Perturbation theory without unperturbed solutions

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A modified version of Rayleigh-Schrödinger (RS) perturbation theory, which has been developed previously, can dispense with the usual RS restriction that the unperturbed Hamiltonian should be diagonal in the chosen basis. This modified RS (MRS) perturbation scheme is discussed in some detail and extended to the degenerate case. The new degenerate MRS perturbation theory remains based upon a rearrangement of the unperturbed and perturbed parts of the Hamiltonian. Basically, an unperturbed Schrödinger equation is thereby produced which may be satisfied trivially and identically for an arbitrary Hamiltonian. The zeroth-order approximation to the energy remains a free parameter of the degenerate version of the MRS formalism. The explicit MRS expressions for the higher-order correction terms also preserve a strict analogy with their counterparts in the nondegenerate formalism. What is new is an enormous increase in the applicability and universality of the whole approach. Thus, *a priori*, the unperturbed Hamiltonian may now be chosen so as to have all of its larger off-diagonal elements much closer to those of the full original Hamiltonian than is permitted in the standard RS approach. This is a particular advantage of the whole MRS approach. By testing the method on two nontrivial model Hamiltonians, the method is demonstrated to have considerably improved convergence properties over the standard RS scheme, and at relatively little extra cost.

I. INTRODUCTION

The bound-state Schrödinger equation

$$H|\psi\rangle = E|\psi\rangle \qquad (1)$$

is most commonly solved by the numerical diagonalization of the (suitably truncated) Hamiltonian matrix $\langle m|H|n\rangle$. Some suitable basis $\{|n\rangle\}$ must be chosen, and this is usually some sufficiently simple and complete set of orthogonal vectors which are not directly related to the particular Hamiltonian H itself.

In many physical applications of perturbation theory, the Hamiltonian H in Eq. (1) is often a simple and particular function of some small parameter or some such set of parameters ρ. Such parameters may arise, for example, as coupling strengths, corrections to coupling constants determined by some experiment, uncertainties of the strengths of some externally applied fields, etc. For these families of Hamiltonians $H = H(\rho)$, we are usually interested in the overall pattern of the observables upon these input parameters ρ. In such a context, the use of numerical methods is not very convenient in obtaining, for example, both $E = E(\rho)$ and $|\psi\rangle = |\psi(\rho)\rangle$ over some range $(\rho_0 - \Delta\rho, \rho_0 + \Delta\rho)$ of the parameters ρ. Indeed, in a purely numerical procedure, one would need to repeat the diagonalization of H for each set of values of the input parameters ρ. Furthermore, the resulting purely numerical information still lacks both the clarity and "bookkeeping" aspects of the comparable results of a perturbation-theory approach.

On the other hand, such standard perturbative procedures as that of the Rayleigh-Schrödinger (RS) type, lead unfortunately, at least in their usual textbook form, to perturbation expansions for the wave function and energy eigenvalue,

$$|\psi\rangle = |\psi^{(0)}\rangle + \lambda|\psi^{(1)}\rangle + \lambda^2|\psi^{(2)}\rangle + \cdots , \qquad (2a)$$

and

$$E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots , \qquad (2b)$$

where $H = H_0 + \lambda H_1$, $H_0 = H(\rho_0)$, and $\lambda = O(\rho - \rho_0)$, which rely too heavily upon a systematic evaluation of the successive correction terms. Indeed, various technical difficulties are frequently encountered in putting the standard RS procedure into effect. In the first place, it may be prohibitively difficult to perform the necessary calculations, as for most realistic calculations in nuclear physics, for example. Second, it often occurs that the results diverge, even for very small values of the perturbation parameters.[1] Third, even if the results do converge, they may do so in such a prohibitively slow fashion that it becomes necessary to find a more suitable method.

It is our belief that these three classes of difficulties are, in fact, quite closely related to each other. One of us has recently proposed a modified formalism,[2] which attempts to identify the underlying source of each of the difficulties with a "bad" (diagonal) choice of the unperturbed system

in the context of the standard RS perturbation theory.[3] Indeed, the choice of unperturbed Hamiltonian in the standard textbook versions of RS theory is based on the two requirements of simplicity of the basis set $\{|n\rangle\}$ and simplicity or ease of solution of the "unperturbed" Hamiltonian $H(\rho_0)$ in the chosen basis. In the proposed modification of the RS theory,[2,4] these two requirements were decoupled from each other by rendering the solution of the unperturbed Schrödinger equation trivial. We are thereby allowed to choose $H(\rho_0)$ to be a general (nondiagonal) matrix in some arbitrary, but otherwise sufficiently simple, basis. The modified RS (MRS) expansions may then be constructed, loosely speaking, as power series in the "truly small" matrix elements V of the perturbations, in which all of the "large" components $H(\rho) - V$ appear conversely in the denominator terms.

The basic idea expressed by, and underpinning, the above achievement of the MRS approach, is scarcely new. Indeed, at the level of its abstract formulation, it has proved to be a continuing source of inspiration for much of the last thirty years or so. For example, in nuclear physics Brueckner theory[5] was able to deal with the large components (namely, the repulsive short-range cores) of the internucleon potential; and in quantum chemistry the problem of the long-range Coulombic forces has been successfully handled by a variety of techniques after an appropriate improvement in the choice of basis states (or molecular orbitals).[6,7] It is therefore clear that the points addressed within our own MRS approach have also been discussed by many other authors. Indeed, the present work should be seen in the larger context of addressing one of the most important topics in modern perturbation theory, namely how to proceed when the exact solutions to the unperturbed Hamiltonian are not known. This problem has been addressed from many different viewpoints, and it is therefore perhaps now appropriate to attempt a brief historical survey of the main related ideas and to emphasize thereby the distinguishing new features of our own approach.

One of the most general formulations of this basic problem, and one of the most penetrating attacks upon it, has been given by Löwdin and his coauthors in a long series of papers which have been reviewed, for example, in Ref. 8. This work is based upon the Brillouin-Wigner (BW) formulation of perturbation theory. As a primary object of interest, the so-called "bracketing function," $\kappa(E)$, is introduced and studied. It is a quantity which vanishes at values of its argument equal to the physical eigenvalues of Eq. (1). The core of this approach lies in the introduction of an arbitrary reference function $|\phi\rangle$ and a wave operator W, such that the exact wave function $|\psi\rangle$ becomes equal to the product $W|\phi\rangle$ in a certain limit. As a consequence it was possible to derive formulas which are not only completely equivalent to infinite-order BW perturbation theory, but which also admit a straightforward and smooth transition to the degenerate case. However, the technical details of this transition are far from trivial. The bracketing function $\kappa(E)$ of the nondegenerate case becomes a matrix quantity in the degenerate case; and the comparable extension of the reference function $|\phi\rangle$ to a set of t reference functions

$\{|\phi_i\rangle, i=0,1,\ldots,(t-1)\}$ made the BW formalism extremely flexible. The basic underlying idea, namely the partitioning of Eq. (1), actually has its origins in the 19th century,[9] but in the hands of Löwdin and those who followed him, it has become extremely popular. When further combined with the so-called "inner projection technique,"[10] the partitioning method became a rather powerful tool. Particularly simple yet illustrative examples of the approach are provided by the applications to both single- and double-well quartic anharmonic oscillators.[11,12]

In principle, the introduction of the concepts of bracketing function or effective Hamiltonian[13] makes the transition from the BW to the RS formulation of perturbation theory straightforward.[8,14] The related technicalities have been discussed in some detail especially by Hirschfelder and his group. In particular, they have developed the so-called double-parameter perturbation theory,[7] after having been inspired by the Dalgarno-Lewis procedure[15] for iteratively improving the choice of the unperturbed Hamiltonian. This same basic "resplitting idea" of reapportioning the division of the original Hamiltonian into unperturbed and perturbed parts has been used by several other authors (see, for example, Refs. 4, 16, and 17 and other references cited therein). It will also be one of the main inspirations for the present work.

It is instructive and easy to understand all of these various resplitting procedures as different attempts to accelerate the convergence properties of the perturbative expansions. Failures in such attempts may then often be traced to a basic conflict between the simultaneous insistence on the "diagonality" or "solvability" of the unperturbed Hamiltonian H_0,

$$H_0 = \sum_n \varepsilon_n |\chi_n\rangle\langle\chi_n| , \tag{3}$$

and the smallness of the perturbative terms. A particularly unfortunate consequence of this insistence on diagonality is our subsequent complete loss of control over the smallness of the off-diagonal elements of the perturbation, $H - H_0$. A nice example is provided by the so-called chain models in solid-state physics, where the role of the off-diagonal elements has proved to be so crucial[18] that the perturbative approaches have largely been abandoned. In this context, the restoration of applicable perturbative techniques seems wholly desirable and may indeed be satisfactorily made by a suitable algebraic elimination of all the large perturbations[4] within the MRS scheme considered here.

At the heart of the above algebraic procedures lies a rearrangement of the perturbative part of $H(\rho)$,

$$H(\rho) = H(\rho_0) + V(\rho) , \tag{4a}$$

where it is postulated that the term $V(\rho)$ is "really small." In what follows, a characteristic further small modification is made,

$$H(\rho) = H_0 + \lambda H_1, \quad \lambda = O(\rho - \rho_0) . \tag{4b}$$

The pair of MRS operators H_0 and H_1 will be constructed in detail in Sec. II A. In a way which parallels the

simpler nondegenerate MRS formalism,[4] the new method still rests on a weakening of the assumptions conventionally made in the standard RS version of perturbation theory. The reader should be warned from the outset that this does not, however, imply that the present generalization of the nondegenerate ($t = 1$) formalism of Ref. 4 to the present degenerate ($t > 1$) case, is trivial. On the contrary, we encounter not only the purely formal problems of dealing with matrix quantities rather than scalars, but also certain key difficulties allied to having a matrix bracketing function (or "error" function) $\kappa(E)$. The gist of this new difficulty is that even when E becomes equal to an exact eigenvalue of Eq. (1), the matrix $\kappa(E)$ satisfies only the single condition that its determinant should vanish. On the other hand, its individual matrix elements may, in principle, still remain large. It is precisely at this point that a naive extension from the nondegenerate to the degenerate case of the multiple perturbation series ideas becomes rather ambiguous and may be expected to fail. We feel that the only natural framework to tackle this problem is within the context of creating a new modified formalism from the "classical" degenerate RS formalism. It is this approach that we discuss in Sec. II B.

A priori, the more we generalize the formalism, the greater is the potential price that we must expect to pay. More specifically, we must anticipate that the broader applicability of the degenerate MRS formalism, and its expected improved convergence properties, will be compensated for by an increased degree of complexity in the individual correction terms at a given order. Even in the nondegenerate case this complexity has manifested itself as an increased number of intermediate summations,[19] by the appearance of analytic[2] and/or matrix[20] continued fractions, by the replacement of the original RS unperturbed energies by the complex fixed-point auxiliary functions,[21] etc. On the credit side, however, the general spirit of the original RS perturbation theory remains unmodified, and such familiar positive features as its simple order-by-order implementation, its explicit analytical display of the parametric dependence of the results, and its convenient methods of keeping track of the various contributions diagramatically are all preserved. Our higher-order version of the degenerate MRS perturbation theory is then described in some detail in Sec. II C.

Finally, the question is formulated in Sec. III whether the good numerical convergence properties which have been demonstrated to some extent for the nondegenerate case in the earlier work cited above, and which we now examine in much greater detail, can survive the extension to the degenerate formalism. This is a crucial question, and in this present initial study we attempt only a partial answer though numerical solutions. We examine two particular model problems to illustrate the salient features. The first is a nontrivial but exactly soluble finite model, which provides a rather stringent test of our formalism. The second system, namely the quartic anharmonic oscillator, is more realistic and has become a standard yardstick against which to measure new approaches. As a testing ground it has the distinctive feature of having a Hamiltonian with entirely non-negligible off-

diagonal matrix elements in the standard harmonic oscillator basis. Although this has often been interpreted as a reason for using nonperturbative methods,[18] we find that our own MRS scheme gives convergent and accurate results. It is clear, therefore, that the strict mathematical reasons[22] for the well-known divergence of the standard RS expansions for *all* values of the strength λ of the quartic anharmonicity in this model, in particular the asymptotic formula

$$E = E(\lambda) = a_0 \lambda^{1/3} + O(\lambda^{-1/3}) \ ,$$

are somehow circumvented in our approach. Finally, even in the context of resummations of Eq. (2b) of the type proposed by Halliday and Suranyi,[23] our technique is shown to be capable of leading to a very rapid rate of numerical convergence.

In comparison with the nondegenerate MRS formalism, it is clear that the degenerate version is a much more demanding test of the whole approach, since the multiplets of energies now have to be evaluated from the same zeroth-order estimate, $E^{(0)}$. We might anticipate that the modification $V \rightarrow \lambda H_1$ of the perturbation term in Eqs. (4a) and (4b) now plays a more crucial role and that whereas the convergence, if it exists, must still ultimately stem from the "smallness" of V, the likelihood of now requiring larger rearrangements in the degenerate case might lead to a deterioration of the convergence properties. We show, however, that the MRS method seems to have the capability of giving very precise and highly converged results in the degenerate case as well. This is one of the main outcomes of our numerical calculations.

II. GENERAL PERTURBATION THEORY IN A MODEL SPACE

In this section we describe perturbation theory in a rather general context and use the model-space concept and notation made familiar by such workers as Feshbach and Löwdin.[13] Our specific modification to the usual decomposition of the Hamiltonian is introduced in Sec. II A 2 where we show how the zeroth-order Schrödinger equation is then satisfied automatically and trivially. One of the advantages of our prescription is that, other than this simple modification, the perturbation theory itself remains formally unchanged. In this way, many of the remaining equations will either be also applicable in the RS formulation, for example, or will be very reminiscent of previous results. Nevertheless, the detailed interpretation of the various elements in our expansions will be considerably different, as is exemplified by the appearance of free parameters not found in earlier versions of perturbation theory.

The problem that we pose ourselves is, given a rather general Hamiltonian $H(\lambda)$ containing a coupling parameter or some such set of coupling parameters indicated by λ, we wish to solve the corresponding Schrödinger equation,

$$H(\lambda)|\psi_i\rangle = E_i(\lambda)|\psi_i\rangle, \quad i = 0, 1, \ldots, (t-1) \tag{5}$$

for some set of (usually the lowest) t bound-state eigen-

vectors and corresponding eigenvalues $\{|\psi_i\rangle; E_i(\lambda)\}$, respectively, where $t = 1, 2, \ldots$. Clearly, the eigenvectors $|\psi_i\rangle$ also depend on the coupling parameter(s) λ, but this dependence is left implicit in our notation. The starting point for all perturbative approaches is a decomposition of the Hamiltonian into two parts,

$$H(\lambda) = H^0 + \rho W(\lambda) \tag{6}$$

with

$$\rho W(\lambda) \equiv H(\lambda) - H^0 , \tag{7}$$

and the (expansion) parameter ρ is inserted as a purely formal device for keeping track of the order of the ensuing expansion. The entire success or otherwise of the method is thus predicated by the initial choice of H^0. The primary focus of the present paper is to address the various possibilities open to us here and to suggest a particular relaxation of the standard choice which is made in Rayleigh-Schrödinger perturbation theory (RSPT). We also note before proceeding that in the decomposition of Eq. (6), the entire dependence on λ is assumed to be carried by the component $W \equiv W(\lambda)$.

A. The formal expansion and zeroth-order considerations

In any perturbative treatment, the eigenvalues E_i and eigenvectors $|\psi_i\rangle$, with $i = 0, 1, \ldots$, are now decomposed as usual into formal power series expansions in the parameter ρ

$$\begin{aligned} E_i &= E_i^{(0)} + \rho E_i^{(1)} + \rho^2 E_i^{(2)} + \cdots , \\ |\psi_i\rangle &= |\psi_i^{(0)}\rangle + \rho|\psi_i^{(1)}\rangle + \rho^2|\psi_i^{(2)}\rangle + \cdots . \end{aligned} \tag{8}$$

By inserting Eqs. (6) and (8) into Eq. (5) and equating the terms of the same order in the expansion parameter ρ, we find

$$H^0|\psi_i^{(0)}\rangle = E_i^{(0)}|\psi_i^{(0)}\rangle , \tag{9}$$

$$(H^0 - E_i^{(0)})|\psi_i^{(1)}\rangle + (W - E_i^{(1)})|\psi_i^{(0)}\rangle = 0 , \tag{10}$$

$$(H^0 - E_i^{(0)})|\psi_i^{(N)}\rangle + (W - E_i^{(1)})|\psi_i^{(N-1)}\rangle$$
$$- \sum_{m=2}^{N} E_i^{(m)}|\psi_i^{(N-m)}\rangle = 0, \quad N \geq 2 \tag{11}$$

for, respectively, the zeroth-, first-, and higher-order ($N > 1$) equations.

Next, we propose a t-dimensional model space in which to solve our original Schrödinger equation (5). We assume that this space is spanned by some appropriate trial set of t orthonormalized vectors $|\phi_\alpha\rangle$, $\alpha = 0, 1, \ldots, (t-1)$. Projection operators P and Q, defined as

$$P \equiv \sum_{\alpha=0}^{t-1} |\phi_\alpha\rangle\langle\phi_\alpha|, \quad Q \equiv 1 - P \tag{12}$$

may then be used to project into and out of the model space, respectively. In particular we focus initial attention on the zeroth-order equation (9), and decompose it as,

$$P(H^0 - E_i^{(0)})(P + Q)|\psi_i^{(0)}\rangle = 0 , \tag{13a}$$

$$Q(H^0 - E_i^{(0)})(P + Q)|\psi_i^{(0)}\rangle = 0 . \tag{13b}$$

We now formally regard the latter of these equations as a means to solve for the out-of-model-space part $Q|\psi_i^{(0)}\rangle$ of the wave function which solves Eq. (9). We thus simply obtain the result

$$Q|\psi_i^{(0)}\rangle = R_i Q H^0 P|\psi_i^{(0)}\rangle , \tag{14}$$

where the resolvent or propagator R_i is defined in terms of the Hamiltonian H^0 as

$$R_i \equiv (E_i^{(0)} - Q H^0 Q)^{-1} . \tag{15}$$

Insertion of Eqs. (14) and (15) into Eq. (13a) then gives

$$P(H^0 + H^0 Q R_i Q H^0)P|\psi_i^{(0)}\rangle = E_i^{(0)}P|\psi_i^{(0)}\rangle \tag{16}$$

as the projected version of the zeroth-order equation (9) into the model space. We now consider alternative ways to proceed beyond Eq. (16).

1. The standard approach (RSPT)

It is, of course, clear that, in general, Eq. (16) is no easier to solve than the original Schrödinger equation (5). The standard way forward is that adopted in Rayleigh-Schrödinger perturbation theory (RSPT), where H^0 is now normally constrained to be *diagonal* in our chosen representation. This is usually, but not necessarily, accomplished by choosing H^0 to be the noninteracting part of the original Hamiltonian $H = H(\lambda)$,

$$H^0 \rightarrow H(\lambda = 0) \equiv H(0) , \tag{17}$$

and the basis states $|\phi_\alpha\rangle$, $\alpha = 0, 1, \ldots, (t-1)$, to be the lowest t bound eigenstates of this Hamiltonian. In this case, Eq. (16) simply reduces to

$$H(0)P|\psi_i^{(0)}\rangle = E_i^{(0)}P|\psi_i^{(0)}\rangle , \tag{18}$$

and hence the zeroth-order wave functions $|\psi_i^{(0)}\rangle$ and energy estimates $E_i^{(0)}$ become, respectively, the corresponding eigenfunctions and eigenvalues of $H(0)$, which it is assumed are known.

There are countless examples of very successful applications of this standard RSPT approach. On the other hand, it can also lead to serious problems, as we have already indicated in our introductory remarks in Sec. I. This is particularly true in the rather commonly occurring situation where the nature of the Hamiltonian changes radically in the $\lambda \rightarrow 0$ limit. A typical example is provided by the well-studied anharmonic oscillators.[24,25] It is to overcome these difficulties that we now propose an alternative approach to the zeroth-order equation (16).

2. A more general approach (MRSPT)

We now wish to remove the usual constraint imposed in RSPT that H^0 be diagonal. However, as we have already indicated, when this constraint is relaxed the resultant zeroth-order equation is, in general, no easier to solve than the original full Schrödinger equation. This

difficulty can be overcome via the modified Rayleigh-Schrödinger perturbation theory (MRSPT) that is now described. We first note that within our t-dimensional model space it is natural to consider and exploit the rather obvious freedom of modifying the decomposition of the Hamiltonian $H(\lambda)$ in Eqs. (6) and (7) by the addition and subtraction of terms which are *separable* in the model space. We thus write as our new decomposition,

$$H(\lambda) = H^0 + \rho W \tag{19}$$

as before, but now with the new definitions,

$$H^0 = \tilde{H}^0 + \rho P \zeta P , \tag{20}$$

$$\rho W \equiv H(\lambda) - \tilde{H}^0 - \rho P \zeta P , \tag{21}$$

where ζ is an as yet arbitrary matrix of dimension $(t \times t)$ in the model space, which is formally of order unity with respect to the parameter ρ.

Insertion of Eq. (20) into the zeroth-order equation (16) and use of the trivial relations $PQ = QP = 0$ and $QR_i = R_i Q$ readily yields the relation,

$$P(\tilde{H}^0 + \rho \zeta + \tilde{H}^0 QR_i \tilde{H}^0) P |\psi_i^{(0)}\rangle = E_i^{(0)} P |\psi_i^{(0)}\rangle . \tag{22}$$

While it is possible to make further progress with Eq. (22) as it stands, a considerable simplification occurs if we now impose a further constraint on our model space, namely that the zeroth-order eigenvalues are degenerate, i.e., $E_i^{(0)} = E^{(0)}$, independent of i for $i = 0, 1, \ldots, (t-1)$. In this way a knowledge of a single input resolvent $R \equiv (E^{(0)} - QH^0 Q)^{-1}$ will suffice. Furthermore, it is also clear that after this simplification the P projection of an *arbitrary* wave function will also satisfy the zeroth-order equation (16). Indeed it is apparent that Eq. (16) may now be satisfied *identically* by the choice

$$\zeta = \rho^{-1} P(E^{(0)} - \tilde{H}^0 - \tilde{H}^0 QRQ\tilde{H}^0) P , \tag{23}$$

for the separable modification to the Hamiltonian. It should be evident that with this specific choice of Eq. (23) we have solved the zeroth-order Schrödinger equation (9) for an arbitrary wave function and energy. In other words, we effectively no longer need to solve it at all. In this way the (t independent model-space projections of each of the t) zeroth-order wave functions $|\psi_i^{(0)}\rangle$ and their degenerate zeroth-order eigenvalue $E^{(0)}$ are now totally arbitrary at this zeroth-order level. In particular, we shall henceforth denote $E^{(0)}$ by ε to stress the fact that it remains a completely free parameter of the MRSPT approach. To summarize, we thus have that the energy eigenvalue expansion of Eq. (8) becomes

$$E_i = \varepsilon + \rho E_i^{(1)} + \rho^2 E_i^{(2)} + \cdots , \tag{24}$$

where ε is a free parameter of our MRSPT, and the zeroth-order resolvent of Eq. (15) becomes

$$R = (\varepsilon - Q\tilde{H}^0 Q)^{-1} , \tag{25}$$

in terms of the same parameter. The Q projections of the wave functions $|\psi_i^{(0)}\rangle$ are obtained from Eq. (14) with $R_i \to R$, in terms of the as yet arbitrary P-space projections. This latter equation, together with Eq. (23), are henceforth regarded as definitions which fix the decom-

position of Eqs. (19)–(21) and which eliminate the zeroth-order equation (9) completely.

At first sight one might imagine that what we have done is essentially trivial. It is certainly clear that this new MRSPT approach must, in some sense, be more demanding on the higher-order corrections. However the one overwhelming advantage of choosing a nondiagonal "unperturbed" Hamiltonian H^0 is that we can now choose our starting Hamiltonian $\tilde{H}^0$ to be arbitrarily close to $H(\lambda)$ and so hope to ensure a rapid convergence of the perturbation expansions (8) and (24) by producing an expansion parameter ρ which is arbitrarily small. Thus, our starting Hamiltonian $\tilde{H}^0$ need not be fundamentally different from the full Hamiltonian $H(\lambda)$, as is frequently the case in the standard approach where H^0 is constrained to be diagonal. For example, in the case of the quartic anharmonic oscillator discussed below, both $\tilde{H}^0$ and $H(\lambda)$ contain quartic terms.

Naturally, there is a price which has to be paid for this extra freedom. Thus, in practice we still need an efficient method to perform the evaluation of the inversion in Eq. (25) to obtain the "unperturbed propagator" or resolvent R. Various such methods have been proposed in the past. Let us consider a zeroth-order Hamiltonian H^0 which has the general representation in some complete orthonormal basis $\{|n\rangle; n = 1, 2, \ldots\}$,

$$H^0 = \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} H_{mn}^0 |m\rangle \langle n| , \tag{26}$$

and, purely for ease of discussion, let us also consider just the case $Q \to 1, P \to 0$ for the moment. Clearly, the usual RSPT depends on the representation being diagonal, $H_{mn}^0 \to H_n^0 \delta_{mn}$, to be able immediately to calculate the associated resolvent as

$$(\varepsilon - H_0)^{-1} \to \sum_{n=1}^{\infty} |n\rangle \frac{1}{(\varepsilon - H_{nn}^0)} \langle n| . \tag{27}$$

When H^0 is not diagonal, perhaps the simplest way to construct the resolvent is simply to truncate the basis to a finite subspace $\{|n\rangle; n = 1, 2 \ldots, M\}$, so that the upper limits in the double summation in Eq. (26) become M, and the truncated $(M \times M)$-dimensional matrix is then inverted numerically. This is the method that will be adopted in the present work, but clearly we do need to address the question of convergence as $M \to \infty$. Indeed, this convergence has been examined elsewhere[2,4,19−21] by one of us in the case where the RSPT condition of diagonality of H^0 has been relaxed to deal instead with more general representations in which $H_{mn}^0 = 0$ for $|m - n| > s$, for some non-negative integer s. The RSPT discussed above is just the case $s = 0$. The more general case $s > 0$ leads to a band-matrix representation for H^0 in which there are $(2s + 1)$ nonzero "diagonals."

In particular, it has been shown[2,4] how the $s = 1$ case (i.e., tridiagonal matrices H^0) may be solved analytically in terms of continued fractions, and the $M \to \infty$ convergence has been reduced to a convergence of such contin-

ued fractions. This procedure has been extended[20] to the case $s > 1$ by using matrix continued fraction techniques to replace the previous continued fractions of the $s = 1$ case by their $(s \times s)$-dimensional matrix analogs. An alternative approach has also been examined,[19] in which the resolvent is itself approximated by a similar band-matrix form $R \rightarrow \tilde{R}$, where $\tilde{R}_{mn} = R_{mn}$ for $|m - n| \leq \tilde{s}$, and $\tilde{R}_{mn} = 0$ for $|m - n| > \tilde{s}$. A final approach to the inversion inherent in the construction of R has been given[21] in terms of an asymptotic fixed-point analysis.

The upshot of all these investigations is that there seem to be no practical problems of convergence in the $M \rightarrow \infty$ limit of the truncated basis representation for H^0. This is, in any case, intuitively obvious since the error caused by the truncation can, in principle, itself be incorporated into the perturbative part W of the full Hamiltonian. In all of our later numerical work we shall, therefore, perform the inversion in Eq. (25) within a suitable finite-dimensional truncated basis. Furthermore, we shall consider only the more interesting question of the convergence of the MRSPT series of Eq. (24).

Finally, we reiterate that our zeroth-order Hamiltonian $\tilde{H}^0$ has been left completely arbitrary. In particular, it may or may not have the same or similar functional form as $H(\lambda)$. Most previous work, for example, has been done for an $H(\lambda)$ that represents the standard quartic anharmonic oscillator and with $\tilde{H}^0$ equal to an appropriately chosen tridiagonal piece of what is a pentadiagonal matrix representation for the full Hamiltonian in the corresponding harmonic oscillator basis. In the present work we shall concentrate on numerical examples where $\tilde{H}^0$ is chosen to have exactly the same form as $H(\lambda)$ but with a different value of the coupling constant(s) λ.

As stated above, the zeroth-order estimate ε for the energy is a free parameter in the MRSPT scheme. If the model-space projector is constructed as in RSPT and if ε is set equal to the degenerate model-space eigenvalue $E^{(0)}$ of the unperturbed Hamiltonian H^0, then the matrix ζ of Eq. (23) will be identically zero, and our new MRS scheme will reduce to the standard RS scheme. Clearly, a main point of interest is now going to concern the behavior of the MRSPT when ε is not equal to an unperturbed eigenvalue. It is clear that the new scheme will offer little practical advantage if it is capable of producing accurate results only for values of ε close to such unperturbed eigenvalues. Obviously we cannot expect the accuracy of the resultant energy eigenvalues to be totally independent of the choice of ε but we can hope that the results are relatively insensitive, at least in large regions centered around the eigenvalues of $\tilde{H}^0$. This point will be examined particularly closely in the ensuing discussion.

After this rather lengthy discussion of the zeroth-order equation in general perturbation theory and its particular form in our MRSPT approach, we now discuss the higher-order MRSPT equations and corresponding corrections to the wave functions and eigenvalues. As already stated at the beginning of this section, many of the results presented below are formally equivalent to those in standard perturbation theory, although a few modifications are also necessary due to the nondiagonality of $\tilde{H}^0$.

B. The first-order MRSPT equations

The general first-order equation (10) now becomes

$$(H^0 - \varepsilon)|\psi_i^{(1)}\rangle + (W - E_i^{(1)})|\psi_i^{(0)}\rangle = 0 . \tag{28}$$

We proceed as before by projecting Eq. (28) into the P and Q subspaces,

$$P(H^0 - \varepsilon)(P + Q)|\psi_i^{(1)}\rangle + P(W - E_i^{(1)})|\psi_i^{(0)}\rangle = 0 , \tag{29a}$$

$$Q(H^0 - \varepsilon)(P + Q)|\psi_i^{(1)}\rangle + Q(W - E_i^{(1)})|\psi_i^{(0)}\rangle = 0 . \tag{29b}$$

The latter equation (29b) may again be formally solved for the Q projection of the wave function $|\psi_i^{(1)}\rangle$,

$$Q|\psi_i^{(1)}\rangle = QR\tilde{H}^0 P|\psi_i^{(1)}\rangle + QR(W - E_i^{(1)})|\psi_i^{(0)}\rangle . \tag{30}$$

The first-order wave function corrections may be eliminated by taking the overlap of Eq. (28) with the states $\langle \psi_j^{(0)}|$ and using our imposed condition

$$(H^0 - \varepsilon)|\psi_j^{(0)}\rangle = 0 . \tag{31}$$

We thus find the compact relation,

$$\langle \psi_j^{(0)}|(W - E_i^{(1)})|\psi_i^{(0)}\rangle = 0, \quad i, j = 0, 1, \ldots, (t - 1) . \tag{32}$$

We may finally write this equation wholly within the projected P space by using Eq. (14) to write the zeroth-order wave functions $|\psi_i^{(0)}\rangle$ in terms of their P-space projections as,

$$|\psi_i^{(0)}\rangle = (I + QRH_0)P|\psi_i^{(0)}\rangle$$

$$= (I + QR\tilde{H}_0)P|\psi_i^{(0)}\rangle , \tag{33}$$

where we have also used Eq. (20) and the trivial relation $QR = RQ$, and where I is the identity operator. Equation (32) thus becomes

$$\langle \psi_j^{(0)}|P(\tilde{H}_0 RQ + I)(W - E_i^{(1)})(I + QR\tilde{H}_0)P|\psi_i^{(0)}\rangle = 0 . \tag{34}$$

If we decompose the P-space projections of the zeroth-order wave functions in terms of our t orthonormalized basis states $|\phi_\alpha\rangle$ as

$$P|\psi_i^{(0)}\rangle = \sum_{\alpha=0}^{t-1} c_{\alpha i}^{(0)}|\phi_\alpha\rangle, \quad i = 0, 1, \ldots, (t - 1) \tag{35}$$

then Eq. (34) may be written as a $(t \times t)$-dimensional matrix generalized eigenvalue problem,[26]

$$\sum_{\alpha=0}^{t-1} \langle \phi_\beta|[(\tilde{H}^0 RQ + I)W(I + QR\tilde{H}^0)$$

$$- E_i^{(1)}(I + \tilde{H}^0 RQR\tilde{H}^0)]|\phi_\alpha\rangle c_{\alpha i}^{(0)} = 0 ,$$

$$i, \beta = 0, 1, \ldots, (t - 1) \tag{36}$$

which we may now solve numerically.

It is clear that Eq. (36) specifies both the first-order corrections $E_i^{(1)}, i = 0, 1, \ldots, (t - 1)$, to the lowest t states of the spectrum as well as the zeroth-order approximations to the corresponding wave functions via Eqs. (33) and (35). This structure is reminiscent of the comparable result from the degenerate version of RSPT.[14] We note,

however, that in our MRSPT approach we do not require that the model-space projector P commutes with the unperturbed Hamiltonian H^0. We also note that the coefficients $c_{\alpha i}^{(0)}, \alpha = 0, 1, \dots, (t-1)$, are only defined by Eq. (36) up to an overall multiplicative constant which determines the normalization of the unperturbed wave function.

C. The higher-order MRSPT equations

From Eq. (11), the Nth-order generalization of Eq. (28) is now given by

$$(H^0 - \varepsilon)|\psi_i^{(N)}\rangle + (W - E_i^{(1)})|\psi_i^{(N-1)}\rangle$$

$$- \sum_{m=2}^{N} E_i^{(m)}|\psi_i^{(N-m)}\rangle = 0, \quad N \geq 2 . \quad (37)$$

By a similar procedure as for the first-order equation above, the Q projection of Eq. (37) becomes

$$Q|\psi_i^{(N)}\rangle = R \left[Q\tilde{H}^0 P|\psi_i^{(N)}\rangle \right.$$

$$+ Q(W - E_i^{(1)})|\psi_i^{(N-1)}\rangle$$

$$\left. - \sum_{m=2}^{N} E_i^{(m)} Q|\psi_i^{(N-m)}\rangle \right] . \quad (38)$$

By inserting Eq. (38) into Eq. (37), the P projection of the latter equation may also be computed. More directly, by taking the overlap of Eq. (37) with the state $\langle \psi_j^{(0)}|$, and using Eq. (31), we find the compact relation

$$\langle \psi_j^{(0)}|(W - E_i^{(1)})|\psi_i^{(N-1)}\rangle$$

$$- \sum_{m=2}^{N} E_i^{(m)} \langle \psi_j^{(0)}|\psi_i^{(N-m)}\rangle = 0 . \quad (39)$$

Equation (39) can be rewritten as a hierarchical set of equations for the energy correction terms,

$$E_i^{(N)} = (\langle \psi_i^{(0)}|\psi_i^{(0)}\rangle)^{-1}$$

$$\times \left[\langle \psi_i^{(0)}|(W - E_i^{(1)})|\psi_i^{(N-1)}\rangle \right.$$

$$\left. - \sum_{m=2}^{N-1} E_i^{(m)} \langle \psi_i^{(0)}|\psi_i^{(N-m)}\rangle \right] ,$$

$$i = 0, 1, \dots, (t-1), \quad N > 1 \quad (40)$$

where we have put $j = i$. In this way the energy corrections $E_i^{(N)}$ may be regarded as known in terms of the lower-order wave functions $|\psi_i^{(n)}\rangle$ with $n = 0, 1, \dots, N-1$. In this way Eqs. (32) and (39) may be regarded as implicit recurrent definitions of the wave-function correction terms, which may be solved for and reinserted into Eq. (39).

If we decompose the P-space projections of the wave-function correction terms,

$$P|\psi_i^{(m)}\rangle = \sum_{\alpha=0}^{t-1} c_{\alpha i}^{(m)}|\phi_\alpha\rangle, \quad i = 0, 1, \dots, (t-1) \quad (41)$$

then Eq. (40) enables us to eliminate the value of $E_i^{(N)}$ as a function of the coefficients $c_{\alpha i}^{(m)}$ with $m = 0, 1, \dots, N-1$. In this way Eq. (39) may be reduced to a set of equations for the coefficients $c_{\alpha i}^{(N-1)}$ ultimately in terms of the coefficients $c_{\alpha i}^{(0)}$ obtained previously from Eq. (36).

We note, however, that after this procedure, Eq. (39) does not uniquely define all of the quantities $c_{\alpha i}^{(n)}$, $\alpha = 0, 1, \dots, (t-1)$, for given values of i and n. The remaining so-called renormalization ambiguity of these recurrence relations stems ultimately from the fact that Eqs. (10) and (11) do not uniquely specify the correction terms $|\psi_i^{(N)}\rangle$ for $N \geq 1$, since an arbitrary renormalization,

$$|\psi_i^{(N)}\rangle \rightarrow |\psi_i^{(N)}\rangle + \alpha_i^{(N)}|\psi_i^{(0)}\rangle , \quad (42)$$

remains compatible with these equations by use of Eq. (9). In the standard RSPT this ambiguity is usually removed by requiring

$$\langle \psi_i^{(0)}|\psi_i^{(N)}\rangle = 0, \quad N = 1, 2, \dots . \quad (43)$$

In the present case, it is simpler to fix directly one of the t coefficients $c_{\alpha i}^{(N)}, \alpha = 0, 1, \dots, (t-1)$, for each fixed N and i or alternatively to fix the norm of each of the wave-function corrections $|\psi_i^{(N)}\rangle$. An obvious replacement of Eq. (43) in MRSPT would appear to be the condition

$$\langle \phi_i|\psi_i^{(N)}\rangle = 0, \quad i = 0, 1, \dots, (t-1), \quad N \geq 1 \quad (44)$$

which implies immediately $c_{ii}^{(N)} = 0$ for all $N \geq 1$ and $i = 0, 1, \dots, (t-1)$. This is not the only choice possible, but it is the one that we adopt in our numerical work discussed below.

We illustrate how the renormalization ambiguity arises in practice by considering Eqs. (39) and (40) in the case $N = 2$. After eliminating $E_i^{(2)}$ from Eq. (39), by use of Eq. (40), we find

$$\langle \psi_j^{(0)}|\hat{q}_i(W - E_i^{(1)})|\psi_i^{(1)}\rangle = 0, \quad i, j = 0, 1, \dots, (t-1) \quad (45)$$

where

$$\hat{q}_i \equiv 1 - \frac{|\psi_i^{(0)}\rangle\langle \psi_i^{(0)}|}{\langle \psi_i^{(0)}|\psi_i^{(0)}\rangle} . \quad (46)$$

Equation (45) is now a set of equations for the wave functions $|\psi_i^{(1)}\rangle$ and may be compared with Eq. (32). We note, however, that the member of the set of equations (45) with $j = i$ is a trivial identity since $\langle \psi_i^{(0)}|\hat{q}_i = 0$ from Eq. (46), and we immediately see this as the cause of the above-mentioned ambiguity. We may proceed as before by projecting $|\psi_i^{(1)}\rangle$ into the P space. We use Eq. (30) to write $|\psi_i^{(1)}\rangle$ as

$$|\psi_i^{(1)}\rangle = (I + QR\tilde{H}^0)P|\psi_i^{(1)}\rangle + QR(W - E_i^{(1)})|\psi_i^{(0)}\rangle . \quad (47)$$

Insertion of Eqs. (41) and (47) into Eq. (45) then yields the result

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

$$+ \langle \psi_j^{(0)}|\hat{q}_i(W - E_i^{(1)})QRQ(W - E_i^{(1)})|\psi_i^{(0)}\rangle = 0 . \quad (48)$$

Since the wave functions $|\psi_i^{(0)}\rangle$ are known, Eq. (48) may now be solved for the coefficients $c_{\alpha i}^{(1)}$, apart from the ambiguity arising from the effective loss of the $j=i$ member of the set. It is clear that we may remove the term $\alpha=i$ from the sum in Eq. (48) by arbitrarily assigning the coefficients $c_{ii}^{(1)}$ any values we choose. The remaining nontrivial ($j\neq i$) linear equations may then be uniquely solved for the remaining parameters $c_{\alpha i}^{(1)}$.

This procedure may be repeated at each higher level to solve both for the energy corrections $E_i^{(N)}$ and the corresponding wave-function correction terms $|\psi_i^{(N-1)}\rangle$. A similar renormalization ambiguity may be explicitly uncovered in each order. As noted already, for the sake of making a definite choice for our numerical work below, we have adopted the zero-overlap requirement of Eq. (44).

In the remainder of this work we now apply the above MRSPT technique to two specific illustrative examples, in order to see how well it converges in practice.

III. NUMERICAL RESULTS

In all of the results that we present below, we have taken the unperturbed Hamiltonian $\tilde{H}^0$ to have the same functional form as $H(\lambda)$ itself. Thus we choose $\tilde{H}^0 \rightarrow H(\lambda_0)$ with some other (arbitrary) value λ_0 of the coupling constant. We are particularly interested in examining the accuracy and convergence properties of the method as a function of both λ_0 and the free parameter ε.

A. Finite tridiagonal matrix

As our first example we consider one of the simplest model Hamiltonians, namely a finite $(M \times M)$-dimensional tridiagonal matrix $H(\lambda)$, with two coupling constants $\lambda \equiv (\lambda_1, \lambda_2)$ and elements specified as

$$H_{mn}(\lambda) = (a + \lambda_2)\delta_{mn} + \lambda_1(\delta_{m,n+1} + \delta_{m+1,n}),$$

$$m, n = 1, 2, \ldots, M . \quad (49)$$

There are a number of reasons why this particular Hamiltonian is well suited for testing our MRSPT procedure. In the first place, the associated Schrödinger equation

$$H(\lambda)|\psi_k\rangle = E_k|\psi_k\rangle, \quad k = 0, 1, \ldots, M-1 \quad (50)$$

is exactly soluble. Indeed the matrix of Eq. (49) is closely related to the Chebyshev polynomials of the second kind,[27] and we may write for the eigenfunctions and eigenvalues, respectively,

$$\langle n|\psi_k\rangle = (-1)^{n+1}\sin(nX_k)/\sin X_k, \quad n = 1, 2, \ldots, M \quad (51)$$

$$E_k = a + \lambda_2 - 2\lambda_1 \cos X_k , \quad (52)$$

where

$$X_k \equiv \frac{(k+1)\pi}{(M+1)}, \quad k = 0, 1, \ldots, M-1 . \quad (53)$$

Second, this Hamiltonian clearly exhibits a strong "discontinuity" at the point $\lambda = (0,0)$, where the energy spectrum becomes completely degenerate. Clearly, standard RSPT will not work at all about the unperturbed Hamiltonian $H(0)$, unless one uses the maximally degen-

erate form, which is the analog of the case $t=M$ for the MRSPT. By contrast, we shall see that the MRSPT can work very well indeed for any subspace size $t \leq M$, even for $t=1$. We also note that for this model, the unperturbed (nondiagonal) propagator R of Eq. (25) is very simple to calculate, since the inverse of a tridiagonal matrix is straightforward to evaluate by numerical or continued fraction techniques.[28] Finally, we remark that the arbitrary parameter ε in this case may rather simply be set equal to the lowest eigenvalue of $\tilde{H}^0 = H(\lambda_0)$, so that the separable modification ζ to the Hamiltonian, given by Eq. (23), becomes identically zero.

We display in Fig. 1 the "ground-state energy" (i.e., the single energy eigenvalue obtained within the subspace of dimension $t=1$) as a function of the parameter ε for the Hamiltonian of Eq. (49) with dimension $M=4$ and with parameters $a=100$, $\lambda=(0.2,0.4)$. We choose an unperturbed Hamiltonian $\tilde{H}^0 = H(\lambda_0)$ of the same form but with $\lambda_0 = (0.19, 0.28)$ and give results up to tenth order in our MRSPT expansion. We note that the present model Hamiltonian has the special property that if the free parameter ε equals any eigenvalue $E_i(\lambda_0)$ of $H(\lambda_0)$ then the MRSPT scheme will produce the corresponding eigenvalue of $H(\lambda)$ exactly at first order. The underlying reason for this is that the eigenfunctions (but not the eigenvalues) of the Hamiltonian of Eq. (49) are actually independent of the coupling parameters λ, as may be seen from Eqs. (51)–(53). This feature of the model would itself cause the steplike behavior seen in Fig. 1, which becomes more and more pronounced with increasing order of perturbation. We also note that there is an essentially flat plateau centered around each eigenvalue. As already mentioned in Sec. II, this insensitivity of the MRSPT estimates of the energies to the choice of ε, at least within certain broad regions, is just what we had hoped for. All one needs in order to obtain a very accurate estimate for
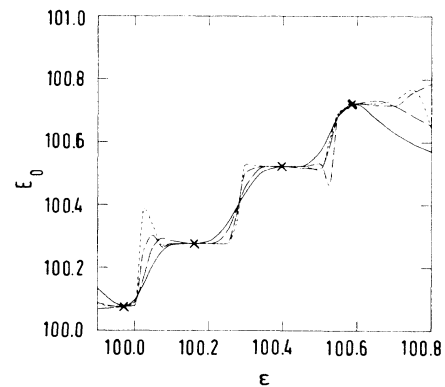
FIG. 1. Results for the energy, calculated via the ground-state formalism, of the tridiagonal Hamiltonian of Eq. (49), with $\lambda = (0.2, 0.4)$ and $\lambda_0 = (0.19, 0.28)$, with a matrix size $M=4$. We have used a subspace size $t=1$, and results are shown as a function of the free parameter ε, for perturbation order $N=1$ (solid line), 2 (long dashes), 5 (medium dashes), and 10 (short dashes). The points $[E_i(\lambda_0), E_i(\lambda)]$ are marked with the symbol $\times$, emphasizing that, for this Hamiltonian, when $\varepsilon = E_i(\lambda_0)$, MRSPT produces the energy $E_i(\lambda)$ exactly, even at first order.

the eigenvalue E_i of the full Hamiltonian H is an extremely rough estimate of the corresponding eigenvalue for the unperturbed Hamiltonian $\tilde{H}^0$. One might still worry that these "plateaus of insensitivity" are an artifact of this special Hamiltonian. We shall see below, however, that the same general behavior also holds for the anharmonic oscillator example, and we postulate that it is a general feature of the MRSPT.

In Table I we present the results for the $M = 8$-dimensional matrix, with the parameters a, λ, and λ_0 taking the same values as above and with ε equal to the exact ground-state eigenvalue $E_0(\lambda_0)$ of $\tilde{H}^0 = H(\lambda_0)$. Results are displayed for the size of the subspace varying from $t = 1$ to the maximum $t = 8$, and for both first and second orders in the perturbation theory in each case. As before, the ground state is produced exactly at first order. Naturally, the entire spectrum is also exact at first order for the $t = 8$ subspace size. Clearly, the excited-state energies are not produced as well as the ground-state energy since the differences between the higher levels and the parameter ε are greater, and we recall that the zeroth approximant for all levels is ε. Certainly a higher-order perturbation calculation would do better. However, for this Hamiltonian at least, we can obtain much better estimates for the excited-state energies by choosing a more appropriate value for ε and working even in the "ground-state" ($t = 1$) formalism.

B. The quartic anharmonic oscillator

As our second model we consider the standard, one-dimensional, quartic anharmonic oscillator defined over the infinite x axis as,

$$H(\lambda) = \tfrac{1}{2}(p^2 + x^2) + \lambda x^4, \quad \lambda > 0 \tag{54}$$

in terms of the coordinate x and canonical momentum p, or equivalently as

$$H(\lambda) = \tfrac{1}{2} + a^\dagger a + \tfrac{1}{4}\lambda(a + a^\dagger)^4 , \tag{55}$$

in terms of the standard creation and destruction operators $a^\dagger$ and a, respectively, defined in terms of the usual commutation relation $[a, a^\dagger] = 1$ and the relation $a|0\rangle = 0$, where $|0\rangle$ is the usual vacuum state.

It is well known[24,25] that standard RSPT diverges for this model for every nonzero value of λ. We have not performed a similar analysis for the MRSPT, although our numerical results below strongly suggest that the method probably converges in certain ranges of the input parameters. A detailed analysis of the convergence properties would be very interesting but would take us too far afield for present purposes. In its absence however, we make two qualitative remarks. In the first place, the standard intuitive argument for why the RSPT series for an energy eigenvalue has a zero radius of convergence in the parameter λ is that the $\lambda \rightarrow 0$ limit is strongly singular in the sense that the coordinate-space representation of Eq. (54) for the potential part of the Hamiltonian, changes from a quartic to a quadratic form. We note that, by contrast, this is not generally the case in our MRSPT scheme, since we may choose to expand about some arbitrary value of $\lambda \rightarrow \lambda_0$, rather than about the value $\lambda \rightarrow 0$. We use our numerical data below to try to ascertain whether values of λ_0 can be chosen so that the corresponding MRSPT series are convergent. Of course, it is impossible to predict the behavior of the neglected higher-order perturbative corrections in this way, but we shall see that the results are nevertheless quite suggestive.

Our second point is that one of the main advantages of our new technique is that we may readily expand about any value of λ_0. Thus, even if our MRSPT techniques do turn out to provide formally divergent series for the energy spectrum, it is still perfectly possible that these series may be able to provide very accurate estimates, by choosing a value of λ_0 "close enough" to λ and by not attempting to go to too high an order in the perturbation theory. That this is true can be seen very clearly even in the standard RSPT. Thus, the results of Bender and Wu[24] show that for $\lambda = 0.01$, for example, the RSPT corrections to

TABLE I. Results for the eigenvalues E_i [$=E_i(\lambda)$] of the tridiagonal Hamiltonian with size $M = 8$, $a = 100$, $\lambda = (0.2, 0.4)$, and $\lambda_0 = (0.19, 0.28)$ for various values of the subspace size t. The free parameter ε has been set to $E_0(\lambda_0)$. For a given t, the first- and second-order energies are displayed above and below each other, respectively. Note that the $t = 8$ results are exact at first order.

t	$E_0 - a$	$E_1 - a$	$E_2 - a$	$E_3 - a$	$E_4 - a$	$E_5 - a$	$E_6 - a$	$E_7 - a$
1	0.024 123							
	0.024 123							
2	0.024 123	0.410 03						
	0.024 123	0.186 08						
3	0.024 123	0.221 12	0.606 93					
	0.024 123	0.113 52	0.494 79					
4	0.024 123	0.147 36	0.417 62	0.687 99				
	0.024 123	0.103 94	0.322 33	0.639 53				
5	0.024 123	0.114 73	0.304 95	0.538 73	0.727 79			
	0.024 123	0.098 27	0.253 00	0.484 51	0.706 79			
6	0.024 123	0.100 03	0.241 07	0.427 92	0.614 04	0.750 18		
	0.024 123	0.094 88	0.218 63	0.394 47	0.587 90	0.741 32		
7	0.024 123	0.094 57	0.208 89	0.358 05	0.519 71	0.664 42	0.764 36	
	0.024 123	0.093 70	0.203 06	0.345 60	0.505 36	0.654 55	0.761 22	
8	0.024 123	0.093 58	0.2	0.330 54	0.469 46	0.6	0.706 42	0.775 88
	0.024 123	0.093 58	0.2	0.330 54	0.469 46	0.6	0.706 42	0.775 88

the ground-state energy decrease monotonically out to 34th order before they start to diverge beyond this and at which point the size of the corrections is of the order of $10^{-12}\%$.

We present our numerical results for the Hamiltonian of Eq. (55) in a Bogoliubov-transformed harmonic oscillator basis and with the specific transformation used determined variationally. This procedure is equivalent to using the Hartree (or Gaussian) approximation as the starting point.[29-33] We first perform a Bogoliubov transformation on the operators a and $a^\dagger$, namely the most general (homogeneous) linear transformation (or "rotation") that leaves the canonical commutation relations unchanged,

$$b = (1-\tau^2)^{-1/2}(a-\tau a^\dagger), \quad |\tau| < 1, \quad [b,b^\dagger]=1 . \quad (56)$$

Without loss of generality we restrict ourselves to real values of the parameter τ. Just as the state $|0\rangle$ is defined to be the original (or "bare") vacuum state $a|0\rangle=0$, we now define $|\phi\rangle$ to be the vacuum state of the unitarily transformed operators, $b|\phi\rangle=0$. Using the easily proved relation,

$$\exp(\tfrac{1}{2}\tau a^{\dagger 2})a \exp(-\tfrac{1}{2}\tau a^{\dagger 2})=a-\tau a^\dagger , \quad (57)$$

it is simple to prove that the normalized state $|\phi\rangle$ is given by the Gaussian form

$$|\phi\rangle = (1-\tau^2)^{1/4}\exp(\tfrac{1}{2}\tau a^{\dagger 2})|0\rangle . \quad (58)$$

We note that the state $\exp(\tfrac{1}{2}\tau a^{\dagger 2})|0\rangle$ is normalizable only if $|\tau| < 1$, which is the condition for the transformation expressed in Eq. (56) to be canonical.

Using the inverse of the transformation of Eq. (56), we can readily write the Hamiltonian of Eq. (55) in terms of the new operators b and $b^\dagger$. It is convenient to write it in explicitly normal-ordered form with respect to these operators, and we find

$$H = \varepsilon_0 + \left[\frac{1-\omega^2}{4\omega}\right](b^2+b^{\dagger 2}) + \left[\frac{1+\omega^2}{2\omega}\right]b^\dagger b$$
$$+ \frac{3\lambda}{2\omega^2}:(b+b^\dagger)^2: + \frac{\lambda}{4\omega^2}:(b+b^\dagger)^4: , \quad (59)$$

where

$$\omega \equiv (1-\tau)/(1+\tau) \quad (60)$$

and

$$\varepsilon_0 \equiv \frac{1+\omega^2}{4\omega} + \frac{3\lambda}{4\omega^2} . \quad (61)$$

The Hartree approximation is finally found by minimizing the expectation value $\langle\phi|H|\phi\rangle=\varepsilon_0$ with respect to the free parameter ω. From Eq. (61), ω is thus a solution to the cubic equation,

$$\omega^3 - \omega - 6\lambda = 0 . \quad (62)$$

It is not difficult to show that for all values of λ, Eq. (61) has only one real root which satisfies the condition $\omega > 0$ imposed by the restriction $|\tau| < 1$. It has been shown elsewhere[33] that this simple approximation itself produces a variational estimate ε_0 for the ground-state energy of the
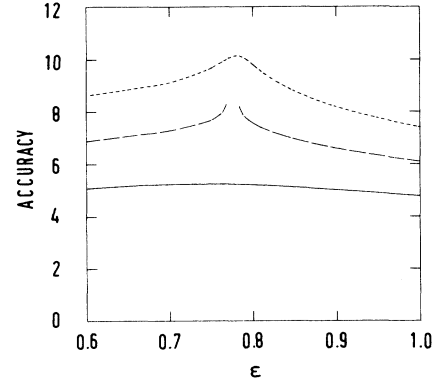

FIG. 2. Accuracy vs ε for the ground-state energy of the anharmonic oscillator, with $\lambda=1.0$, $\lambda_0=0.99$, $t=1$, in a size-19 basis. Results are shown for perturbation order $N=1$ (solid line), 2 (long dashes), and 3 (short dashes). Note that for this case, $E_0(\lambda_0)=0.801\,943\,6$. Accuracy of the energy E has been defined as $-\log_{10}|(E-E^{\text{exact}})/E^{\text{exact}}|$ and is interpreted as the number of correct digits, in base 10, of the approximation E to E^{exact}.

quartic anharmonic oscillator which is accurate to better than about 2% for all (positive) values of λ.

In our numerical work, we use the Hamiltonian of Eqs. (59)–(62) in the orthonormal harmonic oscillator representation specified by the new operators b and $b^\dagger$,

$$|n\rangle = (n!)^{-1/2}(b^\dagger)^n|\phi\rangle, \quad n=0,1,2,\ldots . \quad (63)$$

More specifically we work with an approximate, truncated $(M \times M)$-dimensional representation in which only the states of Eq. (63) with $n < M$ are used, as discussed previously. While this transformed basis will improve the numerical accuracy of our results over those obtained using the original basis, it does not change the fundamental nature of the problem. Thus, the transformed Hamiltonian of Eq. (59) is still "singular" in the limit $\lambda \to 0$.

We turn first to the question of how our results depend on the choice of the input parameter ε. Results for the
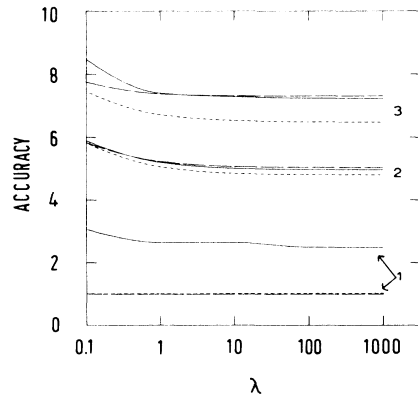

FIG. 3. Accuracy (as defined in Fig. 2) of the ground-state energy for the anharmonic oscillator for various values of λ with $\lambda_0=0.99\lambda$ in a $t=1$-dimensional subspace of a basis of size 19. The free parameter ε has been set to $E_0(\lambda_0)$ (solid line), $0.9E_0(\lambda_0)$ (long dashes), and $1.1E_0(\lambda_0)$ (short dashes), and results are given for perturbation order N from 1 to 3 with N displayed to the right of the curves.

TABLE II. Results for the ground-state formalism energy for the anharmonic oscillator, where the free parameter ε has been set to various values of the eigenvalues $E_i(\lambda_0)$ of the $H(\lambda_0)$ Hamiltonian, with i ranging from 0 to 4. The perturbation parameters are $\lambda = 1.0$, $\lambda_0 = 0.99$, with the subspace size $t = 1$, in a size-19 basis. Results are shown up to perturbation order $N = 10$, with the first row showing the value of ε and the last showing the exact results.

i / N	0	1	2	3	4
ε	0.801 943 626 3	2.730 955 805 6	5.165 126 648	7.919 853 742 7	10.931 714 00
1	0.803 775 642 3	0.804 873 494 5	5.179 334 702	0.847 450 863 0	10.963 739 60
2	0.803 770 633 7	0.803 091 971 5	5.179 291 721	0.734 3	10.963 639 26
3	0.803 770 657 4	0.804 263 748 7	5.179 291 942	1.047 4	10.963 639 79
4	0.803 770 657 3	0.803 389 802 4	5.179 291 941	0.454 4	10.963 639 79
5	0.803 770 657 3	0.804 070 481 0	5.179 291 941	2.148 7	10.963 639 79
6	0.803 770 657 3	0.803 533 391 0	5.179 291 941	-0.851 4	10.963 639 79
7	0.803 770 657 3	0.803 958 597 5	5.179 291 941	8.118 5	10.963 639 79
8	0.803 770 657 3	0.803 621 838 8	5.179 291 941	-6.339 4	10.963 639 79
9	0.803 770 657 3	0.803 888 411 9	5.179 291 941	40.12	10.963 639 79
10	0.803 770 657 3	0.803 677 561 7	5.179 291 941	-25.15	10.963 639 79
E	0.803 770 657 3	2.737 892 359 2	5.179 291 941	7.942 429 339 7	10.963 639 79

accuracy of the ground-state energy are displayed in Fig. 2 for the case $\lambda = 1$, $\lambda_0 = 0.99$, in the same size-19 basis as before. The accuracy of an estimate E for the energy is taken to be the quantity $-\log_{10}|1 - E/E^{\text{exact}}|$, where the exact value E^{exact}, is taken to be that corresponding to the truncated basis. In all of our numerical work we use a basis of size $M = 19$. We point out that this basis size gives results extremely close to the infinite-basis limit. Thus, for the case $\lambda = 1$, for example, the ground-state energy has an error of less than $10^{-7}\%$ due to the finite ($M = 19$) basis size. We note that in each order of perturbation theory, the accuracy is only weakly dependent on ε. In second-order MRSPT in this case the exact answer happens fortuitously to be attained with a value $\varepsilon \approx 0.78$, which may be compared with the corresponding value of $E_0(\lambda_0) \approx 0.80$. We also display in Table II the same $t = 1$ ground-state results, but where $\varepsilon = E_n(\lambda_0)$, $n = 0, 1, \ldots, 4$, the lowest five eigenvalues of the truncated (in the same basis of dimension 19 as previously) unperturbed Hamiltonian $H(\lambda_0)$. We see very clearly the

interesting feature that the "ground-state" ($t = 1$) formalism accurately produces the excited-state energies for all levels which have the same parity as the ground state. We take this as evidence that the steplike feature of Fig. 1 for the case of the tridiagonal Hamiltonian of Eq. (49) is not simply due to the special features of that model, as discussed previously. It seems that as long as the excited state being considered is not too different from the ground state, then our MRSPT always has the rather general feature illustrated by Fig. 1.

In Table III and Fig. 3 we present results for the ground-state energy and its accuracy, respectively, as obtained via the $t = 1$ version of MRSPT in various orders up to the fifth. The coupling parameter λ ranges from 0.1 to 10^3. In each case we have chosen $\lambda_0 = 0.99\lambda$. In Table III we have set ε equal to the exact ground state $E_0(\lambda_0)$ of the (truncated) unperturbed Hamiltonian $H(\lambda_0)$, and in Fig. 3 we have set ε equal to 0.9, 1.0, and 1.1 times $E_0(\lambda_0)$. The data clearly demonstrate that the accuracy of the method at any order in perturbation
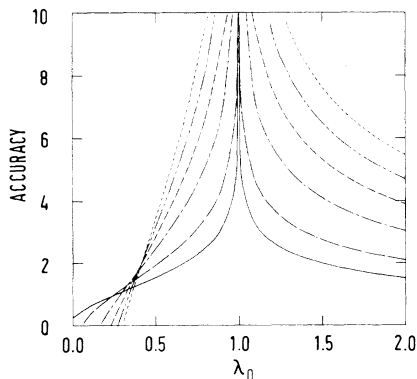

FIG. 4. Accuracy (as defined in Fig. 2) of the ground-state energy for the anharmonic oscillator as a function of λ_0, with $\lambda = 1.0$, $\varepsilon = E_0(\lambda_0)$, with the subspace size $t = 1$ in a basis size of 19. Results are displayed for perturbation order $N = 1$ (solid line), 2 (long dashes), 4 (one long, one short dash), 6 (medium dashes), 8 (one long and two short dashes), and 10 (short dashes).
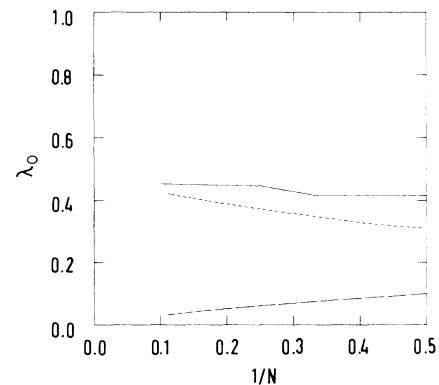

FIG. 5. Crossing points (short dashes) and inflection points (solid line) (as defined in the text) for the anharmonic oscillator, as a function of the inverse of the perturbation order N, with $\lambda = 1.0$, subspace size $t = 1$, in a size-19 basis. Also shown are the crossing points for the standard RSPT results (medium dashes), as derived from Bender and Wu (Ref. 11). For these later data, the vertical axis shows λ and not λ_0.
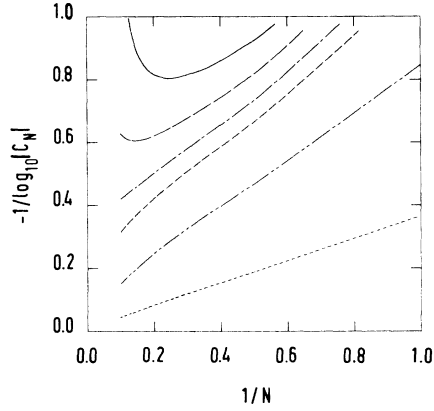
FIG. 6. Size of the Nth-order perturbation correction C_N vs the inverse of N, for the ground state of the anharmonic oscillator with $\lambda = 1.0$, $\varepsilon = E_0(\lambda_0)$, $t = 1$ calculated in a size-19 basis. Results are shown for $\lambda_0 = 0.35$ (solid line), 0.40 (long dashes), 0.45 (one long, one short dash), 0.5 (medium dashes), 0.7 (one long, two short dashes), and 0.99 (short dashes).
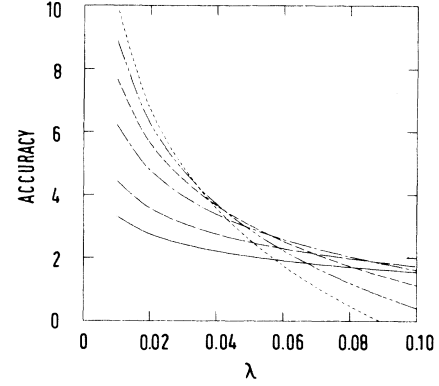

FIG. 7. Accuracy (as defined in Fig. 2) of the ground-state energy of the anharmonic oscillator vs λ calculated via standard RSPT as in Bender and Wu (Ref. 11). Perturbation orders shown are $N = 1, 2, 4, 6, 8$, and 10 and are marked as in Fig. 3.

theory is almost independent of the value of the coupling constant λ, over the four decades displayed, for a fixed-input ratio λ_0/λ, and we see again that they are also quite insensitive to changes in ε.

For a fixed value of λ, the accuracy as a function of the input parameter λ_0 is shown in Fig. 4 for various orders of perturbation theory in the $t = 1$ version of MRSPT. In each case the free parameter ε has been chosen to be the exact ground-state energy of the truncated (in the same basis of dimension 19 as before) "unperturbed" Hamiltonian $H(\lambda_0)$. These curves are quite suggestive concerning the convergence properties of the method. In particular the curves are seen to have an inflection point in the $\lambda_0 < 1$ branch which is almost order independent and which has no counterpart in the $\lambda_0 > 1$ branch. This feature is shown in more detail in Fig. 5 where the inflection point of each curve is plotted against N^{-1}, where N is the perturbation order. We also similarly plot in Fig. 5 the crossing points of the data displayed in Fig. 4, 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. If, in the limit $N \to \infty$, these crossing points would converge to some nonzero value of λ_0 (less than one) our expansion would be convergent for λ greater than this value. Of course the data presented do not constitute a proof, al-

though they are certainly suggestive, and clearly demonstrate the vast improvement over the comparable $(\lambda_0 = 0)$ RSPT results.

It also seems quite plausible from Fig. 4 that the accuracy curves as a function of λ_0 asymptotically approach an infinite step function as the perturbation order increases without bound with a transition from divergence to convergence for values of λ_0, respectively, less than or greater than some critical value of about 0.45. As one last check on this point we display in Fig. 6 the quantity $-1/\log_{10}|C_N|$ against N^{-1}, where $C_N = \rho^N E_0^{(N)}$ is the correction term to the ground-state energy eigenvalue from Nth-order itself. By plotting curves for several values of λ_0, we see again the fundamental change in the behavior of the perturbation series for the ground-state energy at $\lambda = 1$ as we cross a value of $\lambda_0 \approx 0.45$. By way of comparison, we show in Fig. 7 the corresponding accuracy as a function of λ for the standard RSPT as used by Bender and Wu.[24] The corresponding crossing points are also displayed in Fig. 5, where these now indicate the value of λ below which the $(N + 1)$th-order estimate for the energy becomes more accurate than the Nth-order estimate. In this case, the limit $\lambda \to 0$ as $N \to \infty$ of this curve is known,[24] and indicates divergence of the RSPT for all values of λ.

It is our belief that the MRSPT convergence is very good for $\lambda_0 > \lambda_0^{crit}$, where λ_0^{crit} depends on λ. We conjecture that some $\lambda_0^{crit}(\lambda) < \lambda$ is a natural boundary of the convergence domain. At the very least, the data of Fig. 4

TABLE III. Anharmonic oscillator ground-state energies, calculated up to perturbation order $N = 5$, for various values of λ, with $\lambda_0 = 0.99\lambda$, $\varepsilon = E_0(\lambda_0)$, and subspace size $t = 1$ in a size-19 basis. The results in the last row, marked E, are exact.

N \ λ	0.1	1	10	100	1000
0	0.558 656 881 7	0.801 943 626 3	1.500 374 630	3.121 117 646	6.671 928 545
1	0.559 147 038 1	0.803 775 642 2	1.504 987 217	3.131 418 492	6.694 295 996
2	0.559 146 325 2	0.803 770 633 7	1.504 972 389	3.131 384 155	6.694 220 848
3	0.559 146 327 2	0.803 770 657 4	1.504 972 469	3.131 384 346	6.694 221 266
4	0.559 146 327 2	0.803 770 657 3	1.504 972 469	3.131 384 345	6.694 221 266
5	0.559 146 327 2	0.803 770 657 3	1.504 972 469	3.131 384 345	6.694 221 266
E	0.559 146 327 2	0.803 770 657 3	1.504 972 469	3.131 384 345	6.694 221 266

TABLE IV. Results for the anharmonic oscillator, with $\lambda = 1.0$ and $\lambda_0 = 0.99$, in a basis size of 19, for various values of the subspace size t. The column marked ε indicates whether the free parameter ε is equal to $E_0(\lambda_0)$ or $E_1(\lambda_0)$. For a given value of t and ε, first-, and second-order results are displayed above and below each other, respectively. The results in the last row, marked E, are exact.

t	ε	E_0	E_1	E_2	E_3	E_4
1	0	0.803 775 64				
		0.803 770 63				
	1	0.804 873 49				
		0.804 873 49				
2	0	0.803 775 64	2.740 843 83			
		0.803 770 63	2.738 543 46			
	1	0.804 873 49	2.737 912 47			
		0.803 091 97	2.737 892 26			
3	0	0.803 771 05	2.740 843 83	5.225 250 36		
		0.803 770 66	2.738 543 46	5.196 486 06		
	1	0.804 208 35	2.737 912 47	5.200 777 79		
		0.803 666 61	2.737 892 26	5.184 777 22		
4	0	0.803 771 05	2.738 266 72	5.225 250 36	8.170 957 16	
		0.803 770 66	2.737 947 88	5.196 486 06	8.048 220 12	
	1	0.804 208 35	2.737 892 78	5.200 777 79	8.104 641 07	
		0.803 666 61	2.737 892 36	5.184 777 22	8.005 644 30	
5	0	0.803 770 72	2.738 266 72	5.180 180 18	8.170 957 16	11.668 316 4
		0.803 770 66	2.737 947 88	5.179 530 76	8.048 220 12	11.330 342 8
	1	0.803 777 97	2.737 892 78	5.179 652 37	8.104 641 07	11.543 043 0
		0.803 769 78	2.737 892 36	5.179 353 23	8.005 644 30	11.235 496 1
E		0.803 770 66	2.737 892 36	5.179 291 94	7.942 429 34	10.963 639 7

make it clear that we can achieve a high degree of accuracy for $\lambda_0 \gtrsim \lambda_0^{\mathrm{crit}}$.

Finally we present in Table IV some data for subspaces of size $t > 1$, again for the case $\lambda = 1$, $\lambda_0 = 0.99$, and in a size-19 basis. Results are shown for the free parameter ε set equal either to $E_0(\lambda_0)$ or $E_1(\lambda_0)$, and using first- and second-order MRSPT in each case. As one might expect, the energy level produced most accurately in the spectrum of $H(\lambda)$ is that which corresponds to the level in the spectrum of $H(\lambda_0)$ to which the parameter ε has been set equal. We also note that we obtain very accurate results, at low perturbative order, for this favored level by increasing the subspace size t. Thus eight digits of accuracy are obtained at only the second perturbation order for $t = 4(5)$ for the ground (first excited) levels, respectively. We also see that the further away an energy level is from the chosen value of ε, the worse is the accuracy. Given that ε represents the zeroth-order approximant for *all* of the energy levels, this result is to be expected. Overall, the quality of the results is impressive, even for the highest eigenvalues.

IV. SUMMARY AND CONCLUSIONS

The standard versions of perturbation theory first convert the Schrödinger eigenvalue problem into a simplified unperturbed version, which is chosen so that its solutions may easily be determined exactly or, equivalently, so that it has a known diagonal form. This process is then followed by a systematic iterative determination of the correction terms to arbitrary order. Our present MRSPT represents a rather broad and basic generalization which allows easy inclusion of nondiagonal pieces in the starting Hamiltonians about which we perform the corrections. This was achieved by rendering the solution of the unperturbed Schrödinger equation trivial, as a result of which the energy "eigenvalue" for this equation has become a free parameter (denoted by ε) in the theory. If the energy eigenvalues produced by MRSPT turned out to be strongly dependent on the choice of ε, the method would achieve little, since this would imply that a rather accurate knowledge of the unperturbed energy spectrum would be needed as a starting point. The data that we have presented for two very dissimilar models have

shown that the accuracy achievable is, however, quite insensitive to the choice of ε. It was demonstrated that if ε is broadly in the vicinity of, say the ith energy eigenvalue of the unperturbed Hamiltonian $\tilde{H}^0$, then the MRSPT energy will converge to the corresponding eigenvalue for the full Hamiltonian H, as long as the zeroth-order and appropriate exact wave functions are not too dissimilar.

We have seen, however, that the overall structure of the new method is still very akin to that of RSPT, with only relatively slight modifications. Since the unperturbed propagators are no longer diagonal, it is not surprising that the explicit formulas of MRSPT are somewhat more complex then their usual RSPT counterparts. Nevertheless this is a very small price to pay for a procedure that, as shown here and elsewhere[2,4,19-21] has opened up a way towards a new and broad class of self-consistent procedures for use with such nondiagonal unperturbed Hamiltonians, where previously only the diagonal elements had been available in this context.

In physical terms, the main achievement of our modifications has been the possibility of including more, if not all, of the large or otherwise important matrix elements of the full Hamiltonian into a nondiagonal, unperturbed version about which to do perturbation theory. As a consequence, the energy perturbation expansions of the form in Eq. (8) will feel the effects of these large Hamiltonian components only through the energy denominators of the unperturbed propagators of the form of Eq. (18). Conversely, the remaining "small" matrix elements will determine the rate of convergence or the relative decrease in size of the consecutive terms in the perturbation series. It seems intuitively obvious that a much more rapid convergence rate and/or higher quality of approximation at a given perturbative level ought to be achievable in principle by our MRSPT over the standard approach. In our studies here we have presented numerical data to back up these claims, It seems likely for example, that in such important and well-studied examples as the quartic anharmonic oscillator, which are known to diverge for all coupling parameters in the standard approach, the MRSPT does converge for a wide range of choices of unperturbed Hamiltonian. We have explicitly shown that the method is certainly capable of giving results of very high accuracy for a wide range of its input parameters.

Two of the freedoms of the degenerate version of MRSPT presented here are the choice of t-dimensional model space and of the initial energy parameter ε. As already mentioned above, the accuracy achievable is not strongly dependent on the choice of ε, for example. Still, some choice must be made. We believe that this decoupling of the model space and initial energy parameter from the unperturbed Hamiltonian may well be exploited as an asset of the method in future uses. For example, it permits considerable freedom to impose other physical constraints (e.g., variational principles or inequalities) relevant to the problem at hand, in order to determine them separately. We hope to return in the future to such considerations and to other further developments of the method.

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