, 10, 13]**, although we have not yet seen the definitive versions of all of these generalizations. The simplest model of an alpha-emitting nucleus, being a spherical square-well, fits this description, and its sharp resonances are associated with the metastable states caused physically by confinement of particles within the nucleus by a potential barrier at its periphery. It is not obvious, however, that other mechanisms might not also exist for causing resonances. For instance, could some very complicated potential, such as arises in studies of random media, cause as sharp a scattering resonance as a confining barrier? We will find below that the answer is in essence no.

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This paper uses and extends ideas in two earlier works by Harrell [7, 8]. In [7] Harrell studied the one-dimensional Schrödinger equation

$$-d^2\psi/dx^2 + (V(x) - k^2)\psi = 0, \qquad k^2 = E - i\varepsilon, \tag{1.1}$$

with outgoing boundary conditions at 0 and an arbitrary other fixed point L. Positive lower bounds were derived for ε depending only on the support $\subset [0, L]$ and magnitude of V and on the real part of the resonance eigenvalue E, which therefore apply to random or otherwise imperfectly known potentials. That article relied on comparison techniques to generate inequalities, but an alternative approach, which we follow here, is to attempt actually to find the most highly resonant possible potential within some category. This could then be analyzed, if necessary numerically, to furnish optimal bounds on ε. Harrell's other paper [8] investigated the problem of determining the potential that optimizes a different spectral property, namely the ground-state eigenvalue of an n-dimensional Schrödinger operator, and further progress on related problems was made recently in [2]. This provides both a method and a reason for hoping for success in the resonance problem, which is, however, in many ways less tractable, especially because it is not selfadjoint.

In this paper we study equation (1.1) and its higher-dimensional analogue,

$$(-\Delta + V(x))\psi = k^2\psi. \tag{1.2}$$

In the one-dimensional case we shall pose slightly different boundary conditions from those of [7], viz.,

$$\psi(0) = 0 \quad \text{and} \quad \psi(L) = 1, \quad \psi'(L) = ik, \tag{1.3}$$

i.e., Dirichlet conditions at 0 and the traditional outgoing conditions at L. The lower bound derived in [7], which assumed outgoing conditions at both endpoints, carries over immediately with only minor changes. Boundary conditions (1.3) are appropriate if one thinks of the one-dimensional problem as coming from separation of variables in a spherically symmetric three-dimensional problem, and would describe S-wave resonances; it will thus be referred to as the totally spherically symmetric case. Resonances for subspaces of nonzero angular momentum would correspond to an outgoing condition of the form

$$\psi'(L)/\psi(L) \to ik \quad \text{as } L \to \infty$$

and will be discussed further in [15].

Since the boundary conditions (1.3) depend on the eigenvalue parameter k^2, it looks at first as if (1.1) and (1.3) do not constitute an operator eigenvalue problem, but in fact it is easy to show that these equations are equivalent to the eigenvalue problem for the one-dimensional, exteriorly dilated version of the operator $-\Delta + V$, since any eigensolution reduces to a plane wave $C\exp(ikx)$ in the region exterior to the potential but interior to the sphere where exterior dilatation sets in. To sum up, for our purposes:

DEFINITION. A resonance is a triple $\langle k^2, V(x), \psi(x)\rangle$ related by (1.2) and the auxiliary conditions mentioned above, with $\operatorname{Re} k^2 \geqslant 0$ and $\operatorname{Im} k^2 < 0$. We shall frequently refer to k^2 for short as the resonance, and will call ψ (either as a local solution or as an exteriorly dilated solution) the resonance wave-function.

We shall address the following question: Is there a distinguished potential $V_\#$ within a class such as $\{V: 0 \leqslant V \leqslant M, \operatorname{supp} V \subset x: |x| \leqslant L\}$ that minimizes ε in (1.1) or (1.2), and, if so, what is this maximally resonant $V_\#$? We shall also address the question of existence and characterization of potentials that are maximally resonant within a given energy range, and allow a fixed background potential. An analysis of similar questions with other natural classes S over which the potential can vary will appear in [**15**].

A compactness argument will answer the first question in the affirmative, and to characterize $V_\#$ we shall begin by analyzing the effect of small perturbations of it, following an idea of [**8**]. This will give a certain amount of information about $V_\#$; in particular, it will reveal that for the above-mentioned class, $V_\#$ can only equal 0 or M. To get more detailed information on the nature of its support, however, we have to restrict ourselves to the spherically symmetric case and rely on techniques of ordinary differential equations.

II. Preliminaries. The first order of business is to establish the existence of sharp resonances for suitable Schrödinger operators. We shall work in the spaces $\mathbf{R}^+$, $\mathbf{R}^2$, or $\mathbf{R}^3$, and always suppose that the potential V is supported within the ball of radius L centered at the origin. In one dimension this statement will be interpreted as meaning that $\operatorname{supp}(V) \subset [0, L]$. The exterior-wave condition can be incorporated into the eigenvalue problem

$$-\Delta\psi + V\psi = k^2\psi \tag{2.1}$$

most conveniently when the latter is written as an integral equation,

$$\psi = -\int_{|y| \leqslant L} G(x, y; k) V(y) \psi(y)\, dy, \tag{2.2}$$

where we continue onto the second sheet, i.e., with $E = \operatorname{Re}(k^2) > 0$ and $\varepsilon = -\operatorname{Im}(k^2) > 0$,

$$G(x, y; k) = \begin{cases} \exp(ikx_>)\sin(kx_<)/k, & d = 1, \\ iH_0^{(1)}(k|x - y|)/4, & d = 2, \\ \exp(ik|x - y|)/4\pi|x - y|, & d = 3 \end{cases} \tag{2.3}$$

(here H denotes a Hankel function [**16**]). We observe that any solution of (2.2) belongs to $W^2(\Omega)$ for any bounded domain Ω and solves (2.1).

What complex scaling provides for us is a consistent interpretation, in the language of operators on L^2, of this traditional method of defining a resonance. The only facts needed about the exterior scaling formalism are (i) that the associated resonance wave-functions satisfy the Schrödinger equation locally but are modified outside some finite region so as to become square-integrable; and (ii) if J is the antilinear operator of complex conjugation, $Jf = \bar{f}$, then the adjoint of a complex-scaled Hamiltonian operator H_d is simply

$$H_d^* = JH_dJ. \tag{2.4}$$

This prefatory remark should make it clear that our analysis is not strictly tied to the exterior-scaling formalism, but would apply without change to the other alternative complex-scaling techniques that have sprung up recently [**3**, **4**, **10**, **13**]. Since we make only fairly minor use of complex scaling (to justify perturbation theory in Proposition III.1), the detailed discussion of the relationship between it and the integral equation is deferred to [**15**].

It will be helpful to know that there are very sharp resonances for sufficiently large support or potential height, i.e., that ε is exponentially small as a function of these quantities. Suppose that V is supported in the ball of radius L and that $\text{supp}|V| \leqslant M$. There is a scaling relationship between L and M showing that the problem is largely characterized by the combination $L\sqrt{M}$; if x is replaced by $x' = ax$, one finds that the length L becomes aL, while the potential added to $-\Delta'$ becomes $V(x'/a)/a^2$. (The corresponding eigenvalue will also be affected, becoming k^2/a^2.) For convenience, in one dimension we may therefore show the existence of sharp resonances by setting $V = M\chi_{[1,2]}$, a standard textbook variety square-well. It is straightforward to find that the width of the principle resonance is exponentially small, i.e., $\exp(-2\sqrt{M})$ as $M \to \infty$. (A rigorous discussion of this sort of limit, complete with detailed perturbation theory for large barriers of general shape, can be found in [**1**].) For the square barrier $M\chi_{[1,L]}$, there is a resonance whose width is asymptotic to $A\exp(-2L\sqrt{M})$.

Similar analysis of spherically symmetric square-barrier potentials in dimensions 2 and 3 shows that in all cases there are universal positive constants A and B, such that a potential V, $0 \leqslant V \leqslant M$, supported in a ball of radius L, can always be found with a resonance width satisfying

$$\varepsilon < A\exp(-BL\sqrt{M}). \tag{2.5}$$

If necessary, estimates of A and B could be derived without much difficulty. In the totally spherically symmetric case, for example, for any positive A and any $B < 2$, there is a resonance for which (2.5) will hold for L or M sufficiently large.

Fix a function W supported within the ball of radius L and a compact subset Ω of that ball. The function W will play the role of a background potential and will be assumed relatively compact with respect to $-\Delta$. (This will be the case if $W \in L^2$, for example.) Let

$$S = \{V\colon \text{supp}(V) \subset \Omega \text{ and } 0 \leqslant V(x) - W(x) \leqslant M \text{ a.e.}\},$$

let $\varepsilon(V)$ denote any particular resonance width associated with V, and let $E(V)$ be the real part of the corresponding eigenvalue $k^2(V) = E(V) - i\varepsilon(V)$ of $-\Delta + V$.

THEOREM II.1. *Let* $\varepsilon_\# = \inf\{\varepsilon(V)\colon V \in S(C, D)\}$, *where* $S(C, D)$ *is the subset of* S *such that* $0 \leqslant C \leqslant E(V) \leqslant D < \infty$. *We assume* C *and* D *are chosen so that* $\varepsilon_\#$ *is defined* (*i.e., that there is a* V *with a resonance eigenvalue in this energy interval*). *Then*

(i) *There exists a* $V_\# \in S$ *such that* $\varepsilon_\# = \varepsilon(V_\#)$ *and* $C \leqslant E(V) \leqslant D$.

(ii) *If either* $W \geqslant 0$ *a.e. or* $C > 0$, *then* $\varepsilon_\# > 0$.

REMARK. There is no guarantee of uniqueness for the maximally resonant potential, and we expect that there are situations where it is not unique. For instance, suppose that Ω consists of two widely separated disjoint symmetric pieces. There is no physical reason to think that a resonance that would be sharp if only one piece were allowed would necessarily be enhanced if the second piece were equipped with a symmetric bit of potential. On the other hand, we conjecture that the typical situation is uniqueness.

PROOF. Let Ω_1 be an arbitrary finite closed ball containing Ω. Let V_n be a minimizing sequence for ε, i.e., $\varepsilon(V_n) \to \varepsilon_\#$. Let k_n^2 and ψ_n be the associated eigenvalue and eigenfunction. Without loss of generality, since $[C, D]$ is a compact interval, we can pass to a subsequence so that k_n^2 converges. If ψ_n is normalized in $L^2(\Omega_1)$, then (2.1) shows that ψ_n lies in a bounded set in $W^2(\Omega_1)$. By Rellich's theorem this is compactly embedded in $C(\Omega_1)$, so by passing to another subsequence if necessary, it may be assumed that ψ_n converges uniformly on Ω_1. With still another subsequence, we may suppose by the Alaoğlu theorem that V_n converges weakly in $L^2(\Omega_1)$, say to $V_\#$. The limit clearly remains in the set S (integrate V_n by the characteristic function of the set on which putatively $V_\# - W < 0$ or $V_\# - W > M$).

Now note that $V_n\psi_n$ tends weakly to $V_\#\psi_\#$. For fixed $x \in \Omega_1$, the Green function tends to $G(x, y; k_\#)$ in $L^2(\Omega_1, dy)$, so it follows that the right side of

$$\psi_n(x) = -\int_{\Omega_1} G(x, y; k_n)V_n(y)\psi_n(y)\,dy$$

from (2.2) converges pointwise to

$$-\int G(x, y; k_\#)V_\#(y)\psi_\#(y)\,dy.$$

The left side converges uniformly on Ω_1 to $\psi_\#$, so

$$\psi_\#(x) = -\int_{\Omega_1} G(x, y, k_\#)V_\#(y)\psi_\#(y)\,dy \tag{2.6}$$

on Ω_1.

If the minimal value of ε were 0, then the corresponding eigenvalue $k_\#^2$ would either be 0 or a positive embedded real eigenvalue of the selfadjoint realization of the problem (1.2) by the usual argument of dilatation analyticity (see [**12**, §XIII.13], which extends in a straightforward way to exterior scaling). Embedded positive eigenvalues, however, are impossible for bounded, compactly supported potentials (see [**12**, §XIII.13 or **5**]).

It remains to show that if $W \geqslant 0$, there can be no eigenvalue or resonance with $k^2 = 0$. We consider the three-dimensional case only. Suppose the contrary. Then we would have

$$\psi_\# = -(1/4\pi|x|) * V_\#\psi_\#,$$

and because $V_\#$ is compactly supported it would follow that this produces a solution of the Schrödinger equation (without exterior scaling) tending to 0 at ∞. Since (see [**12**, vol. II, p. 183]) in general

$$\Delta|u| \geqslant \mathrm{Re}\big((\bar{u}/|u|)\Delta u\big), \tag{2.7}$$

it follows in this case that

$$\Delta|\psi_\#| \geqslant V_\#|\psi_\#| \geqslant 0. \tag{2.8}$$

Let $f = |\psi(R)| \cos(\sqrt{E}(r - R))$, so $f'' = -Ef$, while $f(R) = |\psi(R)|$ and $f'(R) = |\psi(R)|'$. The Sturm comparison argument now leads to the conclusion that any zero of $|\psi(r)|$ for $r < R$ must lie to the left of the nearest zero of $f(r)$ (see [**9**, p. 334]). Since $\psi(0) = 0$, this means that $\sqrt{E}\, R \geqslant \pi/2$, from which (2.10) follows. □

As for the other regime of high energies, it is known that generally resonance eigenvalues are excluded from a sector in the complex plane of the form $\{0 > \arg(k^2 - \alpha) > -\beta\}$ for some positive α and β. The estimates used by Cycon [**4**], for example, to prove this fact hold uniformly for all $V \in S$. (Although Cycon uses a distorted scaling rather than exterior scaling, the distinction is unimportant in our context.)

COROLLARY II.3. *In the totally spherically symmetric case, if $W \geqslant 0$ a.e. and M or L is sufficiently large, then there exists a potential $V_\#$ that is maximally resonant for the entire range of energies $E(V) \geqslant 0$, and $E(V_\#) > \pi^2/4L^2$.*

DEFINITION. The resonance $\langle k_\#^2, V_\#, \psi_\# \rangle$ with the potential asserted by II.3 to exist will be called the sharpest resonance of all.

III. Characterization of maximally resonant potentials. If a potential is maximally resonant on a set $S(C, D)$, then we term the corresponding resonance maximally sharp, or simply maximal. Thus a resonance is maximal when ε is minimal. It was shown in §II that maximally resonant potentials exist under some physically important circumstances. Suppose now that $V_\#$ is a maximally resonant potential. It will be characterized by a variational analysis, which would equally well characterize minimally resonant potentials or other critical points of the functionals $\varepsilon(V)$. There is no apparent physical significance to other critical points, however. Since the sets S and $S(C, D)$ which we consider here ensure that $V_\#$ is relatively compact with respect to the exteriorly complex dilated version of $-\Delta$, the resonances associated with $V_\#$ are all finitely degenerate and can accumulate only at ∞ or 0. They will always be nondegenerate in the totally spherically symmetric case, and for simplicity we shall restrict ourselves to the problem of characterizing those maximally resonant potentials that have nondegenerate resonance eigenvalues. The functional configuration of $V_\#$ can be probed with small perturbations by appropriate functions. Since this variational analysis is purely local, a convenient definition reads as follows:

DEFINITION. The potential $V_\#$ is locally maximally resonant for the set S (or $S(C, D)$) if it has a resonance eigenvalue $k^2(V_\#)$ such that for sufficiently small δ,

$$\varepsilon(V_\#) = \min\{\varepsilon(V) \colon V \in S, \sup|V - V_\#| < \delta, |k^2(V) - k^2(V_\#)| < \delta\}.$$

The standard methods of perturbation theory allow one to write down a formula for the first-order change in k^2 when $V_\#$ is slightly perturbed, which will be a valuable tool:

PROPOSITION III.1. *Let $P(x)$ be a bounded, real function supported in Ω. If k^2 is a discrete, nondegenerate resonance eigenvalue of $-\Delta + V$, $V \in S$, and ψ_d is the associated eigenfunction $\in L^2$ in the framework of exterior dilatation, then*

$$dk^2(V_d + \kappa P)/d\kappa = \int P\psi_d^2 \Big/ \int \psi_d^2. \tag{3.1}$$

REMARK. With the usual complication of preliminary diagonalization, this formula remains valid for a finitely degenerate eigenvalue.

PROOF. We write $k^2(V + \kappa P)$ for short as $k^2(\kappa)$ and let H_d denote the exteriorly scaled version of $-\Delta + V$ for some fixed scaling parameter. From

$$\left(k^2(\kappa) - k^2(0)\right)(J\psi_d, \psi_d) = \left(J\psi_d, \left(H_d + \kappa P - k^2(0)\right)\psi_d\right),$$

and the differentiability of k^2 and the eigenfunction guaranteed by perturbation theory [**11**, Chapter VII],

$$\begin{aligned} k^{2\prime}(0)(J\psi_d, \psi_d) &= (dJ\psi_d/d\kappa, 0) + (J\psi_d, P\psi_d) + \left(J\psi_d, \left(H_d - k^2(0)\right) d\psi_d/d\kappa\right) \\ &= (J\psi_d, P\psi_d) + \left(\left(H_d^* - \overline{k^2(0)}\right) J\psi_d, d\psi_d/d\kappa\right); \end{aligned}$$

so

$$\left(dk^2(\kappa)/d\kappa\right) \int \psi_d^2 = \int P\psi_d^2.$$

But note that $\int \psi_d^2 \neq 0$, as otherwise the right side would be zero for all the functions P, implying that $\psi_d^2 = 0$ throughout Ω, which is impossible because of the unique continuation property. Therefore we may divide through by the integral, obtaining (3.1). □

THEOREM III.2. *Let $V_\#$ be a maximally resonant potential in the set S. Then*

$$V_\# - W = M\chi_Y \quad a.e. \tag{3.2}$$

except possibly for x on the nodal surface of the corresponding resonance wave function $\{x: \psi_\#(x) = 0\}$.

REMARK. This fact is at first somewhat misleading about the nature of highly resonant potentials, since alternative types of maximally resonant potentials, such as are obtained when V varies over a set with L^p conditions rather than boundedness, turn out to be smooth functions characterized by nonlinear differential equations rather than (3.2) [**15**]. In other words, the discontinuity and two-valuedness of the maximally resonant potential are to some extent artifacts of the particular framework we have erected here. One great advantage that (3.2) brings is numerical feasibility. If a numerical estimate of the minimal resonance width is desired for a potential supported in a given region, the search procedure over this restricted set of potentials is easy to implement. In the spherically symmetric case the maximizers can be further characterized by analytic methods (see §IV).

The nodal surface is necessarily of measure 0 if $V_\#$ is spherically symmetric, and is in any case a nowhere dense set, because of the unique continuation property.

PROOF. Suppose not, and let $F_n = \{x: 0 < 1/n < V_\#(x) - W(x) < M - 1/n\}$ for an arbitrary integer n. For uncluttered notation we call the associated wave-function simply ψ. Recall that ψ and its exteriorly dilated version ψ_d coincide within the undilated region. For almost every $z \in F_n$, we can find a sequence of subsets $G_i \subset F_n$ so that $\mu(G_i) \to 0$, and

$$\psi^2 = \lim_{i \to \infty} \int_{G_i} \psi^2 \, dy/\mu(G_i). \tag{3.3}$$

Now let $P_i(z)$ be the characteristic function of G_i; for $\kappa < 1/n$, $0 < V_\# - W + \kappa P_i(x) < M$, so $\kappa P_i(x)$ is an admissible perturbation for sufficiently small positive or negative κ. If $V_\#$ is maximally resonant, then $\operatorname{Im} dk^2(V_\# + \kappa P_i)/d\kappa = 0$. From (3.1) and (3.3) this means that $\psi^2/\int\psi_d^2 \equiv \alpha\psi^2$ is real for a.e. such z (the denominator must contain the dilated wave-function in order to be finite). Since n is arbitrary, we conclude that $\alpha\psi^2$ is purely real for a.e. $z \in F \equiv \bigcup F_n$.

Consider a point z where, for instance, $\sqrt{\alpha}\,\psi(z) > 0$. We claim that for a.e. such $z \in F$ we can find subsequences $\{z_n\}$ of points of F converging to z from d linearly independent directions. (As before, d denotes the dimension of the space and in our case $d = 1$, 2 or 3. However, if $d = 1$ the statement becomes trivial, so we shall only consider higher dimensions.)

Suppose our claim is false. Let $B(z,\delta)$ be a ball around z of an arbitrarily small radius δ. Then $B(z,\delta) \cap F$ is at most a $(d-1)$-dimensional subset of $\mathbf{R}^d$, so it has measure zero. This, however, contradicts Lebesgue's Theorem on points of density, which states that almost all points of any arbitrary linear set are density points of that set, i.e. for a.e. $z \in F$

$$\lim_{\delta\to 0} \frac{\mu(F \cap B(z,\delta))}{\mu(B(z,\delta))} = 1.$$

Thus our claim is established.

The above claim justifies the next assertion, namely that $\nabla\psi$ can be determined a.e. on F by considering only sequences of points of F. Repeating the same argument one more time we find that $\sqrt{\alpha}\,\Delta\psi$ (or $\sqrt{-\alpha}\,\psi$ where $\alpha\psi^2 < 0$) is real a.e. on F. Then we see that in

$$\sqrt{\alpha}\,(-\Delta + V_\# - E_\#)\psi = -i\sqrt{\alpha}\,\varepsilon_\#\psi$$

the left side would have to be real and the right side imaginary, which means that $\psi = 0$. □

Equation (3.2) is consistent with the expectation that maximally resonant potentials act by confining a particle inside a barrier, i.e., that the potential lies predominantly near the periphery of Ω, but in principle the set Y at this point need have no special position within Ω. The spherically symmetric analysis will bear out the expectation more fully. In one dimension Y will in fact turn out to be (a.e. equivalent to) a finite union of closed intervals (Proposition IV.2).

PROPOSITION III.3. *With α as in the foregoing proof*, $\operatorname{Im}(\alpha\psi^2) \geqslant 0$ *on the set Y of* (3.2), *and* $\operatorname{Im}(\alpha\psi^2) \leqslant 0$ *on the complement of $\overline{Y}$. Moreover, $\alpha\psi^2$ is real on the boundary of Y.*

REMARK. It would thus be possible to modify the normalization of (1.3) and (2.11) so as to make $\operatorname{Im}\psi^2$ respectively $\geqslant 0$ and $\leqslant 0$.

PROOF. For $Z \subset Y$, we may allow a perturbation of the form $V_\# \to V_\# + \kappa\chi_Z$ so long as $\kappa \leqslant 0$, so that the potential remains in S. As in the proof of Theorem III.2, we find that for a.e. $x \in Y$, $\operatorname{Im}(\alpha\psi^2) \geqslant 0$. Similarly, for $Z \subset \overline{Y}'$ we may allow such perturbations so long as $\kappa \geqslant 0$, and the argument of the proof of Theorem III.2 shows that for a.e. $x \notin Y$, $\operatorname{Im}(\alpha\psi^2) \leqslant 0$. Therefore, by the continuity of $\psi_\#$, $\alpha\psi_\#^2$ is real on the boundary of Y. □

IV. The spherically symmetric case. Finally, we embark on the detailed description of the totally spherically symmetric case via a series of propositions and remarks. We will find that the wave-functions of maximal resonances not only suffer from confinement, but they also get kicked when they are down. We show below that, at least for large L or M, maximally resonant potentials must contain a confining barrier stretching to L. We believe that there are locally maximally resonant potentials consisting of more than one barrier, although we do not firmly establish this fact. In particular, as can be seen from (4.1) and (4.3) below, the potential can and will switch on inside the outer barrier if the resonance wave-function has a sufficiently small modulus over a given region. This will happen if the resonance wave-function resembles an excited state of the associated problem with some selfadjoint boundary condition at L, which is ordinarily the case when the resonance width is small. The reason for this conjecture is provided, for example, by [**1**], where resonances are localized near, and asymptotically in one-to-one correspondence with, bound state energies of a related selfadjoint problem. The sharpest resonance of all seems to be generally associated with the ground-state eigenfunction, and its potential contains a confining barrier but no other pieces.

One of the tools for deriving more information about the set Y if there is total spherical symmetry is the formula (2.11) relating any resonance width to the corresponding resonance function on $[0, L]$. It leads to the following:

PROPOSITION IV.1. *In the spherically symmetric case, the argument of any resonance eigenfunction is monotone increasing and twice differentiable. More exactly,*

$$d \arg(\psi)/dr = \varepsilon|\psi(r)|^{-2}\int_0^r |\psi(y)|^2\, dy > 0. \tag{4.1}$$

PROOF. First note that $\psi(r)$ never vanishes except at $r = 0$, as otherwise it would be an eigenfunction of a selfadjoint problem, and ε would have to be 0. If $u = d(\arg\psi)/dr = d(\operatorname{Im}\ln\psi)/dr = \operatorname{Im}(\psi'/\psi)$, then, after the usual Ricatti transformation, the Schrödinger equation becomes

$$u' = \varepsilon - (2\operatorname{Re}(\psi'/\psi))u.$$

Formula (2.11) fixes the limit of integration in the solution of this elementary equation, leading to (4.1). □

PROPOSITION IV.2. *In the spherically symmetric case, the support Y of $V_\# - W$ is a finite union of disjoint intervals, i.e., for some integer $n \geqslant 1$, there are points $0 \leqslant r_1 < r_2 < \cdots < r_{2n} \leqslant L$ for which, if we let $B(j) = [r_{2j-1}, r_{2j}]$, $G(j) = [r_{2j}, r_{2j+1}]$, then*

$$Y = \bigcup_{j=1}^{n} B(j). \tag{4.2}$$

In addition, the following estimates hold for the lengths of the intervals $B(j)$ and gaps $G(j)$: For all j except (i) *$j = 1$ when $r_1 = 0$, or* (ii) *$j = n$ when the associated interval or gap includes the value L,*

$$|B(j)| > \pi \min_{B(j)}|\psi_\#|^2/2K \quad \text{and} \quad |G(j)| > \pi \min_{G(j)}|\psi_\#|^2/2K, \tag{4.3}$$

where, as before, $K = \operatorname{Re} k$.

DEFINITION. We call the intervals $B(j)$ the barriers and the intervals $G(j)$ the gaps.

PROOF. From Propositions III.3 and IV.1 it follows that in one dimension the potential switches on or off exactly at the places where the argument of $\psi_{\#}$ increases by $\pi/2$ from the first point at which it switches on or off. Since $\psi_{\#}$ satisfies a regular Sturm-Liouville equation and vanishes at 0, it is continuously differentiable with $\psi'_{\#}(0) \neq 0$ (else it would vanish everywhere). It follows that the expression in (4.1) is bounded for all r, so there can only be a finite number of switchings. This establishes (4.2).

The estimates (4.3) follow from (4.1). The limiting phase at $r = 0$ is undetermined, so the first switching point is likewise undetermined. Also, the potential is switched off by construction at L regardless of phase. For the other switching points, however, (4.1) implies that

$$\pi/2 = \varepsilon \int_{B(j) \text{ or } G(j)} dr |\psi(r)|^{-2} \int_0^r |\psi(y)|^2 \, dy.$$

Now replace r by L and substitute from (2.11) to get

$$\pi/2 < K \int_{B(j) \text{ or } G(j)} dr |\psi(r)|^{-2},$$

and, finally, estimate the remaining integral by the length of the interval times the maximum of the integrand. □

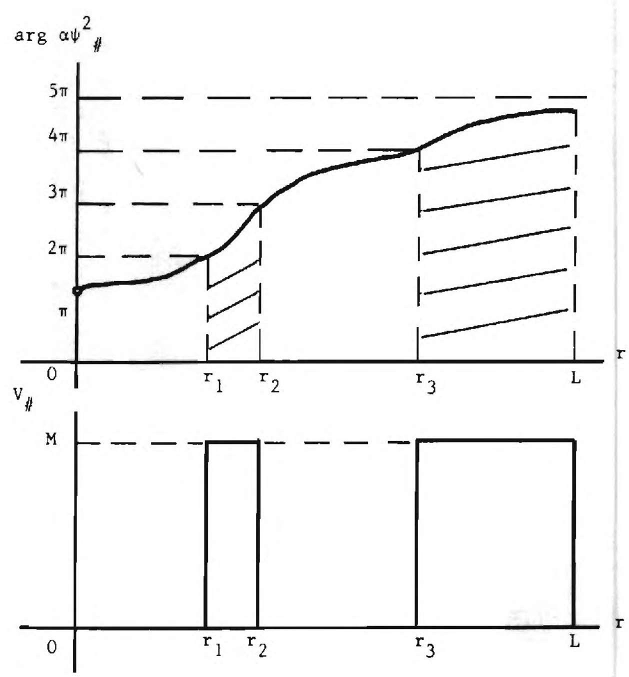

FIGURE 1. The relationship between the argument of the resonance function and the on and off intervals of the maximally resonant potential. The potential equals M in the shaded intervals and 0 otherwise.

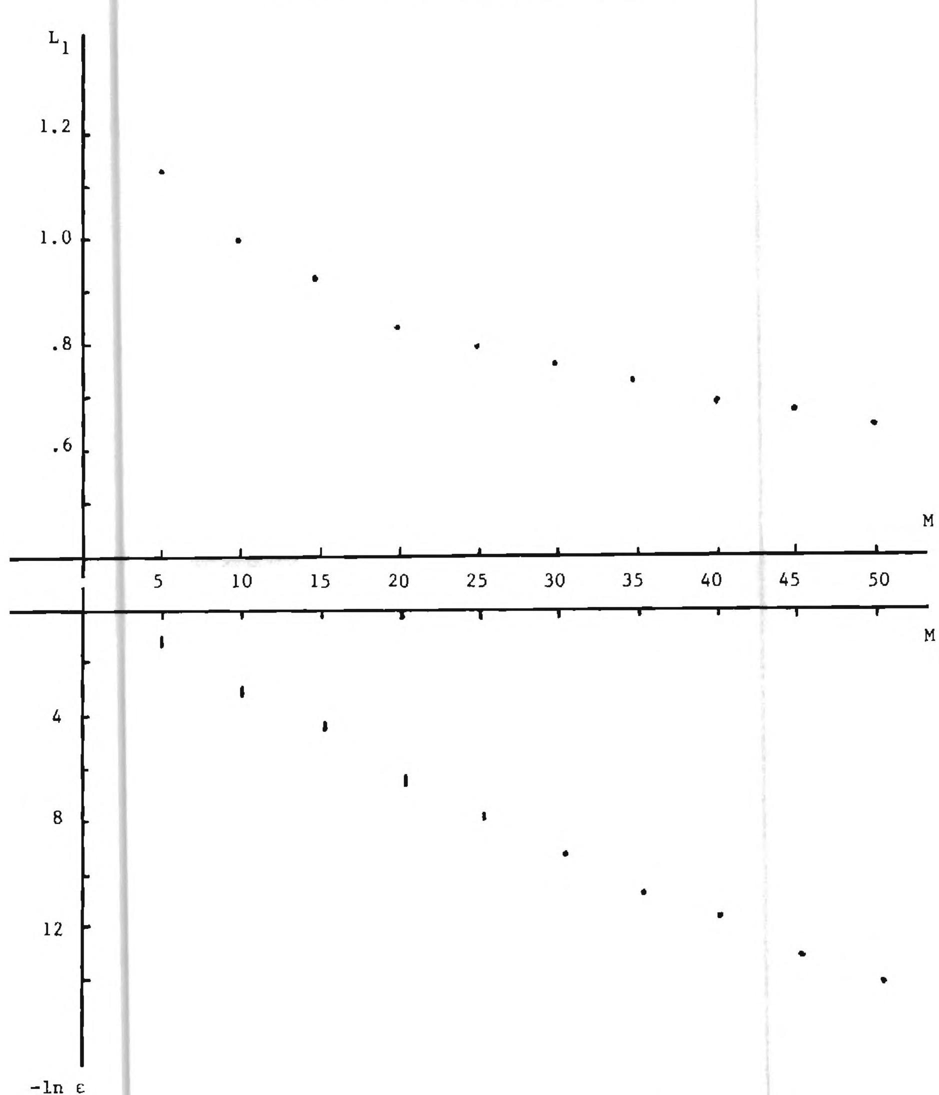

FIGURE 2. We fix $L = 2$ and assume that $V = M\chi_{[L_1, 2]}$. Then we numerically evaluate $\varepsilon(L_1)$ and $d\varepsilon/dL_1$ for different values of L_1. Points on the first graph represent optimal values of L_1 for each fixed value of M and points on the second graph represent corresponding values of ln ε.

From now on we set $W = 0$. Once k^2 is determined for a (locally) maximally resonant potential, there is a simple algorithm for determining the positions of the finite number of "on" and "off" intervals. Since $\psi_{\#}$ is respectively either a linear combination of exponential functions $\exp(\pm k'r)$, $k' = \sqrt{M - k^2}$, or a combination of sinusoidal functions $\sin(kr)$ and $\cos(kr)$ and is continuously differentiable at the switch points, it is a matter of algebra to determine the argument at any given point. The argument steadily increases from the point $r = 0$, and the potential switches on and off whenever it increases by $\pi/2$. The limiting initial phase at $r = 0$ is determined by the condition that the eigenfunction satisfies the resonance condition at $r = L$.

DEFINITION. A resonance will be called typical if $L\sqrt{M} > \pi/2$ and its real part satisfies

(4.4) $$\pi^2/4L^2 < E < 0.9M$$

and

(4.5) $$\max(-\operatorname{Im}(k/\sqrt{M}), \operatorname{Im}(k'/\sqrt{M}), -\operatorname{Im}(k/k'), \operatorname{Im}(k'/k)) < \exp(-L^{1/2}M^{1/4}),$$

where $k' = (M - k^2)^{1/2}$ (conventionally in the first quadrant).

It is not hard to see from Proposition II.2 that for large L or M maximally sharp resonances in this energy range have to be typical, and tunneling estimates indicate that resonances above this energy range are not extremely sharp (some bounds on widths will appear in [**15**]). In particular, the sharpest resonance of all is typical when L or M is sufficiently large. Our last claim states that typical maximally sharp resonances are due at least in part to barrier confinement:

PROPOSITION IV.3. *If a totally spherically symmetric resonance is typical and locally maximal, then r_{2n} (cf. Proposition* IV.2) *equals L.*

PROOF. Suppose not. Then the outermost barrier ends at a point $z < L$. There are then two possibilities: either (a) there is only one barrier stretching from 0 to z, or (b) the argument of $\psi_\#$ increases by $\pi/2$ on the barrier $[y, z]$ with $y > 0$. Possibility (a) is easily checked not to be typical (or maximally sharp), so (b) would have to prevail. But if z is the outermost edge of the potential, then $\psi_\#$ satisfies an outgoing condition at z of the form $\psi'_\#(z)/\psi_\#(z) = ik$. We may modify (1.3) by a fixed multiplicative constant and assume that $\psi_\#(z) = 1$, which means that on $[y, z]$, $\psi_\#(r) = \cosh(k'(z-r)) - i(k/k')\sinh(k'(z-r))$. Hence $\cosh(k'(z-y)) - i(k/k')\sinh(k'(z-y))$ must be purely imaginary. Taking the real part and dividing by a real quantity, we find that

$$0 = 1 + \tanh(\operatorname{Re}(k')(z-y))\operatorname{Im}(k/k') + \tan(\operatorname{Im}(k')(z-y))\operatorname{Re}(k/k').$$

This is impossible if (4.5) holds, as can be seen by substitution and straightforward estimates. □

We close with the result of a representative numerical study of the maximally resonant potentials in the totally spherically symmetric case. We fix $L = 2$ and consider various barrier heights M. Tunneling estimates indicate that the maximal resonance for these values arises from a single barrier with $V = M\chi_{[L_1, 2]}$. The optimal values of L_1 and the corresponding ε are depicted in Figure 2. The error bars are numerical estimates but are not rigorously established.

REFERENCES

1. M. S. Ashbaugh and E. M. Harrell II, *Perturbation theory for shape resonances and large barrier potentials*, Comm. Math. Phys. **83** (1982), 151–170.

2. ______, *Maximal and minimal eigenvalues and their associated nonlinear equations*, preprint 1985.

3. E. Balslev, *Local spectral deformation techniques for Schrödinger operators*, Inst. Mittag-Leffler Report 14, 1982, Resonances, Resonance Functions, and Spectral Deformations, Zentrum für interdisziplinäre Forschung, preprint, 1984.

4. Hans Cycon, *Resonances defined by modified dilations*, preprint, 1984.

5. M. S. P. Eastham and H. Kalf, *Schrödinger-type operators with continuous spectra*, Pitman, Boston, Mass., 1982.

6. S. Graffi and K. Yajima, *Exterior complex scaling and the AC-stark effect in a Coulomb field*, Comm. Math. Phys. **89** (1983), 277–301.[3]

7. E. M. Harrell II, *General lower bounds for resonances in one dimension*, Comm. Math. Phys. **86** (1982), 221–225.

8. ______, *Hamiltonian operators with maximal eigenvalues*, J. Math. Phys. **25** (1984), 48–51.

9. P. Hartman, *Ordinary differential equations*, Wiley, New York, 1964.

10. W. Hunziker, private communication.

11. T. Kato, *Perturbation theory for linear operators*, Springer, New York, 1966.

12. M. Reed and B. Simon, *Methods of modern mathematical physics*, four volumes, Academic Press, New York, 1972–1979.

13. I. Sigal, *Complex transformation method and resonances in one-body quantum systems*, Weizmann Institute, preprint, 1983.

14. B. Simon, *The definition of molecular resonance curves by the method of exterior complex scaling*, Phys. Lett. A**71** (1979), 211–214.

15. R. Svirsky, Johns Hopkins dissertation, 1985.

16. E. C. Titchmarsh, *Eigenfunction expansions associated with second order differential equations*, Part II, Oxford Univ. Press, 1958.

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[3]We are informed by the authors that there are some technical lacunae in this paper. They do not, however, affect the exteriorly complex-scaled resolvent as defined in their equation (2.15).

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L^2 ESTIMATES FOR GALERKIN METHODS FOR SEMILINEAR ELLIPTIC EQUATIONS*

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Abstract. Optimal L^2 error estimates are derived for the usual Galerkin method for the semilinear elliptic problem

$$Lu \equiv -\sum_{i,j=1}^{N} \frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right) + a_0(x)u = f(x, u), \qquad x \in \Omega,$$

$$u = 0 \quad \text{on } \partial\Omega.$$

When f_u is bounded inside the resolvent set of L it is shown that the Galerkin equations can be reformulated as a monotone operator problem. Optimal L^2 error estimates then follow. H^1 error estimates are also derived in the case when f_u touches $\sigma(L)$.

Key words. Galerkin method, finite element method, semilinear boundary value problem

AMS(MOS) subject classifications. Primary 65N30; secondary 35J65

1. Introduction. Consider the semilinear elliptic equation

$$Lu \equiv -\sum_{i,j=1}^{N} \frac{\partial}{\partial x_j}\left(a_{ij}(x)\frac{\partial u}{\partial x_j}\right) + a_0(x)u = f(x, u), \qquad x \in \Omega, \tag{1.1}$$

subject to Dirichlet boundary conditions on $\partial\Omega$

$$u = 0, \qquad x \in \partial\Omega. \tag{1.2}$$

The coefficients of L are assumed to be smooth and L to be uniformly elliptic

$$\sum_{i,j=1}^{N} a_{ij}(x)\zeta_i\zeta_j \geqq a \sum_{i=1}^{N} \zeta_i^2, \qquad a > 0, \quad a_0(x) \geqq 0.$$

Also, assume that the nonlinearity f satisfies the Carathéodory conditions and is Lipschitz in u.

Ciarlet, Schultz and Varga [7] have studied the convergence of the Galerkin method for this problem when $\partial f/\partial u$ is bounded below the smallest eigenvalue of L.

Also, Schultz in [14], [15], has considered the convergence of the Galerkin method to (1.1), (1.2) in the complementary instance where $\partial f/\partial u$ is bounded *between* the eigenvalues of L, as in:

Assumption A1. Assume that there is $p < q$ such that for two consecutive eigenvalues of L, $\lambda_k < \lambda_{k+1}$

$$\lambda_k < p \leqq \frac{\partial f}{\partial u}(x, u) \leqq q < \lambda_{k+1}, \qquad x \in \Omega, \quad u \in \mathbb{R}.$$

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In particular, in Theorem 3.5 of [14] and Theorem 4.1 of [15], Schultz has shown that if $f(x, u)$ is *uniformly bounded*, (A1) holds and the substitution operator $u \to f(x, u)$ is Fréchet differentiable, then the Galerkin method converges to the solution of (1.1) in the norm on the space in which $G: u \mapsto f(x, u)$ is Fréchet differentiable with the same rate as for linear problems.

The proof consists of showing that the method is equivalent to the Galerkin method applied to an integral equation formulation of (1.1), (1.2)

$$(1.3) \qquad u = T(u), \qquad T(u) = L^{-1}[f(x, u)].$$

Specifically, if P_E is the elliptic projection operator associated with the bilinear form derived from L by integration by parts, the Galerkin approximation can be represented as: $U \in S^h$ satisfies

$$(1.4) \qquad P_E U = P_E T(U).$$

Convergence results then follow from the following abstract result (for a proof see, e.g., Schultz [14, Thm. 3.2], or Krasnosel'skii [18, Thms. 3.1 or 3.2]).

THEOREM 1. *Suppose $T: H \to H$ is a Fréchet differentiable (nonlinear) compact operator, H a Hilbert space, and S^h a sequence of subspaces such that*

$$\bigcup_{h_0 \geqq h > 0} S^h$$

is dense in H. Suppose further that the following two conditions hold:

(i) 1 *is not an eigenvalue of $DT(u)$,*

(ii) *$P_h: H \to S^h$ is a sequence of uniformly bounded projections. Then,*

(a) *$U \in S^h$ exists for h sufficiently small ($h \leqq h_1$) and converges to u as $h \to 0$.*

(b) *There is a constant $C > 0$ such that*

$$\|u - U\|_H \leqq C \inf_{\chi \in S^h} \|u - \chi\|_H.$$

The problem considered is also related to the work of Brezzi, Descloux, Rappaz and Raviart in [5], [6], [8], [16], [17] on numerical methods for bifurcation problems (in the case where bifurcation does not occur). For example, in Theorems 1 and 2 of Rappaz [17] (see also [16]) an analogous result is obtained under the added condition that

$$G: \mathring{H}^1(\Omega) \to L^2(\Omega) \quad \text{by } u \to f(x, u)$$

is C^2. Specifically, by specializing his abstract result to this setting one obtains that the Galerkin method converges to u optimally in the H^1 norm.

It is tantalizing to think that L^2-estimates could be obtained by the techniques of Schultz or Rappaz by considering $u \mapsto f(x, u)$ as a map $G: L^2(\Omega) \to L^2(\Omega)$. However, this works *only* in the linear case.

Specifically, it is folklore that if the substitution operator $G: L^2 \to L^2$ is Fréchet differentiable then the function f must be *affine* in u. In this case, the original equation is linear. For completeness, we give a proof of this fact.

PROPOSITION. *If $G: L^2(0, 1) \to L^2(0, 1)$ by $u \to f(u)$ is Fréchet differentiable at $u = 0$ then f is affine:*

Proof. Assume G is Fréchet differentiable at $u=0$. Without loss, we can assume that $f(0)=0=f'(0)$ by considering instead the function

$$\tilde{f}(u)=f(u)-[f(0)+f'(0)u].$$

Assuming this, $DG(0)w=f'(0)w-0$ and

$$\lim_{v\to 0}\frac{\|G(0)-G(v)-f'(0)\cdot v\|}{\|0-v\|}=0. \tag{1.5}$$

Choose k so that $f(k)=Q\neq 0$ (if this is not possible then $f=\tilde{f}$ must be $\equiv 0$, i.e., the original f is affine). Then, let $v_n=k\chi_{[0,1/n]}(x)\to 0$ as $n\to\infty$. Formula (1.5) now becomes

$$\lim_{n\to\infty}\frac{\sqrt{\int_0^{1/n}f(v_k)^2\,dx}}{|k|n^{-1/2}}=\lim_{n\to\infty}\frac{|Q|n^{-1/2}}{|k|n^{-1/2}}=\frac{|Q|}{|k|}\neq 0. \qquad \square$$

In this paper, it is shown that L^2 estimates along the lines of these results of Schultz and Rappaz can be obtained without the Fréchet differentiability condition on G and without assuming G is uniformly bounded C^2 or even differentiable. We weaken (A1) to the following assumption on the function $f(x, u)$.

Assumption A2. Assume $f\in C^0$ is strictly monotone in u. Assume that for some two consecutive eigenvalues $\lambda_k<\lambda_{k+1}$ of L and real numbers p, q, $\lambda_k<p\leqq q<\lambda_{k+1}$, $f(x, u)$ and its inverse are Lipschitz with respect to u with Lipschitz constants bounded by q and $1/p$, respectively.

When $f\in C^1$ in u then (A2) is equivalent to (A1). For general operator equations in a Hilbert space (A1) and (A2) can also be restated as a two sided monotonicity condition.

2. Formalism. Associated with L is a bilinear form $a(\cdot,\cdot):\mathring{H}^1(\Omega)\times\mathring{H}^1(\Omega)\to\mathbb{R}$ by

$$a(v, w)=\int_\Omega\left[\sum_{i,j=1}^{N}a_{ij}(x)\frac{\partial v}{\partial x_i}\frac{\partial w}{\partial w_j}+a_0(x)vw\right]dx.$$

From the assumptions on L it follows easily that $a(\cdot,\cdot)$ is continuous and coercive on $\mathring{H}^1(\Omega)$. The true solution to (1.1), (1.2) satisfies

$$a(u, v)=(f(\cdot, u), v)\quad \forall v\in\mathring{H}^1(\Omega).$$

Let S^h denote a finite dimensional subspace of $\mathring{H}^1(\Omega)$. The Galerkin approximation $u^h\in S^h$ is given by the equations

$$a(u^h, v)=(f(\cdot, u^h), v)\quad \forall v\in S^h.$$

Define the continuous and discrete solution operators T_γ and $T_{\gamma,h}$ to the associated linear problem as follows. For $g(x)\in L^2(\Omega)$ and $-\gamma\notin\sigma(L)$, $T_\gamma g$ is the unique function in $\mathring{H}^1(\Omega)$ satisfying

$$a(T_\gamma g, v)+\gamma(T_\gamma g, v)=(g, v)\quad \forall v\in\mathring{H}^1(\Omega).$$

Similarly, define $T_{\gamma,h}:L^2(\Omega)\to S^h\subset\mathring{H}^1(\Omega)$ by

$$a(T_{\gamma,h}g, v)+\gamma(T_{\gamma,h}g, v)=(g, v)\quad \forall v\in S^h.$$

Assume S^h satisfies the approximation property standard for finite element spaces. For some $r>0$ and all $u\in H^s(\Omega)\cap\mathring{H}^1(\Omega)$, $1\leqq s\leqq r$.

$$\inf_{\chi\in S^h}\{\|u-\chi\|+h\|u-\chi\|_1\}\leqq Ch^2\|u\|_s,\qquad 1\leqq s\leqq r. \tag{2.1}$$

The following convergence result of Schatz [13] for the linear equation will be used.

There is an h_0 such that for $h \leqq h_0$ and $g \in H^s(\Omega)$

$$\|(T_{\gamma,h} - T_\gamma)g\| \leqq Ch^{s+2}\|g\|_s, \qquad -1 \leqq s \leqq r-2. \tag{2.2}$$

Sometimes it will also be convenient work with the discrete operator $L_h = (T_{0,h}|_{S^h})^{-1}$.

3. The convergence theorem.

THEOREM. *Assume* (A2) *holds and* S^h *satisfies* (2.1). *Then, for h sufficiently small* u^h *exists uniquely and satisfies*

$$\|u - u^h\| \leqq C\|[T_\gamma - T_{\gamma,h}]v\|$$

for some $-\gamma \notin \sigma(L)$, *where* $v(x) = \gamma u(x) + f(x, u(x))$.

Rates of convergence then follow immediately.

COROLLARY. (a) *Under the hypotheses of the above theorem*

$$\|u - u^h\| \leqq Ch^{s+2}\|v\|_s, \qquad -1 \leqq s \leqq r-2,$$

holds.

(b) *Suppose t is sufficiently large* ($t > N/2$) *that* $H^t(\Omega) \subset C^0(\Omega)$, $f \in C^s$ *and* $u \in H^s(\Omega) \cap \mathring{H}^1(\Omega)$. *Then,* $\|u - u^h\| \leqq Ch^{s+2}$, $t \leqq s \leqq r-2$, *where C depends on* $\|u\|_s$ *and f.*

Proof of the theorem. Existence and uniqueness of u^h follow from abstract existence results for semilinear equations in, for example, Amann [2, Thm., p. 150] and Mawhin [9, Thm. 2] applied to the equations $L_n u^h = f(\cdot, u^h)$, by noting that (2.2) implies convergence in the operator norm $\|T_{0,h} - T_0\| \to 0$. Thus, $\sigma(T_{0,h}) \to \sigma(T_0)$ as $h \to 0$, so that for h sufficiently small p and q in (A2) are between successive eigenvalues of L_h, so that (A2) is verified for the discrete equations. Thus, for h sufficiently small u^h exists uniquely.

For the error estimate, note that $u - u^h$ satisfies the equation

$$u - u^h = T_{0,h}[f(\cdot, u) - f(\cdot, u^h)] + [T_0 - T_{0,h}]f(\cdot, u).$$

For $-\gamma \notin \sigma(L)$ and h sufficiently small, $-\gamma \notin \sigma(L_h)$. Thus, adding and subtracting terms to the above equation is possible, giving

$$u - u^h = T_{\gamma,h}[F(\cdot, u) - F(\cdot, u^h)] + [T_\gamma - T_{\gamma,h}]F(\cdot, u) \tag{3.1}$$

where $F(x, u) = \gamma u + f(x, u)$.

Note that since f satisfies (A2), F satisfies a condition related to (A2) in an obvious way:

$$(\gamma + q)\|v - w\|^2 \leqq (F(x, v(x)) - F(x, w(x)), v - w) \leqq (\gamma + p)\|v - w\|^2,$$

for all $v, w \in L^2(\Omega)$. This gives an estimate on $\|F(u) - F(u^h)\|$ using the result of Brézis and Nirenberg [4, Appendix A] or Mawhin [9, Lemma 1, p. 270],

$$\|F(u) - F(u^h)\| \leqq \max\{|\gamma + q|, ||\gamma + p|\}\|u - u^h\|. \tag{3.2}$$

Next consider $\|T_{\gamma,h}\|$. Since L_h is a self-adjoint operator, the spectral mapping theorem applied to the function $g(z) = (\gamma + z)^{-1}$ gives

$$\|T_{\gamma,h}\| = \|g(L_h)\| = \operatorname{dist}\{-\gamma, \sigma(L_h)\}^{-1} = \min_j \{|\gamma + \lambda_j^h|\}^{-1} \tag{3.3}$$

where $\{\lambda_j^h\}$ are the eigenvalues of L_h.

Finally, for $v = \gamma u + f(\cdot, u)$, (3.1), (3.2), and (3.3) yield

$$\|u - u^h\| \leqq \alpha_h(\gamma)\|u - u^h\| + \|[T_\gamma - T_{\gamma,h}]v\|,$$

$$\alpha_h(\gamma) = \max\{|\gamma + p|, |\gamma + q|\} \cdot \min\{|\gamma + \lambda_j^h| : j\}^{-1},$$

and the result will follow if there is a choice of $-\gamma \notin \sigma(L)$ such that $\alpha_h(\gamma) < 1$ for h sufficiently small.

Pick $-\gamma = (p+q)/2 \notin \sigma(L)$. Since $T_{0,h} \to T_0$ in the operator norm, $-\gamma \notin \sigma(L_h)$ for h sufficiently small. For the same reason $[p, q]$ is bounded inside $\sigma(L_h)$ for h sufficiently small (Fig. 1).

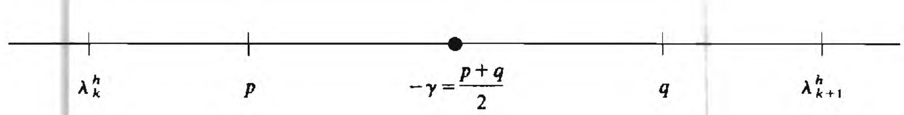

FIG. 1

For this choice of γ, $\alpha_h(\gamma)$ becomes

$$\alpha_h(\gamma) = \left(\frac{q-p}{2}\right) \cdot \max\left\{\left|\lambda_k^h - \frac{p+q}{2}\right|, \left|\lambda_{k+1}^h - \frac{p+q}{2}\right|\right\}^{-1}.$$

Consider Fig. 1. Since the distance from $-\gamma$ to p(or q) is smaller than the distances from $-\gamma$ to λ_k^h or λ_{k+1}^h, it follows that $\alpha_h(\lambda) < 1$. □

Proof of the corollary. The result (b) is a consequence of the Palais lemma (see Palais [12]). Specifically, the map $u \to f(\cdot, u)$ is a C^1 map $H^s(\Omega) \to H^s(\Omega)$ for every $s \geqq t$. Thus $\|f(\cdot, u)\|_s$ is a continuous, finite valued function of $\|u\|_s$. □

Remarks. It is clear that the proof follows for more general methods than considered here. Indeed, whenever a $T_{\gamma,h}$ can be associated with T_γ so that $T_{0,h}$ is self-adjoint positive semidefinite, positive definite on S^h and (2.2) holds, then the theorem holds as well. This includes, for example, the Lagrange multiplier method of Babuška [3] and the methods proposed by Nitsche in [10], [11].

Further, it is clear that the condition (A2) could be weakened to hold only in a neighborhood of the true solution. All the convergence results would then hold for h sufficiently small.

The convergence result is really a statement about nonlinear operators and monotonicity. For example, the following abstract convergence theorem follows by essentially the same argument. Consider a sequence of approximations in a Hilbert space H

$$L_m U^m = N_m(U^m) + f_m, \qquad m = 1, 2, 3, \cdots,$$

to the nonlinear equation for $u \in H$

$$Lu = N(u) + f, \qquad f \in H.$$

Suppose L, L_m are self-adjoint, and each N_m is a continuous gradient operator satisfying

$$p\|v-w\|_H^2 \leqq \langle N_m(v) - N_m(w), v-w\rangle_H \leqq q\|v-w\|_H^2 \quad \forall v, \quad w \in H.$$

Furthermore, suppose that the method is consistent:

$$r_m \equiv L_m u - N_m(u) - f_m \to 0 \quad \text{in } H \text{ as } m \to \infty.$$

THEOREM. *Suppose that either* $\|L_m - L\|_H \to 0$ *or* $\|L_m^{-1} - L^{-1}\|_H \to 0$ *as* $m \to \infty$. *Suppose also* $[p, q] \subset \rho(L)$. *Then, for m sufficiently large, there is a unique* U^m *satisfying*

$$\|u - U^m\|_H \leqq C\|r_m\| \to 0 \quad \textit{as } m \to \infty. \qquad □$$

Of course, the conditions on L_m, N_m, etc. can all be relaxed and the result can be extended to a Banach space, etc.

4. Problems touching an eigenvalue. In this section we consider the case where the nonlinearity just touches a resonance. In this case the approach of Schultz (outlined in the Introduction) can be combined with sharper estimates on the linearized problem to yield convergence results. For simplicity, we consider only one case when f_u touches λ_0.

Let λ_0 be the smallest eigenvalue of L. Assumption (A2) is then weakened as follows to allow f_u to touch λ_0.

Assumption A3. Suppose $u \to f(x, u)$ is Fréchet differentiable as a map: $\mathring{H}^1 \to H^{-1}$. Suppose $f(x, u)$ is C^1 in u for a.e. $x \in \Omega$ and that for a.e. $u \in \mathbb{R}$

$$f_u(x, u) \geqq \alpha(x) \geqq -\lambda_0 \quad \text{a.e. } x \in \Omega$$

where $\alpha(x) > -\lambda_0$ on a set of positive (but possibly very small) measure.

THEOREM 4.1. *Suppose* (A3) *holds and* $L^{-1}: L^2(\Omega) \to \mathring{H}^1(\Omega)$ *compactly. Then, for h sufficiently small, U exists and satisfies*

$$\|u - U\|_1 \leqq C \inf_{\chi \in S^h} \|u - \chi\|_1.$$

Proof. Defining T, P_E as in (1.3), (1.4) the theorem will then follow provided that 1 is not an eigenvalue of $DT(u)$. If 1 is an eigenvalue, we have, for some $w \neq 0$,

$$Lw = f_u(x, u)w, \qquad w \in \mathring{H}^1(\Omega) \cap H^2(\Omega).$$

Letting $q(x) = -f_u(x, u(x))$, we have $q(x) \in L^1(\Omega)$ and $q(x) \geqq -\lambda_0$ for a.e. $x \in \Omega$, with strict inequality holding on a set of positive measure.

Let A denote the self-adjoint realization of $L + qI$, taken as the usual Friedrichs extension. Then, A is positive semidefinite and has purely discrete spectrum with the lowest eigenvalue nondegenerate (see, for instance, Reed and Simon [19]). We now show that the smallest eigenvalue of A is strictly positive by showing it is bounded below by a positive eigenvalue, $E(\theta)$, of an associated problem. This then proves the theorem.

Since q exceeds $-\lambda_0$ on a set T of positive measure, we have for sufficiently small $\mu \geqq 0$

$$\inf_{\substack{\|f\|=1 \\ f \in \mathcal{D}(A)}} (Af, f) \geqq \inf_{\substack{\|f\|=1 \\ f \in \mathcal{D}(A)}} (Lf, f) - \lambda_0 + \mu \int_T |f|^2 \, dx \equiv E(\mu)$$

where $E(\mu)$ is the smallest eigenvalue of $M(\mu) \equiv L - \lambda_0 + \mu \chi_T$.

Note that $E(0) = \inf \sigma(L) - \lambda_0 = 0$, and that χ_T is a bounded perturbation of the principal part L. It follows from standard perturbation theory for linear operators (Reed and Simon [19, Chap. XII], Kato [20]), that $E(\mu)$ is nondegenerate and depends analytically on μ in a sufficiently small neighborhood of $\mu = 0$, and that

$$E'(\mu)|_{\mu=0} = (f_0, \chi_T f_0) > 0$$

where f_0 is the normalized lowest eigenfunction of L, which does not vanish on T. Therefore, $E(\mu)$ is strictly increasing and thus becomes positive. □

One extension of this result would allow appropriate functions to be added to the coefficients a_{ij} as well as in the potential term q.

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REFERENCES

[1] R. A. ADAMS, *Sobolev Spaces*, Academic Press, New York, 1975.

[2] H. AMANN, *On the unique solvability of semilinear operator equations in Hilbert spaces*, J. Math. Pures Appl., 61 (1982), pp. 149–175.

[3] I. BABUŠKA, *The finite element method with Lagrange multipliers*, Numer. Math., 20 (1973), pp. 179–192.

[4] H. BRÉZIS AND L. NIRENBERG, *Characterization of the ranges of some nonlinear operators, and applications to boundary value problems*, Ann. Scuola Norm. Sup. Pisa Cl. Sci., 4 (1978), pp. 275–326.

[5] F. BREZZI, J. RAPPAZ AND P. A. RAVIART, *Finite dimensional approximation of nonlinear problems, Part* I: *Branches of nonsingular solutions*, Numer. Math., 36 (1980), pp. 1–25; *Part* II: *Limit points*, Numer. Math., 37 (1981), pp. 1–28; *Part* III: *Simple bifurcation points*, Numer. Math., 38 (1981), pp. 1–30.

[6] ———, *Approximation of nonlinear problems*, in Nonlinear Partial Differential Equations and their Applications—Collège de France Seminar, vol. III, H. Brézis and J. L. Lions, eds., Pitman, Boston, MA, 1982, pp. 147–153.

[7] P. G. CIARLET, M. H. SCHULTZ AND R. S. VARGA, *Numerical methods of high-order accuracy for nonlinear boundary value problems via monotone operator theory*, Numer. Math., 13 (1969), pp. 51–77.

[8] J. DESCLOUX AND J. RAPPAZ, *Approximation of solution branches of nonlinear equations*, RAIRO Anal. Numér., 16 (1982), pp. 319–349.

[9] J. MAWHIN, *Semilinear equations of gradient type in Hilbert space and applications to differential equations*, in Nonlinear Differential Equations: Invariance Stability and Bifurcation, Academic Press, New York, 1971, pp. 269–282.

[10] J. A. NITSCHE, *On Dirichlet problems using subspaces with nearly zero boundary conditions*, in The Mathematical Foundations of the Finite Element Method with Applications to Partial Differential Equations, A. K. Aziz, ed., Academic Press, New York, 1972, pp. 603–627.

[11] ———, *Über ein Variationsprinzip zur Lösung von Dirichlet-Problemen bei Verwendung von Teilräumen, die keinen Randbedingungen unterworfen sind, Abh. Math. Sem. Univ. Hamburg*, 36 (1971), pp. 9–15.

[12] R. S. PALAIS, *Foundations of Global Nonlinear Analysis*, W. A. Benjamin, New York, 1968.

[13] A. H. SCHATZ, *An observation concerning Ritz–Galerkin methods with indefinite bilinear forms*, Math. Comp., 28 (1974), pp. 959–962.

[14] M. H. SCHULTZ, *Error bounds for the Rayleigh–Ritz–Galerkin method*, J. Math. Anal. Appl., 27 (1969), pp. 524–533.

[15] ———, L^2 *error bounds for the Rayleigh–Ritz–Galerkin Method*, this Journal, 8 (1971), pp. 737–748.

[16] J. RAPPAZ, *Estimations d'erreur dans différentes normes pour l'approximation de problèmes de bifurcation*, C.R. Acad. Sci. Paris, Tome 296, Série 1 (1983), pp. 179–182.

[17] ———, *Numerical Analysis of Bifurcation Problems for Partial Differential Equations*, C. P. Bruter, ed., D. Reidel, Boston, to appear.

[18] M. A. KRASNOSEL'SKII, *Topological Methods in the Theory of Nonlinear Integral Equations*, Pergamon Press, Oxford, 1964.

[19] M. REED AND B. SIMON, *Methods of Modern Mathematical Physics, Vol.* 2: *Fourier Analysis and Self Adjointness* (1975), and *Vol.* 4: *Analysis of Operators* (1978), New York, Academic Press.

[20] T. KATO, *Perturbation Theory for Linear Operators*, Springer, New York, 1976.

On the Asymptotic Distribution of Eigenvalues of Banded Matrices

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Abstract

We consider the abstract measures, known as the DENSITY-OF-STATES measures, associated with the asymptotic distribution of eigenvalues of infinite banded Hermitian matrices. Two widely used definitions of these measures are shown to be equivalent, even in the unbounded case, and we prove that the density of states is invariant under certain, possibly unbounded, perturbations. Also considered are measures associated with the asymptotic distribution of eigenvalues of rescaled unbounded matrices. These measures are associated with the so-called contracted spectrum when the matrices are tridiagonal. Finally, we produce several examples clarifying the nature of the density of states

1. Introduction

The DENSITY OF STATES is a measure of how thickly the eigenvalues of truncated operators fill out the spectrum of the limiting operator as the truncation parameter tends to infinity. It is of physical significance both in scattering theory and in solid-state physics, where it is, for example, a multiplicative factor in the color spectrum of a material. The recent interest in the density of states measure for tridiagonal matrices J has two main underlying causes: 1. It characterizes parts of the spectrum while being relatively accessible in comparison with the spectral measure; and 2. It is related to the Lyapunov exponent for solutions of the associated difference equation by the Thouless formula. The density of states measure has been especially useful for understanding discrete solid-state physics with almost-periodic and random potentials (for an overview see the articles by Kirsch and Simon [4,10]). In addition, it shows up as the limiting measure in the Chebyshev quadrature (Simon [24]) and plays an important role in the asymptotic distribution of the eigenvalues of (modified) Toeplitz matrices (Nevai [15], Maté, Nevai and Totik [12], van Assche [28]. In many cases the density-of-states measure is the equilibrium measure associated with the spectrum of J (Geronimus [8]), and as such figures importantly in the approximation of analytic functions by polynomials (Walsh [31]).

Most earlier work on the density of states has dealt with bounded tridiagonal matrices, and much of it has been restricted to the case of constant off-diagonal elements. In this article we discuss the density of states for unbounded banded matrices, with any band size and with possibly variable off-diagonal elements. There are several justifications for this. The tridiagonal matrices arising in the theory of orthogonal polynomials usually have unbounded off-diagonal elements, so in this context the need for their analysis is obvious. The tendency to work principally with bounded tridiagonal matrices with constant off-diagonal entries has been strongest in mathematical physics, because such matrices arise when one-dimensional Schrödinger equations are made discrete by replacing derivatives with finite differences. The finite-difference method is not, however, necessarily the best way to do this, even in one dimension. If other discretizations are used, such as finite-element methods or the method of Case and Kac [2], then more general types of banded matrices will arise, and higher-dimensional discretizations are even more likely to yield banded or sparse matrices of other types. Potential energies that are unbounded above and below also commonly arise in physical models, and deserve analysis.

After discussing the equivalence of two possible definitions of the density of states, we consider the question of when two matrices may have the same density of states. We then consider density of states measures associated with rescaled unbounded matrices. When J is tridiagonal, these measures are associated with the so-called contracted spectrum (Erdos [7], Nevai and Dehesa [17], Ullman [26]). Finally, we give several examples, e.g., of unbounded matrices with the same density of states as bounded matrices.

Let J be an infinite real Hermitian banded matrix,

$$J_{jk} = (e_j, J e_k),$$

for an orthonormal basis $\{e_j\}$ of a Hilbert space $\mathcal{H}$, which we will regard as either $l^2(\mathbb{Z})$ or $l^2(\mathbb{Z}^+)$, corresponding to whether J is infinite in both directions or only one. We observe that if

$$T e_j = e_{j+1},$$

then J can be written as

$$J = B + \sum_{k=1}^{M} (T^k A_k + A_k T^{*k}), \qquad (1.1)$$

where B and A_k are real diagonal matrices. There are two plausible ways to define the density of states for J by truncation: First, let $\chi^{(L)}$ denote the projection onto the span of $\{e_j\}$, $|j| \le L$, and set $L^\# = \dim \operatorname{Ran}(\chi^{(L)}) = L$ or $2L+1$, depending on $\mathcal{H}$. For any infinite matrix W we define the $L^\# \times L^\#$ matrix

$$W^{(L)} = \chi^{(L)} W \chi^{(L)},$$

which we refer to as the L-truncate of W. Any truncate of J has only discrete eigenvalues, and for one definition we count them as $L \to \infty$:

Definition 1. J has a DENSITY-OF-STATES MEASURE iff the limit

$$\Delta(f) = \lim_{L \to \infty} (1/L^\#) \operatorname{tr}(f(J^{(L)})) \qquad (1.2)$$

exists for all $f \in C_b(\mathbb{R})$, the set of bounded, continuous functions.

Remarks: 1. We always define functions of matrices or operators with the spectral theorem, using any self-adjoint extension of J. That the result is independent of the choice of extension will follow from the results in the next section.

2. Phrased differently, $\Lambda(f) = \int f(\lambda)\, dk(\lambda)$, where dk is the weak limit of

$(L^\#)^{-1} \sum_k \delta(\lambda-\lambda_k^{(L)})$, where $\lambda_k^{(L)}$ are the eigenvalues of $J^{(L)}$. We shall refer to dk as the DENSITY-OF-STATES MEASURE.

3. In the case $\mathcal{H} = l^2(\mathbb{Z})$, we could in principle truncate J at j=L and j=M, and let $L \to +\infty$ and $M \to -\infty$ at different rates. There is no advantage in using this more general definition for our present purposes.

4. For $J_0(n,m) = (\delta_{m,n+1} + \delta_{m,n-1})/2$, i.e., $J_0 = T/2+T^*/2$, which can be regarded as the FREE HAMILTONIAN, the eigenvalues are well known. If J_0 acts on $l^2(\mathbb{Z}^+)$, they are:

$$\mu_k^L = \cos((L+1-k)\pi/(L+1)),$$

and the density-of-states measure is supported in [-1,1], according to the arcsin law,

$$dk(E) = \frac{dE}{\pi\sqrt{1-E^2}}. \qquad (1.3)$$

The density of states is the same if J_0 is interpreted to act on $l^2(\mathbb{Z})$.

Minami [14] has shown, generalizing earlier work, that the density-of-states measure exists when the entries in a tridiagonal matrix are random variables generated in certain ways using ergodic transformations.

The alternative definition truncates functions of J rather than taking functions of a truncate of J:

Definition 2: J has a density-of-states measure iff the limit

$$\lambda'(f) = \lim\, (1/L^\#)\, tr(\chi^{(L)} f(J)) \qquad (1.4)$$

exists for all $f \in C_b(\mathbb{R})$.

These two definitions are known to be equivalent in the bounded case (Simon [22], van Assche [28]). We show that they are equivalent in the unbounded case in the following section:

II. Perturbations that Leave the Density of States Invariant.

Let J be a 2M+1-banded matrix as in (1.1). We first show, in analogy with the argument of Simon [22], section C7), that:

Theorem II.1. Definitions 1 and 2 are equivalent.

Proof. We first consider the case when $f(x) = 1/(z-x)$, z not in sp(J). Let

$$G_1^{(L)}(z) = \chi^{(L)}(zI - J)^{-1}\chi^{(L)}$$
$$G_2^{(L)}(z) = (zI^{(L)} - J^{(L)})^{-1}. \qquad (2.1)$$

We note that both $G_1^{(L)}$ and $G_2^{(L)}$ are $L^\# \times L^\#$ matrices. Both of them satisfy the same inhomogeneous difference equation with different boundary conditions, viz.,

$$\Sigma_{|l-n| \le M} J(n,l)\, G_j^{(L)}(l,k;z) - z\, G_j^{(L)}(n,k,z) = \delta_{nk},\ |k|,|n| \le L-M,\ j=1,2. \qquad (2.2)$$

Therefore the difference $\Phi(n,k;z) = G_1^{(L)}(n,k;z) - G_2^{(L)}(n,k,z)$ satisfies the related homogeneous difference equation in n with k fixed, and is thus expressible as a linear combination of any 2M linearly independent homogeneous solutions $f_j(k;z)$ for $|k|,|n| \le L - M$. Because of the symmetry in the G_j, a similar fact applies in k with n fixed, so Φ is of the form

$$\Phi(n,k,z) = \sum_{j}^{2M} \sum_{k}^{2M} c_{jk} f_j(n,z) \bar{f}_k(k,z)$$

for $|k|,|n| \le L - M$. It is thus a matrix whose rank is finite independently of L, in fact at most $4M^2$. Since

$$\|G_j^{(L)}\| \le 1/|\mathrm{Im}\, z|, \quad j = 1, 2,$$

by the triangle inequality,

$$\|G_1^{(L)} - G_2^{(L)}\| \le 2/|\mathrm{Im}\, z|,$$

so

$$(L^{\#})^{-1} |\mathrm{tr}\, G_1^{(L)} - \mathrm{tr}\, G_2^{(L)}| \le 8m^2/L^{\#} |\mathrm{Im}\, z| \to 0 \text{ as } L \to \infty \tag{2.3}$$

Suppose we begin with Definition 1. By the Stone-Weierstraß theorem, the polynomials in $(x+i)^{-1}$ and $(x-i)^{-1}$ are dense in $C_0(\mathbb{R})$, the continuous functions vanishing at infinity. Equation (2.3) then implies Equation (1.4) for $f \in C_0(\mathbb{R})$. Since by Definition 1 the limiting measure is a probability measure (set f=1), and we know the definitions are equivalent for $f \in C_0(\mathbb{R})$, the limit of the sequence of measures given by Definition 2 is a probability measure, and thus Equation (1.4) is true for all $f \in C_b(\mathbb{R})$ by a standard argument (see Billingsley [1], Page 41, Problem 7).

The argument deducing Definition 1 from Definition 2 is analogous.

□

Remark. The proof also shows that the density-of-states measure is independent of the choice of self-adjoint extension, since different choices amount to making finite-rank perturbations of the resolvents G.

Let $J = J_0 + V$ be infinite matrices with J_0 banded, and denote the associated Green (resolvent) matrices

$$G_0(z) = (J_0 - z)^{-1} \quad \text{and} \quad G(z) = (J - z)^{-1}, \quad z \in \mathbb{C}.$$

We assume that for z ranging over some nonempty open set and A,B > 0,

$$|G_0(z;n,m)| < k \min(1, |n-m|^{-p}) \tag{2.4}$$

for all n,m, with $p > 2$. This is a very weak assumption, the usual situation being an exponential bound of the form

$$|G_0(z;n,m)| < k_1 \exp(-k_2|n-m|). \tag{2.5}$$

We observe that a bound of the form (2.5) holds whenever the off-diagonal elements of J_0 are bounded, by a modification of an argument due to Combes and Thomas [3]. A similar bound is dealt with by Demko et al. [5,6] for bounded banded matrices, using a different argument.

We recall a fundamental concept of perturbation theory (see Kato [9] or Reed and Simon [20]):

Definition. An operator A is **bounded relative to B with bound** b provided that the domain of definition $D(A) \supset D(B)$, and there are finite constants b' and c, with c depending on b', and b = inf b', such that for all $f \in D(B)$,

$$\|Af\| < b' \|Bf\| + c\|f\|.$$

In particular, a bounded operator is bounded relative to any other operator with bound 0.

Proposition II.2. A bound of the form (2.5) holds for $z \notin sp(J_0)$, and any J_0 such that each operator $A_k T^k$ and $T^k A_k$ is bounded relative to J_0.

Proof. Let E_c be the operator that multiplies the n-th component of any vector v by exp(icn), and observe, with a short calculation, that

$$E_c^* J_0 E_c = J_0 + \sum_k (\cos(ck) - 1)(T^k A_k + A_k T^{*k}) + \sum_k \sin(ck)(T^k A_k - A_k T^{*k}), \tag{2.6}$$

which is an analytic family of operators (type A) in the parameter c (see Kato [9] or Reed and Simon [20]) for $|c|$ sufficiently small, because of the relative boundedness. For c real, E_c is a unitary operator, and the analytic family of operators has the same spectrum as J_0. If $z \notin sp(J_0)$, it then follows that $E_c^* G_0(z) E_c = (E_c^* J_0 E_c - z)^{-1}$ is bounded for $|c|$ sufficiently small, even if c is complex. Hence, for some $k_2 > 0$, $\exp(-k_2 n) G_0(z;n,m) \exp(k_2 m)$ is a bounded operator on H, and similarly for $\exp(k_2 n) G_0(z;n,m) \exp(-k_2 m)$ (take $c = \pm i k_2$). Since the operator norm is an upper bound on any entry of a matrix, (2.5) follows.

□

Example. For the tridiagonal matrix $J_0 = T/2 + T^*/2$ on $l^2(\mathbb{Z})$,

$$G_0(z;n,m) = -(z^2-1)^{1/2} \exp(-\operatorname{arccosh}(z)\,|n-m|).$$

The Basic Assumption. We assume henceforth that

$$\lim_{L\to\infty} (1/L^\#) \sum_{|j|<L} \sum_k |V_{jk}| = 0. \tag{2.7}$$

This says that V_{jk} goes to zero on average, but might be arbitrarily large for any given j,k.

Example. V diagonal, $V_{2^{2m}2^{2m}} = 2^m$, $V_{kk} = 0$, otherwise. Although V goes to 0 on average, it is actually unbounded.

Lemma II.3. Suppose that V satisfies the basic assumption (2.7) and

$$|r_{ij}| < A \min(1, |i-j|^{-p}),\ p > 2, \text{ all } i, j.$$

Then $\lim_{L\to\infty} (1/L^\#) \sum_{|j|<L} \sum_m \sum_n r_{jm} V_{mn} = 0.$

Proof. Let $S = \left|(1/L^\#) \sum_{|j|<L} \sum_{m,n} r_{jm} V_{mn}\right|$

$$\le (1/L^\#) \sum_{|j|<L} \sum_{N=0}^{\infty} \sum_{|m|=NL}^{(N+1)L} \sum_n |r_{jm} V_{mn}|$$

$$\le (k/L^\#) \sum_{|m|=0}^{2L} \sum_n |V_{mn}| (1 + \sum_{j=m} |j-m|^{-p})$$

$$+ (k/L^\#) \sum_{|j|<L} \sum_{N=2}^{\infty} \sum_{|m|=NL}^{(N+1)L} \sum_n |V_{mn}|\,|j-m|^{-p}$$

$$\le (k/L^\#) \sum_{|m|=0}^{2L} \sum_n |V_{mn}| (1 + \sum_{s=0} |s|^{-p})$$

$$+ (k/L^\#) \sum_{|j|<L} \sum_{N=2}^{\infty} \sum_{|m|=NL}^{(N+1)L} \sum_n |V_{mn}| (|m|-L)^{-p}$$

The first term tends to 0 as $L \to \infty$ by the basic assumption (2.7), while the second is bounded by a constant times

$$\sum_{N=2}^{\infty} \sum_{m=0}^{(N+1)L} ((N-1)L)^{-p} \sum_{n} |V_{mn}|$$

$$\le (L^{*})^{1-p} \sum_{N=2}^{\infty} (N-1)^{-p}(N+1) \left\{ (1/(N+1)L) \sum_{m=0}^{(N+1)L} \sum_{n} |V_{mn}| \right\}$$

Since the sum in the curly brackets tends to 0 as $N \to \infty$ by the basic assumption (2.7), and $\sum (N-1)^{-p}(N+1) < \infty$, this expression is bounded by a finite number times $(L)^{1-p}$.

□

Theorem II.4 Let J_0 be an N-banded matrix with a well-defined density of states, and suppose that (2.4) and (2.7) hold. Then J has the same density of states as J_0.

Proof As shown above, the functions $1/(\lambda - z)$ are a determining set for the density-of-states measure, so it suffices to analyze the resolvents of J_0 and J, i.e., to show that

$$\lim_L (1/L^{*}) \sum_{|j|<L} |G_0(z,j,j) - G(z,j,j)| = 0$$

From the resolvent formula,

$$(1/L^{*}) \sum_{|j|<L} |G_0(z,j,j) - G(z,j,j)| = (1/L^{*}) \sum_{|j|<L} \sum_{mn} |G_0(z,j,m)V_{mn}G(z,n,j)|$$

$$\le (k/L^{*} |\mathrm{Im}\, z|) \sum_{|j|<L} \sum_{nm} \min(1, |j-m|^{-p}) |V_{mn}|$$

$$\to 0$$

by Lemma II.3.

□

We have thus shown that the basic assumption guarantees the invariance of the density-of-states measure dk under perturbation, for reasonable J_0. Recall that a classic theorem of Weyl states that the essential spectrum, which includes the support of dk, is invariant under compact perturbations. Banded compact matrices are precisely the matrices that tend to 0 at infinity. Here we get invariance for perturbations assumed to tend to 0 only on average.

III. The Contracted Density-of-States Measure.

In this section we shall generalize the definitions given in the introduction so as to extend the notion of the density of states to operators having unbounded essential spectra. The idea here is to renormalize the truncates of J so as to make them essentially bounded. This method has had many applications recently in the theory of orthogonal polynomials (Nevai [16], Lubinsky, Mhaskar, and Saff [12], van Assche [28,29]).

Definition 3. Let c_L be a sequence of positive numbers. We say that J has a CONTRACTED DENSITY-OF-STATES MEASURE associated with the sequence $\{c_L\}$ iff there exists a sequence of positive numbers $\{c_L\}$ such that

$$\Lambda(f) = \lim_{L\to\infty} (L^{\#})^{-1}\, \mathrm{tr}(f(J_L/c_L))$$

exists for all $f \in C_b(\mathbb{R})$.

The notation used here is that of the introduction. The alternative to Definition 3 is:

Definition 4. J has a contracted density-of-states measure associated with the sequence $\{c_L\}$ iff

$$\Lambda'(f) = \lim_{L\to\infty} (L^{\#})^{-1}\, \mathrm{tr}(\chi^{(L)} f(J/c_L))$$

exists for all $f \in C_b(\mathbb{R})$.

Proposition III.1 Definitions 3 and 4 are equivalent.

Proof. The proof is exactly the same as for Theorem II.1. □

Remark. When all the c_L are equal to 1, this reduces to the case considered in sections I and II.

Examples. Suppose J is a Jacobi matrix acting on $l^2(\mathbb{Z}^+)$, i.e., (1.1) with M=1, $A_1 = A = \{a_j\}$, with each $a_j > 0$ and $B = \{b_j\}$ real. Furthermore, suppose that

$$\lim_{n\to\infty} a_n^2/\lambda_n = a > 0 \quad \text{and} \quad \lim_{n\to\infty} b_n/\lambda_n = b,$$

where $\{\lambda_n\}$ is a regularly varying sequence with exponent α (i.e., $\lambda_n = n^{\alpha}L(n)$, where $L(n)$ is a slowly-varying function (Senata [21]). In this case the contracted density of states measure is called an Ullman-Nevai measure. With assumptions on the weight, including symmetry, it has been found by Mhaskar and Saff [13], Rachmanov [19], and Ullman [26]. Starting from the recurrence coefficients (the matrix J) its moments have been found by Nevai and Dehesa [17], and they are given explicitly by van Assche [28,30]. The explicit form of the contracted density-of-states measure is:

$$k(E) = \frac{1}{\pi}\int_0^1 d(t^{1/\alpha}) \int_{(b-2a)t}^{(b+2a)t} dx\, \chi_E(x)\, \frac{t^{1/\alpha}}{\sqrt{(2at)^2 - (x-bt)^2}},$$

where χ_E is the characteristic function of the Borel set $E \subset [b-2a, b+2a]$. For Hermite polynomials, b=0, a=1, and $\alpha = 1/2$. Therefore,

$$k(E) = \frac{1}{\pi}\int_0^1 d(t^2) \int_{-2t}^{2t} dx\, \chi_E(x)\, \frac{1}{\sqrt{4t^2 - x^2}}$$

$$= \frac{1}{\pi}\int_0^1 d(t^2) \int_{-2}^{2} dx\, \chi_E(xt)\, \frac{1}{\sqrt{4 - x^2}}$$

Here we have taken the weight function for the Hermite polynomials as $\sqrt{\frac{2}{\pi}}\exp(-x^2)$. For Laguerre polynomials, b=2, a=1, and $\alpha=1$, and consequently,

$$\kappa(E) = \frac{1}{\pi}\int_0^1 dt \int_0^{4t} dx\ N_E(x)\ \frac{dt}{\sqrt{4t^2-(x-2t)^2}}$$

Theorem. Let J_0 be a $2M+1$-banded matrix with a well-defined density-of-states measure associated with the sequence (c_L). Suppose that $(J_0^{(L)}/c_L)$ is a uniformly bounded sequence of operators and that $J = J_0 + V$ is a banded matrix. If

$$\lim_{L\to\infty} (L\, c_L)^{-1} \Sigma_{|m|<L} \Sigma_{|n|<L} |V_{mn}| = 0,$$

then J has the same contracted density-of-states measure as J_0.

Proof

Again it suffices to show that

$$\lim_{L\to\infty} (L)^{-1} \Sigma_{|j|<L} |G_0^{(L)}(z, j,j) - G^{(L)}(z, j,j)| = 0,$$

where $G_0^{(L)}$ and $G^{(L)}$ are the Green matrices associated with $J_0^{(L)}/c_L$ and $J^{(L)}/c_L$. Since $J_0^{(L)}/c_L$ is a uniformly bounded sequence of operators, $|G_0^{(L)}(z, m,n)| < k_1 \exp(-k_2|m-n|)$ for some $k_{1,2} > 0$ by Proposition II.2. The constants in this estimate are easily seen to be independent of L for $|z|$ sufficiently large.

From the resolvent formula,

$$\begin{aligned}(L^{\#})^{-1} \Sigma_{|j|<L} &|G_0^{(L)}(z, j,j) - G^{(L)}(z, j,j)| \\ &= (L^{\#})^{-1} \Sigma_{|j|, |m|, |n|<L} |G_0^{(L)}(z, j,m)\,(V_{mn}/c_L)G^{(L)}(z, n,j)| \\ &\le \text{const.}\ (L^{\#})^{-1} \Sigma_{|m|, |n|<L} |V_{mn}/c_L| \ \Sigma_{|j|<L} |G_0^{(L)}(z; j,m)| \\ &\le \text{const}\ (L^{\#})^{-1} \Sigma_{|m|, |n|<L} |V_{mn}/c_L| \ \to 0\end{aligned}$$

□

Remark. If J is banded, then it is sufficient to insist, in place of the basic assumption (2.7) that

$$\lim_{l\to\infty} (L^{\#})^{-1} \sum_{|m|<L} \ \sum_{|n|<L} |V_{mn}| = 0, \qquad (3.1)$$

whereas if J is not banded, the equivalence of Definitions 1 and 2 is certainly guaranteed by the stronger assumption (2.7) If one is content with Definition 1 for the density of states and does not insist upon the equivalence of the two definitions, then (3.1) is sufficient to ensure that J and J_0 have the same density of states. In this case the proof above shows that only absolute summability of the columns of G is required.

IV. Some Instructive Examples.

We begin with some curious examples that do not make use of our main results, and then exemplify our results with further examples. We frequently rely on the property of recurrence:

Definition. An infinite matrix W is said to be **recurrent** if for all $L, M \in \mathbb{Z}^+$ and all $\delta > 0$, there exists $N > M$ such that

$$\|(T^{*N} W T^N - W)^{(L)}\|_{\infty} < \delta,$$

where $\|W\|_{\infty}$ is by definition $\max_{|n|,|m| < L} |W_{mn}|$.

This means that given any block of W and any $\delta > 0$, it is possible to translate it arbitrarily far down the diagonal and find another block that matches the original to within δ.

Lemma IV.0. If J, a self-adjoint operator on $l^2(\mathbb{Z})$ (i.e., n, m run from $-\infty$ to $+\infty$), is banded, recurrent, and essentially self-adjoint on the set C, of sequences with finitely many nonzero elements, then sp(J) is a perfect set (there are no isolated eigenvalues).

This is a familiar property of bounded ergodic Jacobi matrices on $l^2(\mathbb{Z})$ [4,10,22], which are recurrent. To sketch the essentially known proof for the minor extension to recurrent operators, we reason as follows: If $\lambda \in$ sp(J), then there are vectors $v \in C$, $\|v\| = 1$, such that $\|(J-\lambda)v\|$ is arbitrarily small. Since J is recurrent, some sequence of disjoint translates of such v's constitutes a Weyl sequence (i.e., a sequence of approximate eigenvectors, cf. Weidmann [32], p. 203), showing that λ belongs to the essential spectrum of J. Essential spectra consist of infinitely degenerate eigenvalues together with accumulation points of the spectrum, but since J is banded, sp(J) contains no infinitely degenerate eigenvalues.

Example IV.1. A bounded operator with a nonconvergent density of states.

We let $J_0 = T/2 + T^*/2$ act on $l^2(\mathbb{Z}^+)$, and let V be diagonal, with

$$V_{00} = 1,$$

$$V_{nn} = (-1)^N, \quad N \le \log\log n < N+1, \quad N \in \mathbb{Z}.$$

Now consider $J = J_0 + V$. (The sequence $(V(n) = V_{nn})_1^{\infty}$ consists of blocks of rapidly increasing length each of which contains only +1 or −1.) The operator J does not have a uniquely defined density of states.

Proof. We will let L run through the integer values L(N) such that log log(L(N)) is the greatest possible value less than than N+1. Recall that the ordered eigenvalues of $J_0^{(L)}$ are $\mu_l^{(L)} = \cos\left(\frac{(L-l+1)\pi}{L+1}\right)$, and observe that if $\lambda_l^{(L)}$ are the corresponding eigenvalues of J, then by the min-max principle, $\mu_l^{(L)} - 1 < \lambda_l^{(L)} < \mu_l^{(L)} + 1$. If $k^{(L)}(\lambda)$ denotes the number of eigenvalues of J that are $\le \lambda$ and $k_0^{(L)}(\lambda)$ is the corresponding number for J_0, then

$$k_0^{(L)}(\lambda-1) < k^{(L)}(\lambda) < k_0^{(L)}(\lambda+1) \quad \text{for all } \lambda.$$

If N is odd, then we claim that

$$0 < \sum_{j=1}^{L(N)} \left(\lambda_j^{(L(N))} - (\mu_j^{(L(N))} - 1)\right) = \sum_{j=1}^{L(N)} \left(V(j) + 1\right) < 2L(N-1) \qquad (4.1)$$

On the other hand, if N is even, then we claim that

$$0 < \sum_{j=1}^{L(N)}((\mu_j^{(L(N))}+1)-\lambda_j^{(L(N))}) = \sum_{j=1}^{L(N)}(1-V(j)) < 2L(N-1) \qquad (4.2)$$

If these claims are granted, then, by dividing by L(N), passing to the limit $N\to\infty$, and noting that $2L(N-1)/L(N) \to 0$, we see that both $k_0^{(L)}(\lambda-1)$ and $k_0^{(L)}(\lambda+1)$ are limit points of $k^{(L)}(\lambda)$ as $L \to \infty$.

To prove (4.1) and (4.2), we use the linearity of the trace to see that

$$\sum_{j=1}^{L}(V(j)+1) = tr(V^{(L)}+I^{(L)}) = tr(J^{(L)}) - tr(J_0-I)$$

$$= \sum_{j=1}^{L}\lambda_j^{(L)} - \sum_{j=1}^{L}(\mu_j^{(L)}-1)),$$

and similarly for $\sum_{j=1}^{L}(1-V(j))$

□

Ullman and Wyneken [27] discuss an analogous situation, beginning with If J is ergodic, then it has a density of states (Minami[14]), but the same is not necessarily true of recurrent operators.

Example IV.2. A bounded, recurrent operator with a nonconvergent density of states.

As in Example IV.1, $J = J_0 + V$ with V diagonal. We construct $V(n) = V_m$ recursively as follows.

Let

$V(n) = 0$ for $-\infty < n \le 10$;

while for n = 0, 1, ...,

$V(10^{10^n}+k) = V(k-n)$ for $1 \le k \le 10^{10^n}+n$;

$V(m) = (-1)^n$ for $2\times10^{10^n}+n < m \le 10^{10^{n+1}}$.

The proof differs from the previous one only in minor ways and will not be repeated. The two distinct limit points are the density-of-states measures for $V_\pm(n) = 0$ for $n \le 0$, $V_\pm(n) = \pm1$ for $n > 0$.

Example IV.3. A bounded operator with a density of states, the support of which is a proper subset of the essential spectrum.

Let R be the set of positive integers of the form

$$\sum_{m=0}^{N} c_m\, 10^{10^m}, \quad \text{with } c_m = 0 \text{ or } 1.$$

Let J be an operator on $l^2(\mathbb{Z})$ of the form $TA + AT^*$, with A diagonal, and

$$A(n) = \begin{cases} 1/2, & n \in R \\ 2, & n \in R. \end{cases}$$

This operator has the density of states (1.3) (same whether we use $\mathbb{Z}$ or $\mathbb{Z}^+$), supported in [-1,1] by Theorem II.4. Since J is easily seen to be recurrent, Lemma IV.0 implies that the spectrum is purely essential. Since the norm of J is larger than 2, this essential spectrum includes values outside [-1,1].

Remark. We conjecture that the thin part of the spectrum outside [-1,1] is a Cantor set, and that other examples could be constructed with spectrum [-2,2], say, but with the density of states supported in [-1,1]. We do not know the nature of the spectrum, e.g., whether there is a dense set of eigenvalues outside [-1,1], or even whether the subset [-1,1] is absolutely continuous. Indeed, a theorem of Rakhmanov [18] casts doubt on the absolute continuity in this example, and also in Example IV.7, below.

Example IV.4. Another bounded operator with a density of states, the support of which is a proper subset, viz. the interval $[-1,+1]$, of the essential spectrum, which is certainly the interval $[-1,+2]$.

According to Theorem II.4, if we take $J = J_0 + V$ on $l^2(Z^+)$, with any V satisfying the basic assumption (2.7), dk will be the same as that of J_0. We take

$$V(n) = 0, \text{ unless } 10^k \leq n < 10^k + k,$$

$$V(n) = 1, \text{ when } 10^k \leq n < 10^k + k.$$

Since $J_0 < J < J_0 + 1$, in the sense of quadratic forms, it is clear that the spectrum of J lies in the interval $[-1,2]$. To show that all such values belong to the essential spectrum of J, recall that λ belongs to the spectrum of J_0 iff for the value λ there is a Weyl sequence, which can be assumed to consist of vectors of finite support. Since J_0 is translation-invariant, we may assume that the support of the vectors v_j in the Weyl sequence begin wherever we want. By choosing their support away from the intervals $10^k \leq n < 10^k + k$, we see that $\|[J - \lambda I]\, v_j\| \to 0$, so every $\lambda \in [-1,+1]$ belongs to sp(J). On the other hand, since the intervals $10^k \leq n < 10^k + k$ are arbitrarily long, we may choose v_j to be supported in such intervals, and we find that

$$\|[J - (\lambda+1)I]\, v_j\| = \|[J_0 - \lambda I]\, v_j\| \to 0,$$

so every point of $[0,2]$ also belongs to sp(J).

Example IV.5. An unbounded operator with a density of states, which is equal to the distribution (1.3) of $J_0 = T/2 + T^*/2$.

According to Theorem II.4, we may take $J = J_0 + V$ on $l^2(Z^+)$, with any V satisfying the basic assumption, e.g.,

$$V(n) = 0, \text{ unless } n = 4^k,$$

$$V(4^k) = 3^k.$$

We observe that the moments of the density of states measure fail to converge in this example, i.e., if

$$\mu^{(L)}_m = |L|^{-1}\, \mathrm{Tr}((J^{(L)})^m)$$

then as $L \to \infty$,

$$\mu^{(L)}_0 \to 1$$

$$\mu^{(L)}_1 \to 0$$

$$\mu^{(L)}_m \to \infty \text{ for } m > 1.$$

Example IV.6. An unbounded operator with a density of states, which is equal to the distribution (1.3) of $J_0 = T/2 + T^*/2$, and for which the truncated moments converge to the moments of the density of states measure.

$$J = TA + AT^* \quad \text{on } l^2(Z^+),$$

where A is diagonal with

$$A_m \begin{cases} = 1/2, & m \neq 2^k, \\ = k/2, & m = 2^k. \end{cases}$$

We calculate the moments:

$$\mathrm{Tr}((J^{(L)})^k) = \sum_{l_1=0}^{L-1} \cdots \sum_{l_k=0}^{L-1} J^{(L)}_{l_1 l_2} J^{(L)}_{l_2 l_3} \cdots J^{(L)}_{l_k l_1}$$

$$= S_1 + S_2, \qquad (4.3)$$

where S_1 contains only terms for which $a_n = 1/2$ and S_2 contains all the other terms. Let $N_k(l_1)$ be the number of k-tuples such that

a) $|l_j - l_{j+1}| = 1, \quad j = 1, \ldots, k-1;$

b) $|l_j - l_{j+1}| = 1$ (4.4)

c) $0 \le l_j \le L-1, \qquad j = 1, \ldots, k-1.$

Then there are precisely $\sum_{l=0}^{L-1} N_k(l)$ terms in the sum (4.3). If a k-tuple satisfying (4.4) has first component l_1, then l_j can at most be $l_1+k/2$ and will never be smaller than $l_1-k/2$. Therefore, a k-tuple for which $|l_1-2^j|>k/2$ for every $2^j \le n-1$ in the sum (4.3) will only contain entries $a_n = 1/2$. This means that there are at most

$$\sum_{\substack{l=0 \\ |l-2^j|<k/2}}^{L-1} N_k(l) \le (\max_l N_k(l))\, k \log_2(L)$$

terms in S_2. Clearly, $N_k(l) \le 2^k$, and each term in S_2 is bounded by $(\log_2(L))^k/2^k$. Therefore

$$|S_2| \le k\,(\log_2(L))^{k+1},$$

so $S_2/L \to 0$ for every k as $L \to \infty$.

In order to calculate S_1, we notice that it is the same as the corresponding sum for J_0. Since the sum corresponding to S_2 for J_0 is o(L) by the same argument as for S_2, the limit of S_1/L converges to the corresponding moment for J_0, i.e.,

$$\frac{1}{\pi} \int_{-1}^{1} \frac{x^k}{\sqrt{1-x^2}}\, dx$$

□

Example IV.7 A bounded operator J with the same density of states (1.3) as $J_0 = T/2 + T^*/2$, and also having the same spectrum [-1,1], but for which

which the perturbation $J - J_0$ is not compact. Take J as in Example IV.3, but with

$$A(n) = \begin{cases} 1/2, & n \notin R \\ 1/3, & n \in R. \end{cases}$$

It is straightforward to calculate (with Weyl sequences) that sp(J) contains sp(J_0), but $\|J\| = 1$, so sp(J) = [-1,1]. Theorem II.4 shows that the density of states is the same as for J_0.

Example IV.8. The contracted density of states. Let

$$(J_0\,\psi)(n) = \sqrt{n+1}\,\psi(n+1) + (2n+1)\psi(n) + \sqrt{n}\,\psi(n-1),\ n = 1, 2, \ldots$$

This is the Jacobi matrix associated with the normalized Laguerre polynomials whose leading coefficients have been made positive (Szegö [25]). Let $J = J_0 + V$, V diagonal with $V(4^m) = 6^m$ and $v(m) = 0$ for $m \neq 4^n$. Then J has the same contracted density-of-states measure associated with $c_L = L$ as J_0. (See Section III.).

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References

1. P. Billingsley (1968): Convergence of Probability Measures. New York: Wiley.

2. K.M. Case and M. Kac (1973): *A discrete version of the inverse scattering problem* J. Math. Phys. **14**: 594-603.

3. J-M. Combes and L. Thomas (1973): *Asymptotic behavior of eigenfunctions for multiparticle Schrödinger operators* Commun. Math. Phys. **34**:251-270.

4. H.L. Cycon, R.G. Froese, W. Kirsch, and B. Simon(1986): Schrödinger Operators, Berlin and New York: Springer.

5. S. Demko, W.F. Moss, and P.W. Smith; *Decay rates for inverses of band matrices* Math. of Computation **43**:491-499.

6. S. Demko: *Inverses of band matrices and local convergence of spline projection* SIAM J. Numer. Anal. **14**:616-619.

7. P. Erdös (1972): *On the distribution of roots of orthogonal polynomials*, pp. 145-150 in: Proc. of the Conf. on Constr. Theory Functions (G. Alexits et al., eds. Budapest: Akademias Klada. **CHECK REF.**

8. L. Ya. Geronimus (1957): *On some finite difference equations and corresponding systems of orthogonal polynomials* Mem. Math. Sect. Fac. Math. Phys. Kharkov State Univ. and Kharkov Math. Soc. **25**:87-100 (in Russian).

9. T. Kato(1966): Perturbation Theory for Linear Operators, Grundlehren der mathematischen Wissenschaften **132**. New York: Springer.

10. W. Kirsch (1985): *Random Schrödinger operators and the density of states*, in: Stochastic Aspects of Classical and Quantum Systems, Lecture Notes in Mathematics, 1109, S. Albeverio, Ph. Combe, and M. Sirugue-Collin, eds. Berlin and New York: Springer.

11. D.S. Lubinsky, H.N. Mhaskar, and E.B. Saff (1987): *A proof of Freud's conjecture for exponential weights* Constr. Approx., to appear

12. A. Máté, P.G. Nevai, and V. Totik (1984): *What is beyond Szegő's theory of orthogonal polynomials?*, pp. 502-510 in: Rational Approximation and Interpolation, Lecture Notes in Mathematics **1105**. New York: Springer.

13. H.N. Mhaskar and E.B. Saff (1984): *Extremal problems for polynomials with exponential weights*. Trans. Amer. Math. Soc. **285**:203-234.

14. N. Minami (1986): *An extension of Kotani's theorem to random generalized Sturm-Liouville operators*. Commun. Math. Phys. **103**:387-402.

15. P.G. Nevai (1980): *Eigenvalue distribution of Toeplitz matrices* Proc Amer. Math. Soc. **80**:247-253.

16. P.G. Nevai (1985): *Exact bounds for orthogonal polynomials associated with exponential weights* J. Approx. Theory **44**:82-85

17. P.G. Nevai and J.S. Dehesa (1979): *On asymptotic average properties of zeros of orthogonal polynomials*. SIAM J. Math. Anal. **10**:1184-1192.

18. E.A. Rakhmanov (1983): *On the asymptotics of the ratio of orthogonal polynomials II*. Math. USSR Sbornik **46**:105-117.

19. E.A. Rakhmanov (1984): *On asymptotic properties of polynomials orthogonal on the real axis* Math. USSR Sbornik **47**:155-193

20. M. Reed and B. Simon (1978): Methods of Modern Mathematical Physics, **IV**: Analysis of Operators. New York: Academic Press

21. E. Senata (1976): Regularly varying functions, Lecture Notes in Mathematics **508**. Berlin: Springer.

22. B. Simon (1982): *Schrödinger semigroups* Bull. Amer. Math. Soc. **7**:447-526.

23. B. Simon (1982): *Almost periodic Schrödinger operators: A review*. Adv. Appl. Math. **3**:463-490.

24 B Simon (1983) *Kotani theory for one dimensional stochastic Jacobi Matrices* Commun. Math. Phys **89**:227-234

25 G Szego (1975) Orthogonal Polynomials, Amer Math Soc Colloq. Publ. **23** (4th ed) Providence Amer Math Soc

26 JL Ullman (1980). *Orthogonal polynomials associated with an infinite interval* Mich. Math J. **27**:353-363

27 JL Ullman and MF Wyneken (1986) *Weak limits of zeros of orthogonal polynomials* Constr Approx. **2**:339-347

28 W van Assche (1987) *Asymptotic properties of orthogonal polynomials from their recurrence formula II* J. Approx Theory, to appear

29 W van Assche (1987) *Eigenvalues of Toeplitz matrices associated with orthogonal polynomials* J Approx Theory, to appear

30 W van Assche (1987) Asymptotics for Orthogonal Polynomials, Lecture Notes in Mathematics **1265** New York and Berlin Springer

31 JL Walsh (1935) Interpolation and Approximation by Rational Functions in the Complex Plane, Amer Math Soc. Colloq. Publ. **9**. Providence: Amer. Math. Soc.

32 J Weidmann (1980) Linear Operators in Hilbert Spaces. New York, Heidelberg, and Berlin. Springer

General Bounds for the Eigenvalues of Schrodinger Operators

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A Schrödinger operator is an elliptic differential operator, usually self-adjoint, of the form

$$H = -\hbar^2\Delta + V(x) \qquad (1)$$

acting on a Hilbert space $\mathcal{H}$ which I will suppose of the form $L^2(\Omega)$, $\Omega \subset \mathbb{R}^n$, thereby ignoring complications arising from various sources, principally spin and the possibility of many particles. The mass has been scaled to ½, and Planck's constant is denoted $\hbar$. It can likewise be scaled to 1, and I shall do so here except where explicitly noted otherwise; but in physics it is a small quantity, about 1.054×10^{-27} erg-sec., so one is frequently interested in the behavior of the spectral properties of H as $\hbar \to 0$, known as the semiclassical limit.

Most of the important problems of mathematical quantum mechanics revolve about the spectral and inverse spectral problem for (1). To get a good mathematical account of the spectral theory of Schrödinger operators, I would recommend looking at the books by Thirring [1979], Reed and Simon, especially vol. IV [1978], and Cycon, Froese, Kirsch, and Simon [1987]. This article will be concerned only with discrete eigenvalues of H. The spectrum of H consists only of discrete eigenvalues when Ω is bounded or when the potential V(x) tends to ∞ as $x \to \infty$, but even when $V(x) \to 0$ as $x \to \infty$, the negative part of the spectrum will be discrete (given some fairly general assumptions on V), and the bounds to be discussed will apply in that situation as well.

Nature has unfortunately chosen to reveal to physicists what only very few of the potentials V that arise look like, leaving physicists with the task of determining V from the data available to them - essentially the inverse spectral problem. The long and interesting history of this problem will not be repeated here. Suffice it to say that in one dimension, if the spectrum is completely known, along with either norming constants or some other information (such as a second spectrum with different boundary conditions), then there are well-established algorithms for determining the potential (Levitan [1984], Marchenko [1986], and Pöschel-Trubowitz [1987]), while the many-dimensional situation is more complicated, and less completely understood (Chadan and Sabatier [1977]).

In more than one dimension, there are two inverse problems for Schrödinger operators, *viz.* to suppose that Ω is known and to determine $V(x)$, or to attempt to deduce both V and Ω. Actually, so long as we impose only Dirichlet boundary conditions, the latter problem is basically a special case of the former, since $\mathrm{ext}(\Omega)$ can at least formally be considered as the set $\{x: V(x) = +\infty\}$ for a problem defined on a domain $\Omega' = \mathbb{R}^n$ (or any domain guaranteed to contain the original Ω). Thus I shall set aside altogether the problem of determining Ω, and will always assume it as given.

Even in a situation that can be reduced to one dimension, allowing a resolution of the inverse spectral problem by, say, the Gel'fand-Levitan or Marchenko algorithms, the requirement that one needs to know the spectrum completely is more than can reasonably be expected. Thus a problem of considerable practical significance is that of determining what properties of V are reflected in *limited* spectral information about H. This problem also turns out to be rather nice theoretically.

Suppose that some general relationship, analogous to the Payne-Pólya-Weinberger inequality, is found to hold for "all" potentials $V(x)$. Then, at the very least, we learn something useful about the feasible set of possible spectra for which the inverse problem is well-posed. I would like to argue that what such relationships teach us is more quantitative, since, in the Schrödinger context at least, general spectral bounds are generally not truly general.

For instance, recall that the Payne-Pólya-Weinberger inequality states that, for the Dirichlet problem of $-\Delta$ on a bounded domain Ω,

$$E_{k+1} - E_k \le \left(\frac{4}{nk}\right) \sum_{j=1}^{k} E_j, \qquad (2)$$

independently of the geometry of Ω. Now, a glance at the proof of this inequality shows that $-\Delta$ can be replaced with no essential change by $-\Delta + V(x)$, provided that $V(x) \ge 0$ a.e., and is sufficiently well-behaved that H can be defined as a self-adjoint operator (e.g., $V \in L^1(\Omega)$). Thus (2) can be replaced by

$$E_{k+1} - E_k \le \left(\frac{4}{nk}\right) \sum_{j=1}^{k} E_j - \left(\frac{4}{n}\right) \mathrm{ess\,inf}(V).$$

In other words, the Payne-Pólya-Weinberger inequality results from the constraint $V(x) \ge 0$ a.e., and can therefore be interpreted as a family of pointwise bounds on $V(x)$, given the values of the first $k+1$ eigenvalues:

$$\mathrm{ess\,inf}(V) \le \left(\frac{1}{k}\right) \sum_{j=1}^{k} E_j - \left(\frac{n}{4}\right) (E_{k+1} - E_k) . \qquad (3)$$

An abstract form of this inequality is proved in the appendix.

Many sorts of general bounds have been studied in the context of the Schrödinger equation, notably bounds on individual eigenvalues, spectral asymptotics, and bounds on ratios and gaps of eigenvalues, especially the fundamental gap, $E_2 - E_1$. I shall concentrate on the last of these problems. There are two questions about gaps: How small can they be, and how large can they be? Both are quite interesting. In their talks at this conference M.S. Ashbaugh and M.H. Protter have surveyed some of the upper bounds for gaps between eigenvalues, and have also spoken about the problem of lower bounds for the fundamental gap, but only with some sort of convexity imposed on Ω or $V(x)$. This article will discuss lower bounds to the gap without such assumptions, and will relate them to the tunneling effect of quantum physics.

In surveying the literature on general bounds for the fundamental gap between eigenvalues, I found that almost all of the techniques can be put into only three categories.

1. One-dimensional estimates
2. Projection coupled with the Rayleigh-Ritz inequality.
3. Special cases or variants of the **basic gap formula**:

$$E_k - E_l = \frac{(u_k,[H,g]u_l)}{(u_k,gu_l)} \qquad (4)$$

In this formula, $E_{k,l}$ are eigenvalues of a self-adjoint operator H, and $u_{k,l}$ are the corresponding eigenfunctions. The brackets denote the commutator, $[H,g] = Hg - gH$, and g can be any operator such that the denominator does not vanish and $g\, u_l \in D(H)$ (actually, even this condition can be relaxed). The proof of (4) is an elementary calculation:

$$\begin{aligned}(u_k, [H,g]\, u_l) &= (H\, u_k,\, g\, u_l) - (u_k,\, g\, Hu_l)\\ &= E_k\,(u_k,\, g\, u_l) - E_l\,(u_k,\, g\, u_l)\end{aligned}$$

Note that if H is a Schrödinger operator and g is a differentiable function, then $[H,g]\phi = -2\nabla g\cdot\nabla\phi$, and (4) becomes

$$E_k - E_l = \frac{-2\int_\Omega u_k\nabla g\cdot\nabla u_l dx}{(u_k,gu_l)} = \frac{2\int_\Omega u_l\nabla g\cdot\nabla u_k dx}{(u_k,gu_l)}$$

$$= \frac{\int_\Omega \nabla g\cdot(u_l\nabla u_k - u_k\nabla u_l)dx}{(u_k,gu_l)} \qquad (5)$$

by symmetrization.

The special choices that have been found useful are

1. $g(x) = x_l$ for some coordinate vector x_l. This, with the aid of some other clever manipulations, leads to the Payne-Pólya-Weinberger inequality.

2. $g(x) = x\, u_l^{a}$. This leads to the improvement of the Payne-Pólya-Weinberger inequality by de Vries [1967].

3. The limiting case as g tends to χ_S for a regular region S corresponds to the expression for the gap obtained from Green's formula:

$$E_k - E_l = \frac{\int_{\partial S}(u_k\mathbf{n}\cdot\nabla u_l - u_l\mathbf{n}\cdot\nabla u_k)da}{\int_S u_k u_l dx} \qquad (6)$$

Equation (6) has been very useful in the study of what is known as the double-well problem (cf. Harrell [1980]). There is a well-known physical mechanism that can make $E_2 - E_1$ very small (in comparison with other quantities with the same dimensions), namely the tunneling effect. If a particle would be classically confined by a potential energy $V(x)$, in quantum mechanics it has a small probability of escaping through a potential barrier. This produces weak coupling effects between the dynamics in regions separated by intervals where $V(x)$ is large, and this can show up as a small gap between eigenvalues, especially if V is symmetric about a central plane, taking on relatively large values on that plane, and lower values elsewhere.

A toy example of a double-well operator is:

$$-\hbar^2 d^2/dx^2 + V(x)$$

acting on $L^2(-1,+1)$, with Dirichlet boundary conditions at ± 1 and

$$V(x) = \chi_{[-a,a]} \qquad (7)$$

Proposition 2. As $\hbar \to 0$,

$$E_2 - E_3 \sim \text{const.} \exp(-\text{const.}/\hbar^2),$$

whereas (8)

$$E_3 - E_2 \sim \text{const.}\, \hbar^2,$$

which is much larger.

To outline the proof of this proposition, note first that the one-dimensional version of (6) with $S = [0,1]$ states

$$E_2 - E_1 = \frac{u_1(0)u_2'(0)}{\int_0^1 u_1(x)u_2(x)dx} \qquad (9)$$

Observe that $u_{1,2}$ are explicitly given in terms of $E_{1,2}$ as hyperbolic cosine or sine functions for $-a < x < a$, and ordinary sine functions for $-1 \le x \le -a$ and $a \le x \le 1$. If $\hbar$ is small it is fairly easy to find that $E_{1,2} \cong (1-a)^2\hbar^2\pi^2$, and (8) is an easy calculation from (9).

Essentially any other potential that qualitatively resembles this $V(x)$ will produce eigenvalues behaving in this way in the semiclassical limit, and analogous things happen in the multidimensional setting (Harrell [1980], Helffer and Sjöstrand [1984]; for the physics connected with this see Landau and Lifshitz [1977]).

The final special choice of $g(x)$ that has been found very useful is

4. $g = u_2/u_1$. In this case (6) becomes

$$E_2 - E_1 = \frac{\int_\Omega |\nabla g|^2 u_1^2 dx}{\int_\Omega u_2^2 dx} \qquad (10)$$

The ratio u_2/u_1 appears in the work of Ashbaugh and Benguria [1987b] and Singer, Wong, Yau, and Yau [1985] on lower bounds for the gap. It is also the key to a recent lower bound due to Kirsch and Simon [1987], which makes no convex assumptions, and which is roughly of the form expected from the tunneling effect, although with nonoptimal constants. Kirsch and Simon estimate (10) from below by applying the Cauchy-Schwarz-Buniakovskii inequality to

$$1 = \left(\int_C |\nabla g|\right)^2 = \left(\int_C |\nabla g| u_1 \cdot \frac{1}{u_1}\right)^2$$

for a subset C of Ω:

$$1 \le \int_C |\nabla g|^2 u_1^2 \int_C u_1^{-2} = \int_C |\nabla g|^2 u_1^2 \int_C u_1^2 \cdot u_1^{-4}$$

$$\le \int_\Omega |\nabla g|^2 u_1^2 \int_\Omega u_1^2 / (\inf_C u_1)^4$$

Since one of the terms on the right is the denominator of (10), with $g = u_2/u_1$, they obtain

$$E_2 - E_1 \ge \frac{\left(\int_C |\nabla g|\right)^2 (\inf_C u_1)^4}{\int_\Omega u_1^2 \int_\Omega u_2^2}$$

Then they choose C to be a ball enclosing the set $\{x: V(x) < E_1+\varepsilon^2\}$ for some small ε and estimate the factors on the right separately. The key estimate is the pointwise estimate on u_1 needed for the infimum; the tendency for solutions of elliptic equations to grow or decay exponentially is the source of the exponential term characteristic of tunneling. They obtain:

$$E_2 - E_1 \ge C(R) \exp(-2^{7/2} n \lambda R), \qquad (11)$$

where n is the dimension, R is the radius of C, C(R) is a polynomial expression in R, and $\lambda = \sup_x \sup_{E \in S} |V(x)-E|^{1/2}$, $S = [E_1, E_2]$.

Ideally, the exponent in (11) would be λr, where $r < R$ would be the radius of a barrier region contained in C. By the way, using different, strictly one-dimensional methods (a Prüfer substitution), Kirsch and Simon [1985] had earlier obtained a lower bound of tunneling type with more nearly the optimal exponent.

Are there other physical mechanisms producing small gaps? The work of Kirsch and Simon shows that if they exist, they cannot produce dramatically smaller gaps than tunneling. A theorem of Davies [1982] provides further evidence that only the double-well phenomenon can produce extremely small gaps, by showing that the existence of a small gap implies a decoupling of Ω into two parts and a generalized symmetry transformation relating the eigenfunctions. In the abstract setting the operator H can be any generator of a positivity-improving semigroup, e.g., if exp(-tH) is an integral operator with a positive kernel, which is the case for Schrödinger operators where the potentials V(x) have some very general properties (see Reed and Simon [1978], Davies [1980], and Simon [1982]).

Theorem 3 (Davies): Let H generate a positivity preserving semigroup on $L^2(\Omega, dv)$, with eigenvalues $E_{1,2}$ nondegenerate, $H u_1 = E_1 u_1$ and $H u_2 = E_2 u_2$ with $\|u_{1,2}\| = 1$. Let $\delta = E_2 - E_1$ and suppose that $\sigma(H) - \{E_1, E_2\} \subset [E_2 + D, \infty)$, with $D/\delta \ge R > 3$. Then there exists a two-valued function called t (for "two"), $t(x) = c_1 \chi_S + c_2 \chi_{S^c}$ for some set S, such that

$$u_2(x) = t(x) u_1(x) + r(x),$$

where

$$\|r\|_2^2 \le C(R)\, \delta/D,$$

and $\lim_{R \to \infty} C(R) = 3^{1/2}$.

Davies has extensions of the theorem to the situation where E_2 has degeneracy or approximate degeneracy m. A proof of this theorem is given below, but first it is convenient to make an elementary transformation to simplify bookkeeping. Change the operator and Hilbert space $L^2(\Omega, d\nu)$ unitarily so that

$$L^2(\Omega, d\nu) \rightarrow L^2(\Omega, d\mu),$$
$$\text{with } d\mu = u_1^2(x)d\nu, \text{ a probability measure,}$$

$$\phi \in L^2(\Omega, d\nu) \rightarrow \left(\frac{\phi}{u_1}\right) \in L^2(\Omega, d\mu),$$

$$H\phi \rightarrow A\left(\frac{\phi}{u_1}\right) = \frac{1}{u_1}(H - E_1)\, u_1 \left(\frac{\phi}{u_1}\right).$$

This has the effect of making the principal eigenfunction 1 with eigenvalue 0: $A\,1 = 0$, and $A\,v = \delta$, where $v = u_2/u_1$. It does not affect the positivity-improving property. The conclusion of the theorem is then that $v = t(x)$ up to a small error.

Lemma 4: Let $v \in Q(A)$, the quadratic-form domain of A, and for any $T \ge 0$, define

$$v^T(x) = \min(v(x), T)$$

Then $v^T(x) \in Q(A)$, and

$$(v^T, Av^T) \le (v, Av).$$

This is the Beuling-Deny criterion of Reed and Simon [1978], p. 209 ff., except that they choose T=0. Since AT = 0, it is clear that one can truncate at any value T, since $v^T = T + (v - T)^T$.

Lemma 5: Let $B = B^*$ on a Hilbert space $\mathcal{H}$ have an eigenvalue E isolated from the rest of the spectrum by a distance d, and denote the spectral projection onto E as P. If $w \in D(B)$, $\|w\| = 1$, then

$$\|(1 - P)\,w\| \le \|(B - E)\,w\|/d.$$

This is a simple exercise with the spectral theorem.

Proof of Theorem 3: The idea is to take the exact eigenfunction v for $Av = \delta v$ and to use its truncate v^T as a trial function to estimate δ. The lemmas will show that $v^T \equiv v$, and the conclusion will follow by simple algebra.

Thus let $w = N(v^T - (v^T, 1)) = N(v^T - \int v^T d\mu)$, where N is a normalization depending on T and use Lemma 1 to see that:

$$(w, Aw) \le N^2 (v, Av) = N^2 \delta. \qquad (12)$$

At this stage N can be assigned any value from 1 to $\sqrt{2}$ by suitable choice of T and possibly multiplying v by -1, since either $\|v^0\|$ or $\|(-v)^0\| \ge 1/2$, but at the end of the proof it will be argued that it can be taken arbitrarily close to the optimal value 2.

Now notice that $A-\delta$ is a positive operator when restricted to the subspace $\mathcal{H}_1$ of $L^2(\Omega, d\mu)$ orthogonal to 1, so with $B = \sqrt{A-\delta}$, we can calculate:

$$\|B\,w\|^2 = (w, (A-\delta)w) \le (N^2 - 1)\delta$$

by (12). Then Lemma 2 applied to this B on $\mathcal{H}_1$ implies that

$$\|(1 - P)\,w\| \le \sqrt{(N^2-1)\delta/D}.$$

This means that

$$v = \frac{w}{\sqrt{1-(N^2-1)\delta/D}} + r_1 = \begin{cases} a v - \int v^T + r_1 & x \in S \\ a T - \int v^T + r_1, & x \notin S \end{cases} \qquad (13)$$

where $S = \{x: v(x) \le T\}$,

$$\alpha = \frac{N}{\sqrt{1-(N^2-1)\delta/D}} \quad \text{and} \quad \|r_1\| < \sqrt{\frac{(N^2-1)\delta/D}{1-(N^2-1)\delta/D}}$$

Now solve (13) for v to find that:

$$v = t(x) + r$$

where

$$t = \begin{cases} \dfrac{\int vT}{\alpha - 1}, & x \in S \\ \alpha T - \int vT, & x \notin S \end{cases}$$

and

$$r = \begin{cases} \dfrac{-r_1}{\alpha - 1}, & x \in S \\ r_1, & x \notin S \end{cases}$$

This establishes the theorem except for the numerical value of lim C(R), which results from the choice N = 2. A straightforward calculation of $\|t^0 - \int t^0\|$ for t(x) a normalized two-valued function orthogonal to 1 shows that $\|t^0 - \int t^0\| = \mu(S)$ or $1-\mu(S)$ depending on whether t is positive or negative on S. Since one of these numbers is ≤ ½, and since we have seen that v(x) is close to t(x) when the gap is small, we can choose $N \equiv 1/\|t^T - \int t^T\| = 2$ for some T≥0.

□

Finally, I would like to discuss an approach to bounds on the gap via direct optimization. In the last few years M.S. Ashbaugh and I and some other people have explored the problem of imposing a constraint on the potential V and then maximizing or minimizing a given eigenvalue subject to that constraint (Harrell [1984], Ashbaugh and Harrell [1984,1987], Egnell [1987] and references therein). I shall briefly recapitulate the argument and discuss its extension to gaps. Most typically, what we have done is to impose a constraint of the form

$$\|V-W\|_p \le M$$

for a reasonable background potential W(x) and some fixed p, $1 < p < \infty$ ($p=\infty$ is trivial and p=1 is a special case, which is also tractable), and searched for the potential within that class that maximizes or minimizes a given eigenvalue $E_k(V)$, subject, say, to Dirichlet boundary conditions.

There is a serious existence question for these spectral optimizing problems, which I don't wish to discuss here, beyond remarking that, for example, if Ω is smooth and bounded and, for the minimizing problem, p is sufficiently large to ensure that the usual Sobolev embeddings apply, then optimizing potentials exist and satisfy

$$\|V-W\|_p = M < \infty, \tag{14}$$

with V-W nonnegative for the maximizing problem and nonpositive for the minimizing problem.

Granting existence of an optimizer V_*, we can then try to find it by variational analysis, by letting $V_* \to V_* + \kappa P$ for generic perturbations P that are tangential to the ball (14) and differentiating with respect to k. "Tangential" here means that

$$\|V_* - W + \kappa P\|_p = M + o(\kappa). \tag{15}$$

A subtle point here is that even when $H + \kappa P$ is an entire family of operators, the function $E_k(V_* + \kappa P)$ may fail to be differentiable. (For perturbation theory see Kato [1966] or Reed and Simon [1978].) If, for example, $E_k(V_*)$ is isolated and nondegenerate, then differentiability is ensured - for instance the lowest eigenvalue E_1 always has this property, and all eigenvalues do if the dimension n = 1 (with, e.g., Dirichlet or Neumann boundary conditions). If these conditions hold, then there is a simple formula for the derivative, *viz.*

$$\frac{dE_\kappa}{d\kappa} = \int_\Omega P(x)u_*^2(x)dx \qquad (16)$$

where u_* is the normalized eigenfunction for $\kappa=0$. Equation (16) is a sort of orthogonality condition between P and u_*^2. Since P is tangential to V_*-W but otherwise generic, this means that u_*^2 must be proportional to a power of V_*-W. Specifically, a calculation using (15) and (16) reveals that

$$V_*(x) - W(x) = C\,[u_*(x)]^{2/(p-1)}. \qquad (17)$$

Combining this algebraic relationship with the eigenvalue equation for $E_* = E_n(V_*)$, we can characterize the solution of the optimization problem as the solution of a semilinear partial differential equation,

$$[-\Delta + W(x) \pm |u_*|^{\alpha-1}]u_* = E_* u_*. \qquad (18)$$

The constant $\alpha = (p+1)/(p-1)$, and V_* is determined from its sign and (17) if u_* is found from (18). The analysis of (18) can be fairly difficult, but in one dimension or numerically it is not too bad in some circumstances. The result is that one can generate functions

$$E_{max}(M, k,p,\Omega,W) \text{ and } E_{min}(M; k,p,\Omega,W).$$

In terms of these functions, knowledge of even one eigenvalue of H implies a whole class of lower bounds on expressions of the form $\|V-W\|_p$.

M.S. Ashbaugh, R. Svirsky, and I are currently investigating how these ideas apply to gaps. Suppose that Ω is smooth and bounded and, for simplicity, set $W = 0$, constraining the potential V so that

$$V \in S = \{V: \|V\|_p \le M < \infty\},$$

for some fixed $p > n/2$ ($p > 1$ when $n = 1$). Let $\Gamma(V) = E_2 - E_1$ for $-\Delta+V$ on $L^2(\Omega)$, with Dirichlet boundary conditions. For $p < \infty$ existence and uniqueness are guaranteed much as described above, and as before we can derive equations characterizing the optimizing potentials, except that in place of (18) we obtain complicated systems of coupled nonlinear equations.

If we let p be infinite, the situation becomes more tractable. In this case, let us write the constraint as:

$$S = \{V: 0 \le V(x) \le M\} \qquad (19)$$

for some finite M. This is tantamount to the restriction $\|V\|_\infty \le M/2$, but is more convenient.

Proposition 6: The existence of optimizers $V^* \in S$ for $\Gamma(V)$ follows as before, and we find that if $E_2(V^*)$ is nondegenerate, then

$$u_2^{*2}(x) = u_1^{*2}(x) \quad \text{a.e. on } \{x: 0 < V^*(x) < M\}. \qquad (20)$$

Actually, for the minimizing problem for V^*, (20) does not require the assumption of nondegeneracy, but applies when u_2^* is any normalized eigenfunction associated with $E_2(V^*)$.

Proof of (20): Let $T = \{x: \varepsilon \le V^*(x) \le M-\varepsilon\}$ for some $\varepsilon>0$. Assume that $E_2(V^*)$ is nondegenerate. Then, if $P(x)$ is any bounded, measurable function supported in T, and we perturb V^* to $V^* + \kappa P$, formula (16) applies. Taking the difference of formula (16) as applied to E_2 and E_1 shows that:

$$\frac{d\Gamma(V^*+\kappa P)}{d\kappa} = \int (u_2^{*2}(x)-u_1^{*2}(x))P(x)dx \qquad (21)$$

Since this derivative must be 0 at $\kappa=0$, it follows that

$$u_2^{*2}(x) - u_1^{*2}(x) = 0 \text{ a.e. on } T.$$

Since ϵ is arbitrary, (20) follows. If the eigenvalue is degenerate, then the perturbation may split the eigenvalue into a cluster of eigenvalues $E_2^{(m)}$, which are all still analytic in κ, provided that the right choice is made of how to define the functions $E_2^{(m)}(V^* + \kappa P)$ as κ passes through the value 0. (This choice is certainly different from the min-max ordering of the eigenvalues; for example the bottom eigenvalue of a cluster will as a rule have a discontinuous slope at $\kappa=0$.) The derivatives at $\kappa=0$ of the functions $E_2^{(m)}$ are the eigenvalues of the symmetric matrix

$$\int u_2^{*(j)}(x) u_2^{*(k)}(x) P(x)\,dx.$$

(Kato [1966], p. 407, Eq. (4.50)), and so by (16) the derivatives at $\kappa=0$ of the functions $E_2^{(m)} - E_1$ are the eigenvalues of the matrix

$$\int (u_2^{*(j)}(x) u_2^{*(k)}(x) - u_1^{*2}(x)\delta_{jk}) P(x)\,dx. \qquad (22)$$

If even one of these matrix elements differs from 0, then Γ is not at minimum. Hence, setting $j=k$, Equation (20) must hold at the minimum V^* for any normalized u_2^*.

□

The ramifications of (21)-(22) will be further discussed elsewhere (Ashbaugh, Harrell, and Svirsky [1987]). I shall confine myself here to some remarks about the simplest case, one dimension, with the constraint (19). We normalize so that $\Omega = [-1,1]$. In this case, we conclude

Proposition 7: In one dimension

$$V^* = M\,\chi_B, \qquad (23)$$

where $B = B^\sharp$ or respectively $B^\flat$, with $B^\sharp = \{x : |u_1^\sharp| > |u_2^\sharp|\}$ and $B^\flat = \{x : |u_1^\flat| < |u_2^\flat|\}$. $B^\sharp$ consists of a single interval $[-a^\sharp, a^\sharp]$, and $B^\flat$ consists of two intervals, $[-1,-a^\flat] \cup [a^\flat,1]$.

Proof: There is no question of degeneracy, and Sturmian comparison ensures that (20) can hold at only a finite number of discrete points. Indeed, we claim that $|u_1^*| = |u_2^*|$ at no more than two interior points of Ω:

> Suppose this is false. Recall that E_2 is the lowest eigenvalue for $H = -d^2/dx^2 + V$ with Dirichlet boundary conditions at 0 and p (or p and 1), where p is the node of u_2. If there are more than two interior points where $|u_1^*| = |u_2^*|$, then at least two of them, s and t, must lie to one side of p - suppose that they are to the left, $0 < s < t < p$, and take $u_1 > u_2 > 0$ on (s,t). Since [s,t] is a subinterval of [0,p], the eigenvalues of the Dirichlet problem for H on [s,t] lie above E_2. The Rayleigh-Ritz inequality then gives
>
> $$E_2 \int_s^t (u_1-u_2)^2 dx < \int_s^t (u_1-u_2) H (u_1-u_2)\,dx$$
>
> $$= \int_s^t E_1 (u_1-u_2)^2 dx - (E_2-E_1) \int_s^t (u_1-u_2) u_2\,dx$$
>
> $$< E_1 \int_s^t (u_1-u_2)^2 dx,$$
>
> which is a contradiction.

Perturbations P(x) supported where $V(x) = M$ are admissible for $\kappa>0$ only when $P(x) < 0$ a.e., else they would violate the constraint (19), and likewise perturbations supported where $V(x) = 0$ must have $P(x) > 0$ a.e. Since for such perturbations,

$$\frac{d\Gamma(V^\sharp+\kappa P)}{dx} \geq 0 \text{ and resp. } \frac{d\Gamma(V^\flat+\kappa P)}{dx} \leq 0,$$

Equation (21) leads readily to the conclusion that (23) holds for $B^\sharp = \{x : |u_1^\sharp| > |u_2^\sharp|\}$ or $B^\flat = \{x : |u_1^\flat| < |u_2^\flat|\}$. That $B^\sharp$ and $B^\flat$ consist of no more than two intervals is implied by the statement that $|u_1^\sharp| = |u_2^\sharp|$ at precisely two interior points. And since the node of $u_2^\sharp$ lies within $B^\sharp$ while that of $u_2^\flat$ lies in the complement of $B^\flat$, we see that $B^\sharp$ is a single interval, while $B^\flat$ consists of two disjoint intervals extending to $\pm l$.

The final fact to prove is that the intervals B are symmetric about 0. To prove this, shift Ω so that the node of $u_2^\sharp$ is at 0 and choose $u_2^\sharp > 0$ for $x > 0$.

Case I: Maximizing Γ, or minimizing Γ with $E_1 \geq M$ (arises when M is small). The Ricatti equation for $r_{1,2} = d(\ln u_{1,2})/dx$, viz.,

$$r_{1,2}' = V - E_{1,2} - r_{1,2}^2,$$

shows that r_1 decreases monotonically for all $-a^< \leq x \leq a^>$, and likewise for r_2 except at $x=0$. Also observe that the greatest value of u_1 on $[-a^<, a^>]$ is attained closer to $a^>$ than to $-a^<$. Therefore we find that

$$-u_2'(-a^<)/u_2(-a^<) \;>\; u_2'(a^>)/u_2(a^>) > u_1'(a^>)/u_1(a^>) > -u_1'(-a^<)/u_1(-a^<) \quad (24)$$

Next notice that $u_2(x+a^>)$ and $-u_2(-x-a^<)$ are positive and solve the same Schrödinger equation for $0 < x$, and likewise for $u_1(x+a^>)$ and $u_1(-x-a^<)$. The Wronski identity ensures that the signs of

$$r_1(x+a^>) + r_1(-x-a^<) \text{ and } r_1(x+a^>) + r_1(-x-a^<)$$

do not change, except when these quantities diverge. $r_1(x+a^>)$ diverges negatively at $x = c^>-a^>$, while $r_1(-x-a^<)$ diverges positively at $x = c^<-a^<$. Because the sign of $r_1(x+a^>) + r_1(-x-a^<)$ is positive at $x=0$, the latter divergence must occur first, i.e., $c^<-a^< < c^>-a^>$. For similar reasons, the first zero of $-u_2(-x-a^<)$ comes after that of $u_2(x+a^>)$, i.e., $c^<-a^< > c^>-a^>$. This is a contradiction.

Case II. Minimizing Γ with $E_1 < M$. It is straightforward to derive the following facts from the observation that $u_{1,2}^{\sharp\prime}$ are monotonic everywhere except possibly at the edges of B and at the node of $u_2^\sharp$:

$$u_1^\sharp(x) > u_1^\sharp(-x) \text{ for } 0 < x < a^<; \quad (25)$$

and

$$u_1^\sharp(a^>) = u_2^\sharp(a^>) > u_1^\sharp(-a^<) = -u_2^\sharp(a^<),\; u_1^{\sharp\prime}(a^>) > -u_1^{\sharp\prime}(-a^<). \quad (26)$$

It follows from (26) for u_1 that $c^>-a^> > c^<-a^<$. Since the functions $-u_2(-x-a^<)$ and $u_2(x+a^>)$ are positive and solve the same Schrödinger equation for $0 < x < c^<$, and the former function is smaller at $x=0$ and $x=c^<$, the Sturm separation theorem implies that

$$u_2^\sharp(x-a^>) > -u_2^\sharp(-x+a^<) \quad (27)$$

for all $0 < x < c^<-a^<$ (otherwise their difference would have two nodes). Moreover, from (26),

$$u_1^\sharp(x+a^>) > -u_1^\sharp(-x+a^<)$$

for all $0 < x < c^<-a^<$. Together with (25) and (27) this implies that

$$\int_0^{c^>} u_1(x)u_2(x)dx \;>\; \int_{-c^<}^{0} u_1(x)|u_2(x)|dx,$$

which contradicts the orthogonality of u_1 and u_2.

□

To summarize, in one dimension, the optimal potential for minimizing gaps is in fact just that of the toy model (7), with an optimized a! The gap Γ is determined from a pair of transcendental equations, and can easily be optimized numerically or asymptotically with respect to a to determine $a^{\#}$ and a^{b}. For example, asymptotically for large M (which corresponds to small $\hbar$)

$a^{\#} \equiv 1 - \left(\frac{\pi^2}{2M}\right)^{1/3}$, and

$$\Gamma(V^{\#}) \equiv 16\sqrt{M}\exp(-2M^{1/2} + 2^{5/3}\pi^{2/3}M^{1/3}) \qquad (28)$$

Appendix. An algebraic version of the inequality of Payne, Pólya, and Weinberger.

Several years ago I became interested in the inequality of Payne, Pólya, and Weinberger [1956], and reduced it to a series of lemmas involving commutator arguments, in particular the basic gap formula (4). While I never published this work, I discussed it with several people, including E.B. Davies in 1984. He then also got interested in the inequality and concocted a completely algebraic version of it. He has agreed to let me publish it here for the first time.

Let $H \geq 0$ have discrete eigenvalues $E_1 \leq E_2 \leq \ldots$, and let P be the spectral projection for $E_1 \ldots E_k$. Let $G = G^*$ and $A = (1-P)GP$. Let us also assume that the domains and ranges of G and H are such that GP, G^2P, HG^2P, and GHGP exist. Inequalities among operators are intended in the sense of quadratic forms, i.e., $R \geq S$ means that for a suitable dense set of ϕ, $(\phi, R\phi) \geq (\phi, S\phi)$. The trace is denoted tr, and the commutator of two operators R and S is denoted $[R,S] = RS - SR$.

Theorem A0: If β, γ_0, and γ_1 are positive numbers such that $\gamma_0 \leq -[G,[G,H]] \leq \gamma_1$ and $-[G,H]^2 \leq \beta H$, then

$$E_{k+1} - E_k \leq \left(\frac{2\beta\gamma_1}{k\gamma_0^2}\right)\sum_{j=1}^{k} E_j. \qquad (A1)$$

The Payne-Pólya-Weinberger inequality results with $H = -\Delta$, $G = x_1$, so $[G,H] = 2\partial/\partial x_1$, and $-[G,[G,H]] = 2$. We can then take $\beta = 4$, and $\gamma_{0,1} = 2$. This inequality would, for instance, apply to certain partial differential operators with nonconstant coefficients. The proof consists of three lemmas:

Lemma A1:

$$\mathrm{tr}(H\,[A,A^*]) = \mathrm{tr}(P[G,H]A) = -(\tfrac{1}{2})\,\mathrm{tr}([G,[G,H]]P)$$

Proof:

$$\mathrm{tr}(HAA^* - HA^*A) = \mathrm{tr}(H(I-P)GPG(I-P) - HPG(I-P)GP)$$
$$= \mathrm{tr}(GH(I-P)GP - HG(I-P)GP), \qquad \text{(A2)}$$

by the cyclic property of traces and the fact that H commutes with P and I-P. The first identity results from writing the right side of (A2) as

$$\mathrm{tr}([G,H](I-P)GP) = \mathrm{tr}(P[G,H]A),$$

and the second results from writing it as

$$\mathrm{tr}(GHGP - HGGP) = \mathrm{tr}((GHG - (HG^2+G^2H)/2) = -(\tfrac{1}{2})\,\mathrm{tr}([G,[G,H]]P).$$

□

Lemma A2:

If $-[G,[G,H]] \le \gamma_1$, then

$$(E_{k+1} - E_k)\,\mathrm{tr}(A^*A) \le k\gamma_1/2.$$

Proof: First note that $\mathrm{tr}(HAA^*) \ge E_{k+1}\,\mathrm{tr}(AA^*) = E_{k+1}\,\mathrm{tr}(A^*A)$ and $\mathrm{tr}(HA^*A) \le E_k\,\mathrm{tr}(A^*A)$, since $\mathrm{Ran}(AA^*) \subset \mathrm{Ran}(1-P)$ and $\mathrm{Ran}(A^*A) \subset \mathrm{Ran}P$. Hence

$$(E_{k+1} - E_k)\,\mathrm{tr}(A^*A) \le \mathrm{tr}(HAA^* - HA^*A)$$
$$\le \frac{1}{2}\,\mathrm{tr}(\gamma_1 P) = \frac{\gamma_1 k}{2}$$

by Lemma A1. □

Lemma A3:

If $-[G,[G,h]] \ge \gamma_0 > 0$, and $-[G,H]^2 \le \beta H$, then

$$\gamma_0^2 k^2 \le 4\beta\,\mathrm{tr}(A^*A) \sum_{j=1}^{k} E_j.$$

Proof: $\gamma_0 k \le -\mathrm{tr}([G,[G,H]]P) = 2\,\mathrm{tr}(P\,[G,H]\,A)$ (by Lemma A1)

$$\le 2\,(\mathrm{tr}(-P[G,H]^2P)\,\mathrm{tr}(A^*A))^{1/2}$$

by the Cauchy inequality for traces (the minus sign originates in the skew-adjointness of the commutator [G,H], which makes $-[G,H]^2 > 0$). Squaring,

$$(\gamma_0 k)^2 \le 4\,\mathrm{tr}(\beta HP)\,\mathrm{tr}(A^*A) = 4\beta\,\mathrm{tr}(A^*A) \sum_{j=1}^{k} E_j.$$

□

The theorem results from concatenating Lemmas A2 and A3.

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Bibliography

M.S. Ashbaugh and R. Benguria (1987a): Optimal Lower Bound for the Gap Between the First Two Eigenvalues of One-Dimensional Schrödinger Operators with Symmetric Single-Well Potentials, preprint.

M.S. Ashbaugh and R. Benguria (1987b): On the Ratio of the First Two Eigenvalues of Schrödinger Operators with Positive Potentials, preprint.

M.S. Ashbaugh and E.M. Harrell II (1984): Potentials having Extremal Eigenvalues Subject to p-Norm Constraints. Argonne Nat. Lab. Technical Report ANL-84-73. (Proceedings of the 1984 Workshop "Spectral Theory of Sturm-Liouville Differential Operators," H.G. Kaper and A. Zettl, eds.)

M.S. Ashbaugh and E.M. Harrell II (1987): Maximal and Minimal Eigenvalues and their Associated Nonlinear Equations. J. Math. Phys., to appear.

M.S. Ashbaugh, E.M. Harrell II, and R. Svirsky (1987), in preparation.

K. Chadan and P.C. Sabatier (1977): Inverse Problems in Quantum Scattering Theory. Berlin, Heidelberg, and New York: Springer.

Isaac Chavel (1984): Eigenvalues in Riemannian Geometry. New York: Academic Press.

G. Chiti (1983): A Bound for the Ratio of the First Two Eigenvalues of a Membrane. SIAM J. Math. Anal. **14**, 1163-1167.

H.L. Cycon, R. Froese, W. Kirsch, and B. Simon (1987): Schrödinger Operators. Berlin, Heidelberg, and New York: Springer.

E.B. Davies (1980): One-Parameter Semigroups. London and New York: Academic.

E.B. Davies (1982): Metastable States of Symmetric Markov Semigroups I. Proc. London Math. Soc. **45**, 13-150; II, J. London Math. Soc. **26**, 541-556.

H. Egnell (1987): Semilinear Elliptic Equations involving Critical Sobolev Exponents. Ann. Scuola Norm. Sup. Pisa, to appear.

E.M. Harrell II (1984): Hamiltonian Operators with Maximal Eigenvalues. J. Math. Phys. **25**, 48-51, erratum **27**, 419.

E.M. Harrell II (1980): Double Wells. Commun Math. Phys. **75**, 239-261.

E.M. Harrell II and R. Svirsky (1986): Potentials Producing Maximally Sharp Resonances. Trans. Amer. Math. Soc. **293**, 723-736.

B. Helffer and J. Sjöstrand (1984): Multiple Wells in the Semi-Classical Limit I. Commun. PDE **9**, 337-408.

T. Kato (1966): Perturbation Theory for Linear Operators, Grundlehren der mathematischen Wissenschaften **132**. New York: Springer.

W. Kirsch and B. Simon (1987) Comparison Theorems for the Gap of Schrödinger Operators. J. Functional Analysis, to appear.

W. Kirsch and B. Simon (1985): Universal Lower Bounds on Eigenvalue Splittings for One Dimensional Schrödinger Operators. Commun. Math. Physics **97**, 453-460.

L.D. Landau and E.M. Lifshitz (1977): Quantum Mechanics, Non-Relativistic Theory. Course of Theoretical Physics 3, Third ed. Oxford and New York: Pergamon. (Translation of Л.Д. Ландау, Е.М. Лифшиц (1974): Квантовая Механика: Нерелятивистская Теория. Москва: Наука.)

V. M. Levitan (1984). Обратные Задачи Штурма-Лиувилля. Москва: Наука.

V. A. Marchenko (1986). Sturm-Liouville Operators and Applications. Basel, Boston, and Stuttgart: Birkhauser.

L. E. Payne, G. Pólya, and H. Weinberger (1956). On the Ratio of Consecutive Eigenvalues. J. Math. and Physics **35**, 289-298.

Jürgen Poschel and Eugene Trubowitz (1987). Inverse Spectral Theory. New York: Academic.

M. H. Protter (1987): Can One Hear the Shape of a Drum? Revisited. SIAM Review **29**, 185-197.

M. Reed and B. Simon (1978). Methods of Modern Mathematical Physics **IV**: Analysis of Operators. New York: Academic.

B. Simon (1982): Schrödinger semigroups. Bull. Amer. Math. Soc. **7**, 447-526.

I. M. Singer, B. Wong, S-T. Yau, and S. S-T. Yau (1985). An Estimate of the Gap of the First Two Eigenvalues in the Schrodinger Operator. Annali Scuola Norm. Sup. Pisa, ser. IV, **XII**, 319-333.

R. Svirsky (1987). Maximally Resonant Potentials subject to p-Norm Constraints. Pac. J. Math., to appear.

H. L. de Vries (1967). On the Upper Bound for the Ratio of the First Two Membrane Eigenvalues. Z. Naturforschung A **22**, 152-153.

Q. Yu and J-Q. Zhong (1986). Lower Bounds of the Gap Between the First and Second Eigenvalues of the Schrodinger Operator. Trans. Amer. Math. Soc. **294**, 341-349.

W. Thirring (1979). A Course in Mathematical Physics 3. Quantum Mechanics of Atoms and Molecules. New York and Vienna: Springer.