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RAYLEIGH-SCHRÖDINGER PERTURBATION THEORY REVISITED AND EXTENDED

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1. INTRODUCTION

It is an unfortunate fact of life that for virtually any physically interesting problem in quantum many-body theory, our present state of knowledge is such that the convergence properties of any of the existing forms of many-body perturbation theory are far from clear. It is also the case that apart from the purely variational techniques or the various 'exact' numerical calculations that are largely based on Monte Carlo or other stochastic simulation techniques, most of the available fundamental or microscopic many-body methods are still ultimately rooted in perturbation theory. This is true even for such methods as the coupled cluster method[1-3] and the extended coupled cluster method[4-6] that have seemingly left their humble perturbative origins far behind. Many of the variational techniques (e.g., the hypernetted chain method) are themselves also built upon some (diagrammatic) cluster decomposition, only some elements of which are included at any given level of approximation. In *all* such cases we are therefore faced with a formal series expansion, for which the precise definition of the expansion parameter is often far from clear, let alone its smallness.

Information about the convergence properties of such typical series solutions as that for the ground-state energy of a many-body system, for example, is important for a number of reasons. Most obviously, if the series is divergent, we would like to know how many terms in the series are worth keeping (i.e., beyond which the series approximation deteriorates) for a given value of the expansion parameter or relevant coupling constant. Secondly in most problems of physical interest (e.g., Coulomb fluid, hard sphere systems), a partial resummation of the original series is vital to avoid infinities. If the original series is not convergent, such rearrangements of the series are dangerous and must, in principle, be handled with great care. In practice however, little attention is usually paid to such matters. This point has been particularly stressed by Baker[7] in the context of the necessary resummation of the original series in powers of the two-body potential to one in terms of the 'ladder-summed' T-matrix, in the case of hard-core potentials. Thirdly, and perhaps most importantly, we are interested nowadays less in

the local properties of many-body systems than in such global properties as their phase transitions. In this case, we may envisage the Hamiltonian of the system as depending on some parameter or set of parameters which may, for example, determine the strengths of either some externally applied fields or the internal interparticle forces. Typically we are then interested in considering the whole *family of Hamiltonians* (and the corresponding energy eigenvalues) as a function of these parameters. Phase transitions might then be expected to show up as suitable instabilities or singularities in the relevant parameter space. Perturbation theory is a very convenient method of handling such families of Hamiltonians, but it is clear that the convergence properties of the resulting series expansions play a very crucial role.

It is well known that even for relatively simple model problems, the usual forms of perturbation theory can easily diverge for *all* values of the relevant coupling constants. Indeed it is not necessary to deal with many-body systems to make this manifest. Since the full many-body problem is clearly much more difficult than the quantum-mechanical one-body problem, which however itself already displays many of the same difficulties in this respect, we may for present purposes restrict the ensuing discussion to the one-body problem.

An archetypal system in this respect is the quartic anharmonic oscillator in one dimension with Hamiltonian,

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}x^2 + \lambda x^4 \quad ; \lambda > 0, \tag{1}$$

for which it has been shown[8,9] that Rayleigh-Schrödinger perturbation theory (RSPT) for the ground-state energy diverges for *all* values of λ, if the unperturbed Hamiltonian is taken to be that of the corresponding harmonic

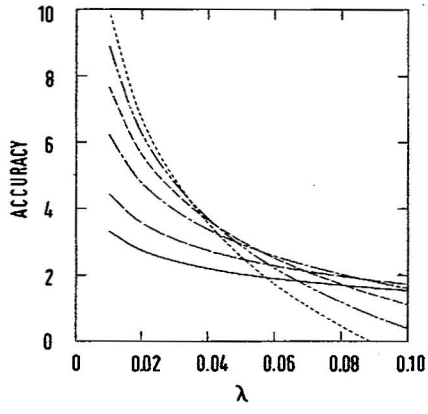

Fig. 1. Accuracy of the ground-state energy of the quartic anharmonic oscillator as a function of λ, in standard RSPT. Results are displayed for perturbation order N = 1 (solid line), 2 (long dashes), 4 (one long and one short dash, 6 (medium dashes), 8 (one long and two short dashes), and 10 (short dashes). Accuracy of the energy is defined as $-\log_{10}|(E/E_{exact} - 1)|$.

oscillator (with $\lambda = 0$). The most that we can therefore expect is that successive terms in the perturbation series decrease in magnitude out to some specific order before they start to increase. This behaviour is illustrated in Fig. 1. Whereas RSPT can still give very accurate results for very small values of λ, the optimal accuracy decreases rapidly as λ is increased. Thus for $\lambda = 0{\cdot}01$ the series apparently converges out to 34th order, at which point the optimal accuracy is reached with a relative error of about $10^{-12}\%$, before successive terms start to worsen the accuracy. On the other hand for $\lambda = 0{\cdot}5$ the magnitude of the correction increases at each order. The optimal asymptotic approximation is then obtained already at first order and the minimum relative error is then about 26%. Even for values as small as $\lambda = 0{\cdot}1$, we see from Fig. 1 that fourth-order perturbation theory gives worse results than second order, and the relative error may not be reduced below a few percent simply by taking more terms in the series.

It is worth pointing out that several techniques for rearranging this perturbation series have been considered (see, e.g., Ref. [10] and further references cited therein). One such technique of particular interest for many-body theory applications is the coupled cluster method (CCM). [1-3] The CCM has been applied by several authors to the quartic anharmonic oscillator. [11-14] In the previous volume in this series, the CCM results were summarised by Kümmel.[13] The errors for the ground-state energy are smaller than 0·1% for $0<\lambda<1000$ at a relatively low level of truncation, namely SUB (6). However, the relevant correlation amplitudes S_n behave rather irregularly for larger n and larger truncation levels. In particular the quality of the energy starts to deteriorate, and the relevant series *still* seems to be asymptotic, although it is clearly much more accurate at the optimal truncation than ordinary RSPT.

Faced with such divergent or seemingly divergent series, one possibility is to develop various "resummation techniques" to try to extract physics from the available terms in the series. Typically in this case, one rigorously needs methods for studying the behaviour of the large order terms in the series. Two such techniques which have been quite widely applied are Borel summation [15] and Padé approximants.[16] In the case of the anharmonic oscillator, Bender and Wu [8,17] first calculated the asymptotic expansion of the ground-state energy as a function of λ using the WKB method. In the context of many-body theory applications, comparable techniques for finding the asymptotic behaviour of the series have involved functional integrals. [18] The interested reader is referred to Ref. [19] for a succinct resumé of the Borel and Padé techniques as applied specifically to the quartic anharmonic oscillator. For this case, it has been proved [20] that the diagonal [N,N] Padé approximants converge to the exact ground-state energy as $N\to\infty$, and even relatively low values of N can give quite accurate approximations, for all values of λ. On the other hand there are few rigorous such results for similar applications to realistic many-body problems.

An alternative approach to the divergence of the RSPT (and similar) series is to abandon the original formulation or, more precisely, to try to generalise it by relaxing some of its implicit constraints that we might suspect of causing the divergent behaviour in the first place. It is from this philosophical viewpoint that we propose the modified Rayleigh- Schrödinger perturbation theory (MRSPT) that we now describe. In keeping with the above discussion we limit the description here to the one-body problem, although we hope ultimately to apply it to realistic many-body systems also.

2. THE BASIC IDEA

Suppose that we wish to solve for the lowest t bound-state eigenvectors $|\psi_i\rangle \equiv |\psi_i(\lambda)\rangle$ and eigenvalues $E_i(\lambda)$ of some general Hamiltonian $H(\lambda)$ which contains a coupling parameter, or some set of such parameters, denoted by λ,

$$H(\lambda)|\psi_i\rangle = E_i(\lambda)|\psi_i\rangle \quad ; \quad i = 0,1, \cdots, (t-1). \tag{2}$$

In all perturbative approaches the Hamiltonian H is decomposed as,

$$H(\lambda) = H^0 + \rho W(\lambda), \tag{3}$$

where the parameter ρ is introduced simply to keep track of the order of the ensuing expansions in powers of the perturbation W. We then have to decide how to choose both (i) the unperturbed Hamiltonian H^0, and (ii) the single-particle basis $|n\rangle$ in which to evaluate the resulting formal expansion for the eigenfunctions $|\psi_i\rangle$, for example. As is well known, and as we describe more fully below, the formal perturbation expansion may be most easily expressed in terms of the resolvent, $R(z) \equiv (z-H^0)^{-1}$. The choice of H^0 is then usually dictated by requiring R to be easily able to be constructed.

In the standard RSPT these two choices above are coupled together, and both are essentially decided by requiring H^0 to be simple enough so that it is diagonal in the chosen basis. That is, we are required to be able to solve explicitly the unperturbed problem

$$H^0|n\rangle = E_n^{(0)}|n\rangle, \tag{4}$$

for the basis $|n\rangle$. It is clear that these two restrictions imposed simultaneously so severely restrict the choice of H^0 that the $\rho \to 0$ limit of Eq. (3) may be so singular as to cause the subsequent divergence of the perturbation series.

By contrast, the key element of the MRSPT scheme that we now propose, is to decouple the two previous requirements by giving up the diagonality of H^0, but in such a way that *the unperturbed eigenvalue problem is satisfied identically*. This is achieved within the framework of an exact projection of the original Schrödinger equation (2) into a (finite) t-dimensional model space, by the usual introduction of P and Q projection operators into and out of the model space, in the usual Feshbach spirit, [21] and as described below. The Hamiltonian H^0 is then written as,

$$H^0 = \tilde{H}^0 + \sum_{i,j=0}^{t-1} z_{ij}|\phi_i\rangle\langle\phi_j| \ , \tag{5}$$

in terms of a set of t^2 parameters z_{ij}, and where our model space is spanned by some suitable set of orthonormalised vectors $|\phi_i\rangle$. All that we then require is that some well-defined resolvent associated with $\tilde{H}^0$ out of the model space be calculable by any suitable means. In particular $\tilde{H}^0$ can otherwise be arbitarily chosen to share some or all of the essential properties of H itself. In this way the remaining perturbation term W can be made "really small" so that the possibly quite large off-diagonal components of H can be shifted into the energy denominator terms arising from the usual resolvent expansion, and the convergence properties of the perturbation series may thereby be improved. Furthermore, the parameters z_{ij} can be chosen, as we see below, so as to make the zeroth-order eigenvalue equation trivially satisfied, and the corresponding zeroth-order eigenvalue itself becomes a truly free parameter in the MRSPT scheme.

3. FORMAL DETAILS

We now first describe more fully the general prescription for setting up perturbation theory in a suitable model space, and then compare and contrast the standard RSPT scheme with the MRSPT scheme. We first make the standard decompositions,

$$E_i \equiv E_i(\lambda) = E_i^{(0)} + \rho E_i^{(1)} + \rho^2 E_i^{(2)} + \ldots ,$$

$$|\psi_i\rangle \equiv |\psi_i(\lambda)\rangle = |\psi_i^{(0)}\rangle + \rho|\psi_i^{(1)}\rangle + \rho^2|\psi_i^{(2)}\rangle + \ldots , \tag{6}$$

and insert them into Eq. (2). By equating powers of ρ we correspondingly find the zeroth-order equation,

$$H^0|\psi_i^{(0)}\rangle = E_i^{(0)}|\psi_i^{(0)}\rangle , \tag{7a}$$

and its Nth -order ($N \geq 1$) counterpart,

$$(H^0 - E_i^{(0)})|\psi_i^{(N)}\rangle + W|\psi_i^{(N-1)}\rangle - \sum_{m=1}^{N} E_i^{(m)}|\psi_i^{(N-m)}\rangle = 0. \tag{7b}$$

We may now project any of these equations into and out of the model space defined by the projectors P and Q,

$$P \equiv \sum_{\alpha=0}^{t-1} |\phi_\alpha\rangle\langle\phi_\alpha| \quad ; \quad Q \equiv 1-P , \tag{8}$$

where the orthonormalised vectors $|\phi_\alpha\rangle$ define and span the model space. For example the zeroth-order equation (7a) may be exactly mapped onto its equivalent for the P-projected wavefunction, $P|\psi_i^{(0)}\rangle$,

$$P[H^0 + H^0 Q R_i Q H^0]P|\psi_i^{(0)}\rangle = E_i^{(0)} P|\psi_i^{(0)}\rangle , \tag{9a}$$

$$|\psi_i^{(0)}\rangle = (1+R_i Q H^0)P|\psi_i^{(0)}\rangle , \tag{9b}$$

in terms of the resolvent operator R_i defined as,

$$R_i \equiv (E_i^{(0)} - QH^0Q)^{-1} , \tag{10}$$

Of course, Eq. (9a) is no easier to solve than Eq. (7a). However, we may now contrast the usual RSPT scheme to proceed beyond this point with our proposed new MRSPT scheme.

3.1. RSPT: The Standard Approach

Equation (9a) is now particularly tractable if $H^0P = PH^0$, and hence if the states $P|\psi_i^{(0)}\rangle$ are the eigenstates of H^0. This is usually, but not necessarily, accomplished in the standard RSPT by choosing $H^0 \rightarrow H(\lambda=0)$, the 'non-interacting' part of H, and by choosing the basis states $|\phi_i\rangle$ to be the corresponding $|\psi_i^{(0)}\rangle$. The energy corrections $E_i^{(n)}$ may then be regarded as functionals of the lower-order wavefunctions $|\psi_i^{(m)}\rangle$ with $m < n$, obtained as usual by taking the overlaps of the general nth-order correction equation (7b) with the state $\langle\psi_i^{(0)}|$, and then employing the zeroth-order equation (7a). In this way all of the corrections $|\psi_i^{(n)}\rangle$ and $E_i^{(n)}$ with $n>0$, may be regarded as being reduced by the hierarchy of equations (7b) to functions of $|\psi_i^{(0)}\rangle$ and $E_i^{(0)}$. The RSPT scheme may thus be viewed as a systematic

reduction of the full (perturbed) equation (2) to its simplified (unperturbed) counterpart of Eq. (7a) or, equivalently, Eqs. (9a,b).

3.2. MRSPT: A Different Approach

As we have already sketched in Sect. 2, it seems natural at this point to exploit the freedom of modifying H^0 by terms *separable in the model space*. Thus, in MRSPT we now write H^0 as already indicated in Eq. (5), or equivalently in the form,

$$H^0 = \tilde{H}^0 + \rho P \zeta P \ , \tag{11}$$

where ζ is some (as yet, arbitrary) t×t matrix, and we are still free to choose $\tilde{H}^0$. Inserting Eq. (11) into the zeroth-order Eq. (9a), we find,

$$P[\tilde{H}^0 + \rho\zeta + \tilde{H}^0 Q R_i \tilde{H}^0]P|\psi_i^{(0)}\rangle = E_i^{(0)}|\psi_i^{(0)}\rangle \ . \tag{12}$$

Further progress is now simplified if we choose as a constraint (c.f., the usual *degenerate* form of RSPT),

$$E_i^{(0)} = \varepsilon \quad , \forall \ i = 0,1, \ \ldots, \ (t-1) \ ; \tag{13}$$

namely, that the zeroth-order eigenvalues are all degenerate. In this case, the zeroth-order MRSPT Eq. (12) may now be satisfied identically if we choose ζ as,

$$\zeta = \rho^{-1} P[\varepsilon - \tilde{H}^0 - \tilde{H}^0 Q R Q \tilde{H}^0]P \ , \tag{14}$$

$$R \equiv (\varepsilon - Q\tilde{H}^0 Q)^{-1} \ . \tag{15}$$

We note that the MRSPT scheme at this point contains ε as a *totally free parameter*, and that the choice of $\tilde{H}^0$ is still open. In particular $\tilde{H}^0$ may, as necessary, be chosen so as to share as many of the properties of the full $H(\lambda)$ as may be needed (for example, to try to improve the convergence properties). The price that we have paid for this freedom and for the essentially total elimination of the unperturbed problem is that the explicit construction of R is now not so simple if $\tilde{H}^0$ is not diagonal. Once ε has been chosen however R has only to be calculated *once*. Clearly, if the formalism in practice turns out to be very sensitive to the choice of ε, most of its possible practical advantages would be lost. We note that if the model space projector P would be constructed as in the RSPT scheme, and if ε were then also set equal to the exact degenerate unperturbed eigenvalue, then the matrix ζ vanishes identically, and our new MRSPT scheme would reduce to the old RSPT scheme. We shall need to investigate, for example, whether the actual MRSPT convergence depends on ε being very close to such unperturbed eigenvalues. We shall return in the later Sections to a critical discussion of this important point, and indicate now only that for the applications that we have made to date, the results are remarkably *insensitive* to the choice of ε.

First-order MRSPT now proceeds just as in standard RSPT. Thus, the overlap of the N=1 member of the hierarchy of equations (7b) is taken with the state $\langle\psi_j^{(0)}|$. Using both the relation,

$$(H^0 - \varepsilon)|\psi_j^{(0)}\rangle = 0 \ , \tag{16}$$

and Eq. (9b), to write the resulting equation entirely in the model space, and writing the P-projected nth-order wavefunction in terms of the model-space spanning functions,

$$P|\psi_i^{(n)}\rangle = \sum_{\alpha=0}^{t-1} c_{\alpha i}^{(n)} |\phi_\alpha\rangle \ , \tag{17}$$

we find the (txt) - dimensional *generalised eigenvalue problem*,

$$\sum_{\alpha=0}^{t-1} \langle\phi_\beta|[(\tilde{H}^0RQ+1)W(1+QR\tilde{H}^0) - E_i^{(1)}(1+\tilde{H}^0RQR\tilde{H}^0)]|\phi_\alpha\rangle c_{\alpha i}^{(0)} = 0;$$
$$i, \beta = 0,1, \ldots, (t-1), \qquad (18)$$

for the first-order energy correction terms $E_i^{(1)}$ and the coefficients $c_{\alpha i}^{(0)}$ of the P-projected zeroth-order energy eigenfunctions. We note that these coefficients are defined only up to a multiplicative constant which can be fixed by a normalisation condition.

Higher-order MRSPT proceeds very similarly. If the overlap of Eq. (7b) is taken with the state $\langle\psi_i^{(0)}|$, the resulting equations can be regarded as a set of recurrence relations for the energy corrections $\{E_i^{(N)}\}$. By employing Eq. (17), these relations formally allow us to eliminate the $\{E_i^{(N)}\}$ in terms of the coefficients $c_{\alpha i}^{(m)}$ with $m < N$. The corresponding overlaps of Eq. (7b) with the state $\langle\psi_j^{(0)}|$ may then be formally reduced to a set of equations for the coefficients $\{c_{\alpha i}^{(N-1)}\}$ to be ultimately given in terms of their lowest-order counterparts $\{c_{\alpha i}^{(0)}\}$. We note however that there still remains a *renormalisation ambiguity* since Eq. (7b) is left unchanged by the transformation $|\psi_i^{(N)}\rangle \to |\psi_i^{(N)}\rangle + \alpha_i^{(N)}|\psi_i^{(0)}\rangle$ with arbitrary constants $\alpha_i^{(N)}$, for all $N \geq 1$. This ambiguity is normally resolved in standard RSPT by choosing the normalisation condition $\langle\psi_i^{(0)}|\psi_i^{(N)}\rangle = 0$; $N \geq 1$. In MRSPT it is more natural to fix directly one of the t coefficients $c_{\alpha i}^{(N)}$ for each fixed value of i and N. An obvious (but not necessary) choice that we shall use in Sect. 4 in the numerical applications, is $c_{ii}^{(N)} = 0$, which follows from the normalisation condition $\langle\phi_i|\psi_i^{(N)}\rangle = 0$. We can make this renormalisation ambiguity explicit by exhibiting the second-order MRSPT equation which results from the above procedure. We find,

$$\sum_{\alpha=0}^{t-1} \langle\psi_j^{(0)}|\hat{q}_i(W-E_i^{(1)})(1+QR\tilde{H}^0)|\phi_\alpha\rangle c_{\alpha i}^{(1)}$$
$$+ \langle\psi_j^{(0)}|\hat{q}_i(W-E_i^{(1)})QRQ(W-E_i^{(1)})|\psi_i^{(0)}\rangle = 0, \qquad (19)$$

where the operator $\hat{q}_i$, defined as,

$$\hat{q}_i \equiv 1 - (\langle\psi_i^{(0)}|\psi_i^{(0)}\rangle)^{-1} |\psi_i^{(0)}\rangle\langle\psi_i^{(0)}|, \qquad (20)$$

clearly renders the j=i member of the t equations (19) a trivial identity. The remaining (j≠i) set of (t-1) equations may then be solved for the coefficients $c_{\alpha i}^{(1)}$ with $\alpha \neq i$.

4. APPLICATIONS

In order to utilise the MRSPT approach in practice, we need a method to construct the resolvent R of Eq. (15) given a particular (and generally non-diagonal) choice for $\tilde{H}^0$. The most straightforward way to construct R is probably a brute-force numerical inversion in some appropriate complete basis, suitably truncated at a given (M x M) level. The convergence of this procedure as $M \to \infty$ has been examined by one of us [22] in the case of tridiagonal matrix representations for $\tilde{H}^0$, where continued-fraction techniques may be employed for the inversion. This procedure has also been extended [23] by use of matrix continued fractions for more general representations in which $\tilde{H}^0_{mn} = 0$ for $|m-n| > s$ for some non-negative integer $s > 1$. An alternative

approach to the construction of R has also been given in terms of an asymptotic fixed-point analysis. [24]

While it is certainly interesting to speculate on which method for the construction of R is likely to be the most suitable for large-scale applications of the MRSPT, for present illustrative purposes we shall simply construct R by a straightforward numerical inversion of a suitably truncated (M×M) representation. In this way we shall focus attention solely on the question of the convergence properties of the MRSPT series representations.

Finally, we note that our choice of zeroth-order Hamiltonian $\tilde{H}^0$ is still undefined. In the present work we shall choose $\tilde{H}^0 \to H(\lambda_0)$, so that the "unperturbed" problem is of the same form as the "perturbed" problem, but with a different value of the coupling constant. We now wish to examine the accuracy and convergence properties as functions of the free parameters ε and λ_0. We may also examine the method as a function of the model space (or degeneracy) size t, and the perturbation order N.

4.1. Numerical Example: Anharmonic Oscillators

In order to illustrate the MRSPT techniques, we now apply it to the well-studied quartic anharmonic oscillator of Eq. (1), which has already been discussed in some detail in Sect. 1. In order to facilitate comparison with other recent calculations [11-14] on this system, we present our numerical results for this Hamiltonian in a Bogoliubov-transformed harmonic oscillator basis, with the specific transformation parameter determined variationally to minimise the expectation value of the Hamiltonian in the ground state of the basis. This procedure, which is equivalent to using the Hartree (or optimised Gaussian) approximation as the starting-point, has been fully described elsewhere. [14] It has also been shown [14] that this simple starting-point itself produces a variational estimate for the ground-state energy of Eq. (1) which is accurate to better than about 2% for *all* values of λ. We perform all of the calculations discussed below in a truncated (M×M) representation in which only the lowest M states are kept of the otherwise complete basis of the (optimally Bogoliubov-transformed) harmonic oscillator. All of our numerical results are shown for the case M = 19, for which the error in the ground-state energy E_0 for $\lambda = 1$, for example, is approximately 10^{-7}% due to the basis truncation. We note that while the transformed harmonic oscillator basis will improve the numerical accuracy of our results over those obtained using the original (λ=0) basis, it does not change the fundamental nature of the problem. Thus the Hamiltonian in the new basis is still 'singular' in the limit $\lambda \to 0$.

In order to investigate the sensitivity of the results to the input parameter ε, we first restrict ourselves to a non-degenerate (t=1) 'ground-state' calculation, and examine in Fig. 2 the accuracy of the ground-state energy as a function of ε, for the first few orders of the MRSPT scheme. We observe that in each order the accuracy obtained is very insensitive to ε over a rather wide range of values around the exact eigenvalue. Comparable 'ground-state' (t=1) results are also shown in Table 1, but where the parameter ε has in turn now been set equal to the lowest five eigenvalues $E_i(\lambda_0)$ of the (truncated) 'unperturbed' Hamiltonian $\tilde{H}^0 = H(\lambda_0)$. We see very clearly that the so-called 'ground-state' (t=1) formalism can also very accurately reproduce the excited-state energies for all levels which have the same parity as the ground state.

The accuracy of the non-degenerate (t=1) version of MRSPT is also displayed at various orders in Fig. 3 as a function of coupling constant λ, where in each case the 'unperturbed' Hamiltonian $\tilde{H}^0 = H(\lambda_0)$ is chosen to have $\lambda_0 = 0.99\lambda$. Results are shown for a range of values of the parameter ε. The data show that the accuracy is almost independent of λ over a very wide

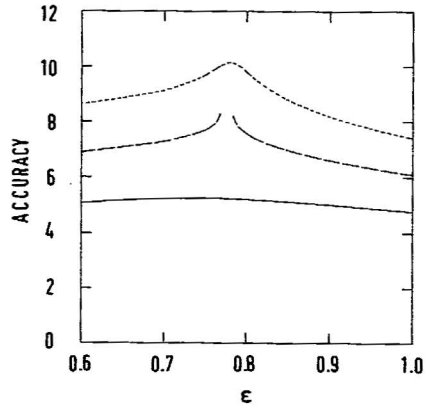

Fig. 2. Accuracy (as defined in Fig.1) versus ε for the ground-state energy of the quartic anharmonic oscillator with $\lambda=1$, $\lambda_0=0.99$ via the non-degenerate (t=1) version of MRSPT. Results are displayed for perturbation order N=1 (solid line), 2(long dashes), and 3(short dashes).

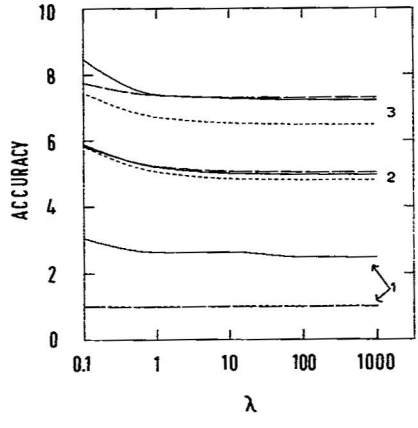

Fig. 3. Accuracy (as defined in Fig.1) for the ground-state energy of the quartic anharmonic oscillator as a function of λ, in the non-degenerate (t=1) version of MRSPT. In each case, $\lambda_0=0.99\lambda$. The free parameter ε has been set equal to $E_0(\lambda_0)$ (solid line), $0.9E_0(\lambda_0)$ (long dashes), and $1.1\ E_0(\lambda_0)$ (short dashes). Results are displayed in each case for perturbation order N=1,2,3 as shown to the right of the curves.

Table 1. Results for the energy of the λ=1 quartic anharmonic oscillator in the non-degenerate (t=1) MRSPT scheme, with λ_0=0.99 and ε set equal to one of the five lowest eigenvalues $E_i(\lambda_0)$ of the 'unperturbed' Hamiltonian $\tilde{H}^0=H(\lambda_0)$. Results are shown for various values of the perturbation order N, with the first row showing the value of ε, and the last row showing the exact lowest five eigenvalues, $E_i(\lambda)$.

N ↓ \ i →	0	1	2	3	4
ε	0.80194363	2.73095581	5.16512665	7.91985374	10.9317140
1	0.80377564	0.80487349	5.17933470	0.84745086	10.9637396
2	0.80377063	0.80309197	5.17929172	0.7343	10.9636393
3	0.80377066	0.80426375	5.17929199	1.0474	10.9636398
8	0.80377066	0.80362184	5.17929199	-6.3394	10.9636398
9	0.80377066	0.80388841	5.17929199	40.12	10.9636398
10	0.80377066	0.80367756	5.17929199	-25.15	10.9636398
E	0.80377066	2.73789236	5.17929199	7.94242934	10.9636398

range of values, for a fixed ratio λ_0/λ. Furthermore, the relative insensitivity to ε is again apparent.

Comparable (t=1) MRSPT results are also shown in Fig. 4 as a function of the imput parameter λ_0 for the important case where λ is fixed. In this case, ε is chosen to be the exact ground-state energy $E_0(\lambda_0)$ of the (truncated) 'unperturbed' Hamiltonian $\tilde{H}^0= H(\lambda_0)$. The curves are seen to have an inflection point in the $\lambda_0 < 1$ branch which is almost independent of perturbation order. This feature is shown in more detail in Fig. 5 which displays both these MRSPT inflection points and the comparable crossing points which are defined to be the values of λ_0 *above* which the (N+1)th-order estimate for the ground-state energy becomes more accurate than the Nth-order estimate. The comparable crossing points for the RSPT curves of Fig. 1 are also displayed in Fig. 5, where these now indicate the value of λ (rather than λ_0) *below* which the (N+1)th-order estimate for the energy becomes more accurate than the Nth-order estimate. In the latter case the limit $\lambda \to 0$ of this curve as $N \to \infty$ is known, [8] and the curve indicates graphically the divergence of RSPT for all values of λ. By contrast, our numerical data using MRSPT seem to indicate the convergence of this scheme for $\lambda_0 > \lambda_0^{\text{crit}}$ where λ_0^{crit} depends on λ, and has the approximate value of 0.45 for the displayed case $\lambda = 1$. We conjecture that some $\lambda_0^{\text{crit}}(\lambda) < \lambda$ is a natural boundary of the convergence domain.

Finally, we also present some results in Table 2 for the degenerate (t>1) version of MRSPT with model spaces of dimension t up to five. For these data, the parameter ε has again been set equal to $E_0(\lambda_0)$, and it is clear by inspection that it is the lowest eigenvalue $E_0(\lambda)$ which is then obtained to the highest accuracy in a given order. Similarly, when ε takes other values, one finds, roughly speaking, that the energy level calculated most accurately is that closest to ε. We note that we can obtain extremely accurate results for *all* levels at even very low perturbation order; and that the accuracy for a given level increases quite rapidly with the dimensionality t of the model space.

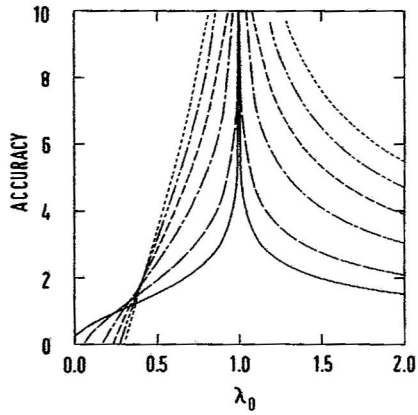

Fig. 4. Accuracy (as defined in Fig.1) for the ground-state energy of the λ=1 quartic anharmonic oscillator, as a function of λ_0, in the non-degenerate (t=1) version of MRSPT. Perturbation orders shown are N=1,2,4,6,8 and 10, marked as in Fig.1.

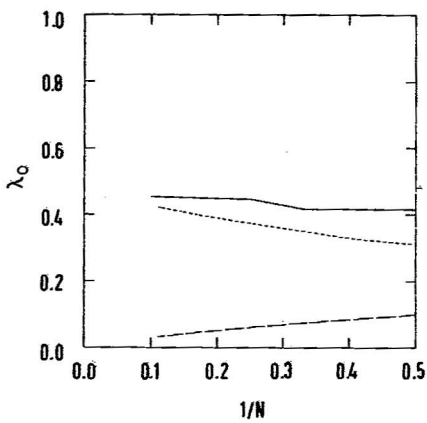

Fig. 5. Crossing points (short dashes) and inflection points (solid line), as defined in the text for λ=1 quartic anharmonic oscillator via the t=1 MRSPT scheme, as a function of the inverse of the perturbation order N. The comparable RSPT crossing points of Fig.1 are also shown (medium dashes), where the vertical axis now shows λ, rather than λ_0.

Table 2. Results for the energy levels of the λ=1 quartic anharmonic oscillator in the degenerate MRSPT scheme for various dimensions t of the model space, with λ_0=0.99 and ε set equal to the lowest eigenvalue $E_0(\lambda_0)$ of the 'unperturbed' Hamiltonian $\tilde{H}^0=H(\lambda_0)$. For each value of t the first and second lines show respectively the results of first and second orders (N=1,2). The last row, labelled E, indicates the exact results.

t	E_0	E_1	E_2	E_3	E_4
1	0.80377564 0.80377063				
2	0.80377564 0.80377063	2.74084383 2.73854346			
3	0.80377105 0.80377066	2.74084383 2.73854346	5.22525036 5.19648606		
4	0.80377105 0.80377066	2.73826672 2.73794788	5.22525036 5.19648606	8.17095716 8.04822012	
5	0.80377072 0.80377066	2.73826672 2.73794788	5.18018018 5.17953076	8.17095716 8.04822012	11.6683164 11.3303428
E	0.80377066	2.73789236	5.17929194	7.94242934	10.9636397

5. DISCUSSION AND SUMMARY

It is clear both from the data on the quartic anharmonic oscillator presented here, and from comparable applications to various other one-body systems, that the MRSPT seems capable of yielding very high precision in situations where the standard RSPT does not work at all well or is difficult to implement. Furthermore, the extra complexity of the MRSPT scheme causes little practical difficulty and only a relatively modest increase in the numerical computations. The convergence properties of the scheme look particularly promising. Both the 'ground-state' or non-degenerate (closed shell) and the 'excited-state' or degenerate (open-shell) versions have been seen to be capable of giving very good quantitative results.

One of the key features of the method is the decoupling of the model space (i.e., the unperturbed wavefunctions) from the unperturbed Hamiltonian. We believe that the extra freedom which this opens up is ripe for future exploitation. The free choice of the input parameter ε may also be utilised to improve the rate of convergence, as may the freedom in choosing the unperturbed Hamiltonian $\tilde{H}^0$. An example of how these extra freedoms may be put to practical advantage is the possibility of simultaneously imposing on the formalism such other physical constraints as conservation laws or sum rules or inequalities, that one may wish to preserve at any level of approximation.

In conclusion, we believe that these preliminary tests on one-body Hamiltonians are sufficiently encouraging to warrant the further development and application of the method to many-body and field-theoretic systems.

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