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ABSTRACT

An iterative method for determining bound-state eigenvalues and properties of the radial Schrödinger equation is appraised. The method stems from iterating the integral equation

$$\psi = \mu(T + \tfrac{1}{2}\gamma^2)^{-1}(-V\psi)$$

where T and V are the kinetic and potential energy operators. The basic theory is briefly reviewed, and calculations are performed for the Coulomb and Screened Coulomb potentials. The lowest three μ-eigenvalues together with expected values of $(\gamma r)^{-1}$, γr and $(\gamma r)^2$ are obtained from a single iterated eigenfunction sequence. Convergence is rapid for eigenvalues but slow for expected values. There is some sensitivity to the choice of numerical integration formula. Regarded as a numerical

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method, this approach may be most competitive for the determination of zero-energy potential-strength eigenvalues. Its disadvantages are listed.

Analytical improvements to eigenfunctions can be easier to obtain by iteration than by perturbation, and some success has been achieved. A simple example suggests that the rate of convergence of an iterated eigenfunction sequence is less than that of a related perturbation sequence unless the choice of starting function is bad.

I. INTRODUCTION

In this paper we report on the utility of an iterative method for calculating bound-state eigenvalues and properties associated with the radial Schrödinger equation

$$(T + \mu V)\psi = -\tfrac{1}{2}\gamma^2\psi \ , \qquad \gamma \geq 0 \tag{1}$$

where

$$T(r) = -\tfrac{1}{2}\, d^2/dr^2 \ , \qquad 0 \leq r < \infty \ , \tag{2}$$

is the kinetic energy operator, $V(r)$ is the potential energy, and $\psi(r)$ is the r-multiplied radial wave function. The method is based on an integral-equation equivalent of (1), namely

$$\psi = \mu(T + \tfrac{1}{2}\gamma^2)^{-1}(-V\psi) \ , \tag{3}$$

which is formulated using the bound-state free-particle Green's operator $(T + \frac{1}{2}\gamma^2)^{-1}$ with kernel

$$\gamma^{-1}\left\{\exp[-\gamma|r-r'|] - \exp[-\gamma(r+r')]\right\} . \tag{4}$$

The alternative form (3) of the Schrödinger equation has been called the conjugate eigenvalue equation. When γ is regarded as a fixed parameter, equation (3) gives rise naturally to eigenvalues and eigenfunctions for the potential strength μ ; often (most simply by scaling procedures) it is possible to relate them to energy eigenvalues and eigenfunctions for a prescribed μ .[1]

We employ the iterative sequence $\{\phi_k\}$ specified by

$$\phi_{k+1} = (T + \tfrac{1}{2}\gamma^2)^{-1}\,(-V\phi_k), \qquad k = 0,1,2,\ldots, \tag{5}$$

which ultimately behaves like a constant times the eigenfunction ψ_o of (3) which corresponds to $\mu_o(\gamma)$, the μ-eigenvalue of smallest magnitude. Illustrative numerical calculations are performed for the Coulomb potential, and also for the screened Coulomb potential. Properties of the lowest three eigenstates are obtained from a single iterative sequence. The convergence of expected values is slow but steady, and the convergence of bounding sequences for eigenvalues is rapid.

Regarded as a numerical technique, the iterative method is akin to the power method for finding the eigenvalues of a matrix. It is likely to be competitive only for the lowest eigenstates, and most competitive for zero-energy states where more sophisticated methods[2,3] might run into difficulties because of their dependence on the adjustment of γ.

As an analytical method of improving approximate wave functions and estimating eigenvalues, this iterative approach has enjoyed success from time to time. Activity has been mainly in momentum space where an integral equation arises naturally as the Fourier Transform of the Schrödinger equation.[4-9] But there has been some work in coordinate space[10,11] and recently considerable attention has been paid to eigenvalue bounds derived from the conjugate eigenvalue equation.[12-16] The present paper is concluded with a simple example which suggests that the rate of convergence of the sequence $\{\phi_k\}$ is less than that of a related perturbation sequence unless the choice of ϕ_o is a bad one. However, analytical improvements to wave functions are in principle easier to obtain by iteration than by perturbation.

II. GENERAL THEORY

The theory is clear-cut when the operator $(-V)$ is positive-definite, thus admitting a square root, and given that the operator

$$K = (-V)^{\frac{1}{2}} (T + \tfrac{1}{2}\gamma^2)^{-1} (-V)^{\frac{1}{2}} \tag{6}$$

is a Hilbert-Schmidt operator (i.e. K has finite double-norm). Equation (3) may then be written as

$$\left\{(-V)^{\frac{1}{2}}\psi\right\} = \mu K\left\{(-V)^{\frac{1}{2}}\psi\right\} , \tag{7}$$

and the standard Hilbert-Schmidt theory of integral equations invoked.[17,18] The potential-strength μ has a discrete spectrum $\{\mu_n\}$ whose members can be arranged in ascending order of magnitude

$$0 < \mu_0 < \mu_1 < \cdots < \mu_n < \cdots \quad . \tag{8}$$

(In general there could be some equalities here, but not for a one-dimensional radial problem.) If $\{\psi_n\}$ are the corresponding eigenfunctions, orthonormalized so that

$$(\psi_n,(-V)\psi_m) = \int_0^\infty \psi_n(-V)\psi_m \, dr = \delta_{nm} , \tag{9}$$

then it follows from the Hilbert-Schmidt theorem that

$$\phi_k = \sum_{n=0}^{\infty} a_n \mu_n^{-k} \psi_n , \qquad k = 1,2\cdots , \tag{10}$$

where

$$a_n = (\phi_0,(-V)\psi_n) \tag{11}$$

and the initial function ϕ_0 need not necessarily be in the domain

spanned by $\{\psi_n\}$. Assuming that a_0 is not zero, the sequence $\{\phi_k\}$ ultimately behaves like a constant times ψ_0, and (if a_1 is also non-zero) the rate of convergence is governed by the ratio μ_0/μ_1. Thus if $\mathcal{L}(r)$ is an operator of interest and

$$L_k = (\phi_k, \mathcal{L}\phi_k)/(\phi_k, \phi_k), \tag{12}$$

the sequence $\{L_k\}$ will tend to the expected value of $\mathcal{L}(r)$ in the bound state which is specified by the parameter values μ_0 and γ.

It can also be shown that[19]

$$A_0 \geq B_0 \geq A_1 \geq B_1 \quad \cdots \geq A_k \geq B_k \geq \cdots \geq \mu_0 \tag{13}$$

where

$$A_k = v_{kk}/v_{k,k+1} \quad , \qquad B_k = v_{k,k+1}/v_{k+1,k+1} \quad , \tag{14}$$

and

$$v_{ij} = \int_0^\infty \phi_r(-V)\phi_j \, dr \, . \tag{15}$$

The sequences $\{A_k\}$ and $\{B_k\}$ actually have limit-point μ_0, and their rate of convergence is governed by the ratio (μ_0/μ_1).

If a_0 (but not a_1) happens to be zero, then ϕ_k tends to a constant times ψ_1, and we obtain bounding sequences for μ_1. If μ_0 is known, then the sequence $\{\tilde{\phi}_k\}$ defined by

$$\tilde{\phi}_k = \mu_0 \, \phi_{k+1} - \phi_k \tag{16}$$

always has a zero $\tilde{a}_0$ since

$$\tilde{a}_0 = (\tilde{\phi}_0, (-V)\psi_0) = (\mu_0\phi_1, (-V)\psi_0) - (\phi_0, (-V)\psi_0) \, , \tag{17}$$

and from equations (3) for ψ_0 and (5) with $k=0$ the terms on the right of (17) are seen to cancel. Similarly if

$$\approx\!\!\approx\!\!\phi_k = \mu_1 \tilde{\phi}_{k+1} - \tilde{\phi}_k \tag{18}$$

then $\approx\!\!\approx\!\!a_0$ and $\approx\!\!\approx\!\!a_1$ are zero and $\approx\!\!\approx\!\!\phi_k$ tends to a constant times ψ_2, and so on. These ideas were first developed and applied to vibration problems by Temple[20-22] and Bickley.[22] In the event that the powers of the dominant eigenvalue make ϕ_k too small as k increases (so that accuracy is lost), powers of an appropriate scale factor can be introduced. We can work with $\phi_k P^{-k}$, $\tilde{\phi}_k Q^{-k}$ etc., when P, Q are very rough estimates of μ_0, μ_1 etc.

Certain relaxations of the Hilbert-Schmidt condition on K are possible[23]; as far as μ_0 and ψ_0 are concerned, the method is not likely to be affected by the presence of a continuum at the upper end of the μ-spectrum. If the operator $(-V)$ is indefinite, equation (3) must be treated in the form

$$(-V)\psi = \mu\left\{(-V)(T + \tfrac{1}{2}\gamma^2)^{-1}\ (-V)\right\}\psi\ . \tag{19}$$

The operator on the right of (19) is positive-definite and self-adjoint, but the signs of the eigenvalues are now uncertain and negative eigenvalues may well not be physically relevant. The inequalities (8) and (12) are replaced by[19]

$$0 < |\mu_0| < |\mu_1| < \cdots < |\mu_n| < \cdots \tag{20}$$

and

$$|B_0| \geq |B_1| \geq \cdots \geq |B_k| \geq \cdots \geq |\mu_0|\ . \tag{21}$$

Nothing can be said here about the sequence $\{|A_k|\}$.

Whenever for a given value of μ the quantity $-\frac{1}{2}\gamma^2$ is a discrete energy which is not embedded in a continuum, physical considerations indicate that the entire μ-spectrum is discrete for that value of γ.

III. SCREENED COULOMB POTENTIAL

The negative screened Coulomb potential has been studied in connection with the deuteron[7-9], hydrogen plasmas[24], scattering theories[25], and has recently been the subject of a perturbation treatment[26]. Let

$$V(r) = -r^{-1} \exp(-\beta r), \qquad \beta \geq 0 , \tag{22}$$

Then the double-norm of K is, from (4), (6), and (22),

$$I(\beta,\gamma) = \gamma^{-2} \int_0^\infty \int_0^\infty (rr')^{-1} \exp[-\beta(r+r')] \left\{ \exp[-\gamma|r-r'|] - \exp[-\gamma(r+r')] \right\}^2 dr\, dr' \tag{23}$$

which satisfies the relations

$$0 < I(\beta,\gamma) < I(0,\gamma) = \Pi^2/\gamma^2 , \tag{24}$$

$$I(\beta,0) = 4\beta^{-2} \ln(4/e) , \tag{25}$$

and is thus finite unless both β and γ are zero. Hence K is Hilbert-Schmidt.

Remembering that $\psi(r)$ is r-multiplied, we set

$$\phi_k = r\theta_k , \qquad k = 0, 1, 2, \ldots \tag{26}$$

so that equation (5) becomes

$$r\theta_{k+1}(r) = \gamma^{-1} \int_{r'=0}^\infty \left\{ \exp[-\gamma|r-r'|] - \exp[-\gamma(r+r')] \right\} \exp(-\beta r')\theta_k(r')\, dr' \tag{27}$$

which reduces to

$$\theta_{k+1}(0) = 2 \int_{r'=0}^{\infty} \exp[-(\beta+\gamma)r'] \, \theta_k(r') \, dr' \qquad (28)$$

at zero r. If γ is zero (corresponding to zero-energy bound states), equation (27) simplifies to

$$r\theta_{k+1}(r) = 2 \int_{r'=0}^{\infty} \min\{r,r'\} \, \exp(-\beta r') \, \theta_k(r') \, dr' \, . \qquad (29)$$

Whenever suitable, equations (27) and (28) can be recast in terms of a variable (γr); likewise equation (29) in terms of (βr).

IV. NUMERICAL RESULTS

Illustrative calculations of iterative sequences for eigenvalues (μ_n/γ) and expected values of $(\gamma r)^{-1}$, γr and $(\gamma r)^2$ were performed for the Coulomb potential (Table 1) and also for the screened Coulomb potential with $\gamma = 0.313\beta$ (Table 2). This particular ratio was used by Goldstein and Salpeter[8] for a deuteron model; they found an estimated value of 3.797 for (μ_0/γ) in comparison with our 3.91770. In Table 3 appear the eigenvalue sequences for the zero-energy screened Coulomb potential. Here our values of $(2\mu_n/\beta)$ for the lowest three states are 1.68374, 6.5066 and about 14.6. Gilda Harris[24] has obtained approximate values 1.74, 7.14 and 13.33 by a variational method, and the directly-calculated value for $(2\mu_0/\beta)$ of 1.683 by Sachs and Goeppert-Mayer[27] is still quoted in the more recent literature[25,28]. (Expected vulues of powers of r are not relevant for this latter system.)

A typical iteration integral like (27) was replaced by the discrete approximation

Table 1. Hydrogenic States; $\beta = 0$

	k	$(\mu_n/\gamma)_+$	$\langle(\gamma r)^{-1}\rangle$	$\langle \gamma r \rangle$	$\langle(\gamma r)^2\rangle$
n=0	2	1.02058	1.21845	1.23336	2.04225
	5	1.00031	1.02174	1.46395	2.85934
	8	1.00000	0.99978	1.49538	2.98162
	11	1.00000	0.99707	1.49943	2.99769
	16	1.00000	0.99669	1.49999	2.99995
	Exact	1	1	1.5	3
n=1	2	2.04856	0.65904	2.51028	7.50855
	5	2.00418	0.53968	2.84926	9.52412
	8	2.00036	0.51011	2.95426	10.20061
	11	2.00003	0.50179	2.98630	10.41303
	16	2.00000	0.49877	2.99821	10.49287
	Exact	2	0.5	3	10.5
n=2	2	3.08672	0.47910	3.69947	16.2225
	5	3.01531	0.38479	4.15840	19.9559
	8	3.00268	0.35286	4.35433	21.6771
	11	3.00079	0.34032	4.43927	22.4466
	Exact	3	0.33333	4.5	23
n=3	2	4.13443	0.39205	4.80276	27.6378
	5	4.03504	0.30827	5.40371	33.7558
	8	4.00214	0.27294	5.72726	37.2586
	Exact	4	0.25	6	40.5

Table 2. Screened Coulomb Potential: $\gamma = 0.313\beta$

	k	$(\mu_n/\gamma)_+$	$\langle(\gamma r)^{-1}\rangle$	$\langle \gamma r \rangle$	$\langle(\gamma r)^2\rangle$
n=0	2	3.96021	2.09677	0.78233	0.90407
	5	3.91771	2.31556	0.73404	0.82038
	8	3.91770	2.31973	0.73328	0.81916
	11	3.91770	2.31982	0.73327	0.81913
	16	3.91770	2.31982	0.73327	0.81913
n=1	2	14.9319	1.23822	1.08014	1.47862
	5	14.1578	1.47790	0.97406	1.24966
	8	14.1538	1.49632	0.96807	1.23784
	11	14.1538	1.49768	0.96761	1.23694
n=2	2	37.367	0.92969	1.30628	2.02770
	4	33.497	1.10295	1.17606	1.69953
	6	33.281	1.15282	1.14950	1.63902
	7	33.266	1.16213	1.14524	1.62963
n=3	2	78.8	0.773	1.492	2.550
	4	66.7	0.909	1.344	2.132
	6	63.4	0.944	1.308	2.036

Table 3. Screened Coulomb Eigenvalues at Zero Energy: $\gamma = 0$

k	$(2\mu_0/\beta)_+$	$(2\mu_1/\beta)_+$	$(2\mu_2/\beta)_+$	$(2\mu_3/\beta)_+$
2	1.75493	6.6309	15.3334	28.698
4	1.68406	6.5112	14.6989	28.609
6	1.68374	6.5068	14.6420	26.424
7	1.68374	6.5066	14.6235	- - -
8	1.68374	6.5066	- - -	- - -
16	1.68374	- - -	- - -	- - -

$$x_i\theta_{k+1}(x_i/\gamma) = \sum_j \left\{ \exp[-|x_i - x_j|] - \exp[-(x_i+x_j)] \right\} \exp[-\beta x_j/\gamma]\theta_k(x_j/\gamma)\omega_j, \tag{30}$$

where $x = \gamma r$ and (x_j, ω_j) are the points and weights of the numerical integration formula. The same integration formula was used to evaluate all the integrals in a single program, thus saving a factor of about a hundred in time. The particular formula used to give the results in Tables 1-3 was a trapezoidal rule with 100 equal intervals from 0.0 to 10.0, combined with a 19-point Gauss-Laguerre quadrature formula from 10.0 to ∞. The trapezoidal rule was chosen becuase the discontinuity in the slope of the kernels should have no effect on it. Beyond $x = 10.0$ there is little contribution to the integral and different means used to integrate the tail of the integrand gave similar results. In each case the starting function was $\theta_0 = \exp(-3x/2)$, but the iteration is insensitive to choice of starting function. After one or two cycles, similar results were obtained with for example $\theta_0 = 1$.

Sixteen iterations were performed, and the bounding sequences $\{A_k\}$ and $\{B_k\}$ given by (14) were stable through eight figures after twelve iterations. Only the sequence $\{B_k\}$ is quoted in the tables, (designated by $(\mu_n/\gamma)_+$ and $(2\mu_n/\beta)_+$) since $A_k \geq B_k$, and only some of the k-values are shown to save space. Appropriate $\{L_k\}$ sequences are also given. Only a single sequence $\{\theta_k\}$ was calculated for each of the three systems, and sequences suitable for the next highest states were deduced from it, as indicated in equations (16) and (18). Although this method of finding sub-dominant eigenvalues is highly subject to round-off errors, the calculations were stable thorugh 16, 11, and 8 iterations for the next three hydrogenic states, and through rather less

iterations for the other systems (the highest k-value shown is the last stable one for $n = 1, 2, 3$). Better accuracy could of course be obtained for $n > 0$ if a fresh iterative sequence were generated for each state, with renormalization at appropriate stages. But such refinements consume more machine time, and were felt to be unjustified in the present context. The calculations were run in FORTRAN on a CDC 3600 computer in single precision arithmetic which is good to about 10 significant figures, and the average running time including compilation was about 40 seconds.

In an attempt to improve the expected value of $(\gamma r)^{-1}$ for hydrogen (which for $n=0$ is 0.3% too low), an alternative integration formula was tried with 40 equal intervals in 0.0 to 2.0, 80 intervals in 2.0 to 10.0 and the same 19-point Gauss-Laguerre formula past 10.0. The main effect of this change was to lower the eigenvalue results in about the fourth significant figure, but the $(\gamma r)^{-1}$ values were improved slightly. This fact, combined with the stable convergence of the eigenvalue sequence with each formula; would seem to indicate that the iterative method is somewhat sensitive to the particular integration formula in use. Because of the excellent results for the first two hydrogenic eigenvalues, we put our faith in the trapezoidal rule with equal intervals from 0.0 to 10.0.

V. COMPARISON WITH PERTURBATION THEORY

As a simple example let us consider the hydrogenic ground state where $\mu_0 = 1$, $\gamma = 1$ and $\psi_0 = r \exp(-r)$ (not normalized). The overlap of ϕ_k $(= r\theta_k)$ with $r \exp(-r)$ is

$$S_k = \int_0^\infty \theta_k(r) \exp(-r)\, r^2 dr \,. \tag{31}$$

If we also define

$$C_k = \int_0^\infty \theta_k(r) \exp(-r)\, r\, dr \tag{32}$$

then it follows from (27) with $\beta = 0$, $\gamma = 1$ that

$$C_k = C_0 \qquad \text{(independently of } k\text{)} \tag{33}$$

and

$$S_k = C_0 + (S_0 - C_0)2^{-k} \tag{34}$$

The rate of convergence of the overlap integral S_k is thus exactly 1/2 (the value of μ_0/μ_1) and this is independent of the initial trial function θ_0.

If we take

$$\chi_0 = \exp(-\alpha r), \qquad \alpha \neq 1 \,, \tag{35}$$

as the unperturbed wave function for a Rayleigh-Schrödinger perturbation expansion, the perturbation is $(\alpha-1)/r$ and it is possible by standard methods[29] to determine χ_k, the wave function corrected through order k in the perturbation. For comparison with θ_k, the normalization is arranged so that

$$C_k' = \int_0^\infty \chi_k \exp(-r)\, r\, dr = C_0 \qquad \text{(independently of } k\text{)}, \tag{36}$$

and the consequent overlap integral

$$S_k' = \int_0^\infty \chi_k \exp(-r)\, r^2\, dr \tag{37}$$

has the value

$$S_k' = C_0 - C_0\left(\frac{\alpha-1}{\alpha+1}\right)^{k+1} . \tag{38}$$

Thus judging by the overlap integrals S_k and S_k', the perturbation approach to the true eigenfunction converges more rapidly than does the iterative approach whenever

$$\frac{\alpha-1}{\alpha+1} < \tfrac{1}{2}, \quad \text{i.e. } \alpha < 3 . \tag{39}$$

Since $\alpha=1$ gives the true eigenfunction, the iterative approach is only superior when a bad initial trial function is chosen.

Qualitatively one might expect a perturbation treatment to be better; ideally such a treatment involves corrections resulting from a small perturbation to the potential, whereas in the iterative approach corrections are generated by the operator $(T + \tfrac{1}{2}\gamma^2)^{-1}(-V)$, involving the whole potential. However the single quadrature required for an iterative correction to a wave function is in principle easier to carry out analytically than the double quadrature required for a first-order perturbed wave function[29]. Thus in some cases it may be possible to improve a wave function analytically by iteration but not by perturbation. It has been pointed out[10] that the first iterated improvement to a hydrogenic 1s function is a so-called 0s function.

VI. CONCLUDING REMARKS

As a numerical tool, this iterative method is conceptually very simple but it has shortcomings. These are:

(i) the difficulties with the basic theory if K is not Hilbert-Schmidt;

(ii) the slow convergence of expected-value sequences;

(iii) the difficulties in dealing with sub-dominant-eigenvalues;

(iv) the sensitivity of results to integration formulas;

(v) the possible difficulties in relating the two different types of eigenvalue equations.

Perhaps these help to explain its relative lack of popularity. The method may well be seen to best advantage in the calculation of zero-energy potential-strength eigenvalues, which are useful in determing the number of bound states admitted by a given potential[1].

As an analytical method, the approach has enjoyed some success devolving from its simple Green's operator. It may be useful occasionally when perturbation theory fails.

Equation (1) which we considered was for s-states. For states with higher orbital angular momentum, one can either work with the operator

$$\left\{ T + 2\ell(\ell+1)r^{-2} + \tfrac{1}{2}\gamma^2 \right\}^{-1} \tag{40}$$

which has kernel

$$2(rr')\ I_{\ell+\frac{1}{2}}(\gamma r_<)\ K_{\ell+\frac{1}{2}}(\gamma r_>), \quad (r_< \equiv \min[r,r'],\ r_> = \max[r,r']), \tag{41}$$

where $I_{\ell+\frac{1}{2}}$ and $K_{\ell+\frac{1}{2}}$ are the modified spherical Bessel functions, or alternatively the r^{-2} might be absorbed into the potential.

If the Schrödinger equation is many-dimensional and non-separable the difficulties mount. But some analytical progress has been made for He and H_2^+ [5,6,15], and the numerical approach may well be feasible, certainly in two dimensions. The free-particle Green's function in n-dimensions is known[30].

Methods which combine features of the two types of eigenvalue equation (1) and (3) have been suggested[11,31].

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