Modified Rayleigh-Schrödinger perturbation theory

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A new version of perturbation theory is described. It extends the admissible class of Hamiltonians H_0 to nondiagonal matrices via use of the nondiagonal unperturbed propagators. Numerically, its efficiency is demonstrated on the standard anharmonic-oscillator example where it works as an effective resummation technique.

I. INTRODUCTION

Let us consider a Schrödinger bound-state problem

$$H|\psi\rangle=E|\psi\rangle \tag{1.1}$$

and its approximate (tentative) solution

$$|\psi\rangle\approx|\chi_n\rangle,\quad E\approx\varepsilon_n,\quad n=0,1,\ldots . \tag{1.2}$$

Obviously, this solution may be treated as corresponding to a tentative component

$$\sum_{n=0}^{\infty}|\chi_n\rangle\varepsilon_n\langle\chi_n|=H_t \tag{1.3}$$

of the complete Hamiltonian $H\approx H_t$. Thus, an improved solution of Eq. (1.1) may be constructed by the perturbative methods in principle.

The textbook Rayleigh-Schrödinger (RS) perturbation theory usually starts from the explicit knowledge of (1.2). In this paper we shall try to get rid of such a strong requirement—we shall assume that H_t is a nondiagonal matrix in our (*a priori* chosen or constructed) working basis $|0\rangle,|1\rangle,\ldots$.

For this sake of definiteness, let us assume that

$$H_t=\begin{bmatrix} a_0 & b_0 & 0 & 0 & \cdots & \\ c_1 & a_1 & b_1 & 0 & 0 & \cdots \\ 0 & c_2 & a_2 & b_2 & 0 & 0 \\ 0 & 0 & c_3 & a_3 & b_3 & 0 \\ \vdots & \vdots & 0 & c_4 & a_4 & \vdots \\ \vdots & \vdots & & & & \end{bmatrix} \tag{1.4}$$

is an infinite tridiagonal matrix. Such a structure is the simplest form of nondiagonality and appears in a number of applications. For example, we may recall the strong-coupling scheme appearing in nonequilibrium statistics,[1] "chain models" used in solid-state physics,[2] etc. At the same time, matrix (1.4) is sufficiently general—we encounter a tridiagonalization of Hamiltonian within the universal numerical Lanczos method of solving (1.1), e.g., in nuclear physics computations.[3]

An important formal merit of the tridiagonal choice (1.4) lies in its connection with the analytic continued fractions.[1–4] In this framework, unfortunately, an inclusion of corrections seems rather complicated.[5] In this paper we shall avoid the generalized continued fractions used in Ref. 5 and describe a simpler technique of a systematic perturbative inclusion of the higher-order corrections related to the general small perturbation $\lambda V=H-H_t$.

Within the Rayleigh-Schrödinger (RS) standard formalism,[6] an evaluation of (1.2) or (1.3) with the "simplified" unperturbed Hamiltonian H_t is possible in a few exceptional cases only. For a general operator H_t, this task becomes almost as difficult as a complete solution of the original Eq. (1.1) itself. A removal of this difficulty is the main purpose of this paper.

The continued-fraction tractability of Eq. (1.1) with $H=H_t$ is closely related to an algebraic factorization of the resolvent.[5] A similar idea will be employed here. We shall see that, in terms of the analytic continued fractions, the modified RS-type expansions may be constructed even without an explicit solution (1.3) of the unperturbed eigenvalue problem. This will be our main result.

The common features of the RS and our modified Rayleigh-Schrödinger (MRS) perturbation theories will be summarized in Sec. II. The essence of the new, modified version of the formalism will be described in Sec. III. In particular, a trial wave function $|0\rangle$ will be employed in place of the RS zero-order solution $|\chi_0\rangle$ (Sec. III A) and the need for a basis $|\chi_n\rangle$ when using RS theory will completely be eliminated (Sec. III B). In Sec. IV the further formal details will be added—we construct the unperturbed propagator $R(E_0)$ as an analytic continued-fraction chain-model resolvent (Sec. IV A) and show that E_0 plays a role of a free parameter (Sec. IV B).

The efficiency and good convergence of the new formalism will be analyzed numerically in Sec. V and documented by its application to the standard anharmonic oscillator example in Sec. VI.

II. THE RS FORMALISM

The extreme popularity of the RS technique stems from the flexibility and universality of its basic ansatz

$$\begin{aligned}|\psi\rangle&=|\psi_0\rangle+\lambda|\psi_1\rangle+\cdots+\lambda^N|\psi_N\rangle+O(\lambda^{N+1}),\\ E&=E_0+\lambda E_1+\cdots+\lambda^N E_N+O(\lambda^{N+1}).\end{aligned} \tag{2.1}$$

An insertion of Eq. (2.1) in Eq. (1.1) is the main idea. The resulting relation

$$[H_t-E_0+\lambda(V-E_1)-\lambda^2E_2-\cdots]$$
$$\times(|\psi_0\rangle+\lambda|\psi_1\rangle+\cdots)=0 \quad (2.2)$$

is to be satisfied for each value of the parameter λ_1 so that we get the unperturbed equation

$$H_t|\psi_0\rangle=E_0|\psi_0\rangle\ , \quad (2.3)$$

complemented, term by term, by the relations

$$(H_t-E_0)|\psi_k\rangle=-V|\psi_{k-1}\rangle+\sum_{m=1}^{k}E_m|\psi_{k-m}\rangle\ ,$$
$$k=1,2,\ldots . \quad (2.4)$$

Their $\langle\psi_0|$ projection defines the energies

$$E_1=\kappa\langle\psi_0|V|\psi_0\rangle,\quad \kappa=(\langle\psi_0|\psi_0\rangle)^{-1}\ , \quad (2.5)$$

and

$$E_k=\kappa\left[\langle\psi_0|V|\psi_{k-1}\rangle-\sum_{m=1}^{k-1}E_m\langle\psi_0|\psi_{k-m}\rangle\right],$$
$$k=2,3,\ldots \quad (2.6)$$

in a recurrent (implicit) way. Their explicit form $E_k=E_k(\psi_0,\psi_1,\ldots,\psi_{k-1})$ may, of course, be inserted back in Eq. (2.4).

After an elimination of energies, we may treat Eq. (2.4) as a recurrent specification of the wave-function corrections $|\psi_k\rangle$, $k=1,2,\ldots$. Obviously, it is not unique—an arbitrary "renormalization"

$$|\psi_k\rangle\rightarrow|\psi_k\rangle+\alpha_k|\psi_0\rangle \quad (2.7)$$

remains compatible with Eq. (2.4). This ambiguity is usually removed by an RS requirement

$$\langle\psi_0|\psi_k\rangle=0,\quad k=1,2,\ldots . \quad (2.8)$$

Then, expansions (2.1) become uniquely defined whenever we pick up an unperturbed solution, say,

$$|\psi_0\rangle=|\chi_0\rangle,\quad E_0=\varepsilon_0\ . \quad (2.9)$$

In accord with Eq. (1.3), this converts the unperturbed RS problem (2.3) into an identity.

III. THE MRS FORMALISM

A. A MRS normalization

In nuclear physics calculations where the tridiagonal approximants H_t appear in a purely numerical context,[3] the first basis state $|0\rangle$ is carefully being constructed as the best available approximation to the exact wave function $|\psi\rangle$. In this case, it is of course natural to replace the RS requirement (2.8) by

$$\langle 0|\psi_k\rangle=0,\quad k=1,2,\ldots . \quad (3.1)$$

In accord with (2.7), this may be achieved via an appropriate $\alpha_k\neq0$ shift of the RS wave functions $|\psi_k\rangle$.

On a purely formal level, we may simplify the preceding construction, assuming that $\langle 0|0\rangle=\langle 0|\psi_0\rangle=1$, by introducing the projector $Q=1-P$, $P=|0\rangle\langle 0|$. It does not appear in the MRS normalization (3.1) and enables us to rewrite Eq. (2.4) as the requirements

$$Q(H_t-E_0)Q|\psi_1\rangle=-QVQ|\psi_0\rangle-QV|0\rangle+E_1Q|\psi_0\rangle\ , \quad (3.2)$$

$$Q(H_t-E_0)Q|\psi_k\rangle=-QVQ|\psi_{k-1}\rangle+\sum_{m=1}^{k}E_mQ|\psi_{k-m}\rangle\ ,$$
$$k=2,3,\ldots ,$$

complemented by the definitions (2.5) and (2.6) of energies. This follows from a formal equivalence between the $\langle\psi_0|$ and $\langle\psi_0|(P+Q)$ projections of Eq. (2.4), and enables us to specify the explicit MRS corrections by the formulas

$$|\psi_1\rangle=R(V-E_1)|\psi_0\rangle\ ,$$
$$|\psi_k\rangle=RQVQ|\psi_{k-1}\rangle-\sum_{m=1}^{k}E_mR|\psi_{k-m}\rangle\ , \quad (3.3)$$
$$k=2,3,\ldots .$$

Here, the MRS unperturbed propagator is defined formally,

$$R=Q(E_0-QH_tQ)^{-1}Q\ . \quad (3.4)$$

Its non-numerical construction will be discussed later.

B. Getting rid of the unperturbed Schrödinger equation

Let us write Eq. (2.3) as a pair of projected equations

$$PH_t(P+Q)|\psi_0\rangle=E_0P|\psi_0\rangle\ ,$$
$$QH_t(P+Q)|\psi_0\rangle=E_0Q|\psi_0\rangle\ . \quad (3.5)$$

Precisely in the Feshbach spirit,[7] we may eliminate here

$$Q|\psi_0\rangle=RH_t|0\rangle\ , \quad (3.6)$$

and reduce Eq. (3.5) to its effective one-dimensional form

$$\langle 0|H_t|0\rangle+\langle 0|H_tR(E_0)H_t|0\rangle=E_0\ . \quad (3.7)$$

This is the standard chain-model secular equation.[2,3]

Within our one-dimensional model space, we may introduce a free parameter ζ and modify the original decomposition of the Hamiltonian,

$$H=H_t'+\lambda V'\ ,$$
$$H_t'=H_t+|0\rangle\zeta\langle 0|,\quad V'=V-|0\rangle\frac{\zeta}{\lambda}\langle 0|\ . \quad (3.8)$$

In contrast to the RS formalism with $|0\rangle=|\chi_0\rangle$, this is a nontrivial transformation of the MRS solutions and, in fact, a core of the present proposal. Its first consequence may be seen immediately: the primed form of the secular Eq. (3.7) defines

$$\zeta=E_0-\langle 0|H_t|0\rangle-\langle 0|H_tR(E_0)H_t|0\rangle \quad (3.9)$$

as a function of E_0. In this way, we may reinterpret E_0

as a free parameter and treat (3.9) as a mere definition of the primed decomposition (3.8).

After replacing all the unprimed H_t and V by the primed ones, the unperturbed secular equation becomes satisfied identically. There is just one other change in the preceding formulas: in place of Eq. (2.5), we may write

$$E_1=\kappa(\langle\psi_0\,|\,V\,|\,\psi_0\rangle-\zeta/\lambda)\,, \tag{3.10}$$

and avoid any explicit use of the primed components (3.8) of H.

IV. THE EXPLICIT CONTINUED-FRACTION MRS FORMULAS

A. The unperturbed propagator

Up to now, the MRS definitions of energies [(3.9), (3.10), and (2.6)] and wave functions [(3.6) and (3.3)] contain $R(E_0)$ as a numerical inverse of the operator E_0-QH_tQ. Due to its tridiagonality, we need not even use the numerical techniques—its analytic continued-fraction inversion is a well-known procedure.[5] It is based on the algebraic identities

$$E_0I-\begin{bmatrix} a_n & b_n & 0 & \cdots & \\ c_{n+1} & a_{n+1} & b_{n+1} & 0 & \cdots \\ 0 & c_{n+2} & a_{n+2} & \cdots & \\ & \cdots & & & \end{bmatrix}=\begin{bmatrix} 1 & -b_nf_{n+1} & 0 & \cdots \\ 0 & 1 & -b_{n+1}f_{n+2} & \cdots \\ 0 & 0 & 1 & \cdots \\ & \cdots & & \end{bmatrix}$$

$$\times\begin{bmatrix} 1/f_n & 0 & \cdots & \\ 0 & 1/f_{n+1} & 0 & \cdots \\ & \cdots & & \end{bmatrix}\begin{bmatrix} 1 & 0 & \cdots & & \\ -c_{n+1}f_{n+1} & 1 & 0 & \cdots & \\ 0 & -c_{n+2}f_{n+2} & 1 & 0 & \cdots \\ \cdots & & & & \end{bmatrix} \tag{4.1}$$

and

$$f_k=(E_0-a_k-b_kf_{k+1}c_{k+1})^{-1},\quad k=n,n+1,\ldots, \tag{4.2}$$

with $n=1$. When we put, formally, $f_{N+1}=0$ in the limit $N\to\infty$, we may interpret Eq. (4.2) as a definition of the analytic continued fractions.[4] Then, after an explicit inversion

$$\begin{bmatrix} 1 & \omega_{11} & \omega_{12} & \cdots \\ 0 & 1 & \omega_{21} & \cdots \\ & \cdots & & \end{bmatrix}=\begin{bmatrix} 1 & -b_nf_{n+1} & 0 & \cdots \\ 0 & 1 & -b_{n+1}f_{n+2} & \cdots \\ \cdots & & & \end{bmatrix}^{-1},$$

$$\omega_{kl}=\prod_{m=1}^{l}(b_{m+n+k-2}f_{m+n+k-1}),\quad k,l=1,2,\ldots \tag{4.3}$$

of the two-diagonal factors in (4.1), we may determine the unperturbed MRS propagator (3.4) completely,

$$\langle m\,|\,R\,|\,n\rangle=\sum_{i=0}^{M}d_{m-i}f_{i+1}d^*_{n-i},\quad M=\min(m,n)-1,\quad m,n=1,2,\ldots,\quad d_0=d^*_0=0,\quad d_1=d^*_1=1\,,$$

$$d_k=c_kf_kd_{k-1},\quad d^*_k=d^*_{k-1}b_{k-1}f_k,\quad k=2,3,\ldots. \tag{4.4}$$

All its matrix elements are simple products of the auxiliary continued fraction f_n. Moreover, any finite subset of these elements may be also expressed as elementary expressions containing a single continued fraction only. This is a consequence of another algebraic identity

$$f_nf_{n+1}\cdots f_m=1/\det\begin{bmatrix} E_0-a_n & -b_n & & & \\ -c_{n+1} & E_0-a_{n+1} & -b_{n+1} & & \\ & \ddots & & & \\ & -c_{m-1} & E_0-a_{m-1} & -b_{m-1} & \\ & & -c_m & 1/f_m & \end{bmatrix}. \tag{4.5}$$

The matrix elements of R have a simple alternative interpretation: when we denote $\langle k\,|\,\psi_0\rangle=d_k\langle 1\,|\,\psi_0\rangle$ and $\langle\psi_0\,|\,k\rangle=\langle\psi_0\,|\,1\rangle d^*_k$, $k\geq 1$, we see immediately their relation to the components of the unperturbed vector $|\,\psi_0\rangle$.

TABLE I. The divergent RS energies and their MRS resummation for $H=H_{2-\varphi,\varphi}$ and $E^{\text{exact}}=3\sqrt{2}\doteq 4.242\,640\,687$.

Method	RS ($\varphi=1$)		MRS ($\varphi=0$)	
E_0	5.0	5.5	5.0	5.5
$E^{(1)}$	4.5	4.5	4.2487	4.263
$E^{(2)}$	3.75	3.5	4.2418	4.237
$E^{(3)}$	5.25	6.5	4.242 76	4.2439
$E^{(4)}$	2.22	−2.44	4.242 626	4.242 37
$E^{(5)}$	8.09	22.91	4.242 642 3	4.242 688
$E^{(6)}$	−2.47	−43.65	4.242 640 55	4.242 635
$E^{(7)}$	14.38	111.60	4.242 640 695	4.242 640 46

B. The lowest-order MRS approximants

In Sec. III B, Eq. (2.3) has been replaced by the modified unperturbed equation

$$T\,|\,\psi_0\rangle=E_0\,|\,\psi_0\rangle\ ,\qquad T=H_t+\,|\,0\rangle\zeta\langle 0\,|\ . \tag{4.6}$$

As a consequence, we may combine its projection

$$E_0\langle\psi_0\,|\,\psi_0\rangle=\langle\psi_0\,|\,H_t\,|\,\psi_0\rangle+\zeta$$

with the formula (3.10),

$$\lambda E_1\langle\psi_0\,|\,\psi_0\rangle=\langle\psi_0\,|\,\lambda V\,|\,\psi_0\rangle-\zeta\ ,$$

and eliminate the auxiliary quantity ζ,

$$E^{(1)}=E_0+\lambda E_1=\kappa\langle\psi_0\,|\,H\,|\,\psi_0\rangle\ . \tag{4.7}$$

This slightly simplifies the formalism—we may treat Eq. (4.7) as the first nontrivial contribution in the present MRS context.

In comparison with the RS formalism, we may expect an increase in complexity of the comparable formulas. This is the price to be paid for our complete elimination of the strong assumption (1.3). For example, in contrast to the arbitrary RS normalization of $|\,\psi_0\rangle$ (paralleled here by the choice of $\langle 0\,|\,0\rangle=\langle 0\,|\,\psi_0\rangle=1$), we must compute it now as an infinite sum

$$\langle\psi_0\,|\,\psi_0\rangle=1+\langle\psi_0\,|\,Q\,|\,\psi_0\rangle=1+\langle 0\,|\,H_tR^2H_t\,|\,0\rangle$$
$$=1+b_0f_1\left[\sum_{k=1}^{\infty}d_k^*d_k\right]f_1c_1 \tag{4.8}$$

over the intermediate states. Similar interpretation should be given to the other MRS formulas as well.

V. A NUMERICAL ANALYSIS OF THE MRS RATE OF CONVERGENCE

For an illustration of the various new features of the present MRS formalism, let us choose the simplest possible example

$$H=H_{\chi,\varphi}=H_t+\lambda V\ ,\qquad H_t=-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+\chi r^2,\quad \lambda V=\varphi r^2 \tag{5.1}$$

with the basis specified as eigenstates of $H_{1,0}$

$$H_{1,0}\,|\,n\,\rangle=2\tilde{a}_n\,|\,n\,\rangle\ ,\qquad \tilde{a}_n=\langle n\,|\,r^2\,|\,n\,\rangle=2n+l+\tfrac{3}{2}\ , \tag{5.2}$$
$$\langle n\,|\,r^2\,|\,n+1\rangle=\tilde{b}_n=(n+1)^{1/2}(n+l+3/2)^{1/2}\ .$$

TABLE II. A uniformity of the MRS convergence for small E_0 ($H=H_{2,\varphi}$).

φ	0.25	0.50	0.75	1.00	1.25
E_0	1.5	1.5	1.5	1.5	1.5
$E^{(1)}$	5.6	5.8	6.1	6.3	6.6
$E^{(2)}$	5.45	5.67	5.87	6.07	6.26
$E^{(3)}$	5.42	5.63	6.82	6.01	6.19
$E^{(4)}$	5.411	5.615	5.811	6.0000	6.183
$E^{(5)}$	5.4089	5.6127	5.8092	5.9992	6.1834
$E^{(6)}$	5.408 38	5.612 37	5.809 22	5.999 66	6.184 31
$E^{(7)}$	5.408 31	5.612 42	5.809 38	5.999 92	6.184 63
$E^{(8)}$	5.408 31	5.612 46	5.809 46	5.999 999	6.184 68
$E^{(9)}$	5.408 320	5.612 480	5.809 475	6.000 008	6.184 672
$E^{(10)}$	5.408 325	5.612 485	5.809 477	6.000 004	6.184 662
E^{exact}	5.408 327	5.612 486	5.809 475	6.000 000	6.184 658

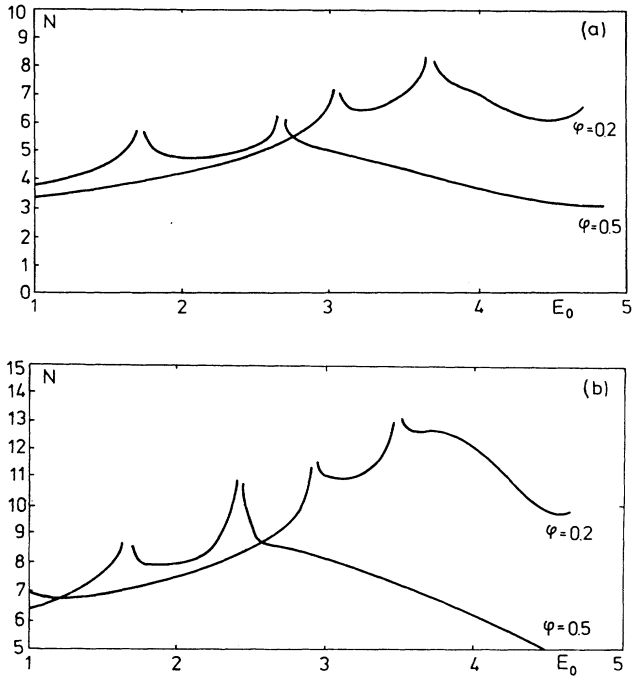

FIG. 1. Precision of the ground-state energies for $H=H_{2,\varphi}$, i.e., a number of correct significant digits $N=-\log_{10}|E^{(k)}-E^{\text{exact}}|$, as a function of the free parameter E_0. (a) The fifth-order MRS approximants $E^{(5)}$. (b) The tenth-order MRS approximants $E^{(10)}$.

These well-known elementary functions $\langle r \mid n \rangle$ (Laguerre polynomials[6]) enable us to treat (5.1) as a nondiagonal operator simulating the general and realistic quantum systems.

A. An improvement of self-consistency

Our choice of the solvable model (5.1) proved its suitability immediately. In a comparison between the RS and MRS formalisms, the RS energy approximants proved to diverge, while their MRS counterparts seem to represent their convergent and numerically reliable resummation. This is illustrated in Table I.

In full analogy with the more realistic examples (cf. e.g., Sec. VI below), the RS divergence reflects here the non-negligibility of the off-diagonal matrix elements of H. In fact, a shift of these components of the perturbation λV into the denominators of $R(E_0)$ has been one of our main motivations in developing the MRS formalism. The example confirms nicely our *a priori* expectations.

In Table I, for the sake of simplicity, we have chosen an absolutely self-consistent unperturbed operator $H_t=H$ with $\lambda V=0$. Indeed, in Table II, an inclusion of the $\lambda V\neq 0$ components is seen to preserve the convergence pattern. For the Hamiltonians $H=H_{2,\varphi}$, it does not change up to perturbations $\lambda V=\frac{5}{4}r^2$.

TABLE III. The sensitivity of the MRS convergence rate to a large variation of E_0 ($H=H_{3,0}$, $E^{\text{exact}}=5.196\,152\,42$).

E_0	1.0	5.0	6.0
$E^{(1)}$	5.31	5.1967	5.209
$E^{(2)}$	5.24	5.196 166	5.1947
$E^{(3)}$	5.21	5.196 152 72	5.196 28
$E^{(4)}$	5.201	5.196 152 428	5.196 145

B. Freedom in choosing the parameter E_0

For the values of E_0 which are safely separated from the spectrum of QH_tQ, the numerical experiments recover a surprisingly stable MRS convergence achieved in spite of a large distance between E_0 and E^{exact}. Once more, we may recall Table II as a sample of this type of result. Indeed, the unperturbed energy $E_0=1.5$ is strongly underestimated even in comparison with the lowest eigenvalue $E_t\sim 5.196$ of the unperturbed operator H_t.

Table III demonstrates an improved rate of convergence achieved with the zero-order values of E_0 chosen from a vicinity of the exact energy $E^{\text{exact}}\sim 5.196$. This has inspired a more detailed analysis of the E_0 dependence for the approximate number $N=-\log_{10}|E-E^{\text{exact}}|$ of correct digits. In Fig. 1 we see the results—$N(E_0)$ is a smooth curve with a broad maximum and irrelevant fluctuations reflecting the change of sign of $E-E^{\text{exact}}$. The good MRS convergence remains compatible with E_0 chosen from a large interval of its admissible zero-order estimates.

VI. AN APPLICATION OF THE MRS EXPANSION TO THE QUARTIC ANHARMONIC OSCILLATOR

The quartic anharmonic oscillator

$$H=-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+\mu r^2+\nu r^4 \tag{6.1}$$

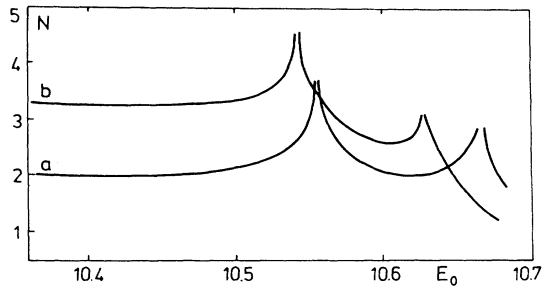

FIG. 2. Precision $N=N(E_0)$ of the first excited anharmonic oscillator energy in the fifth (curve a) and tenth (curve b) MRS approximation.

TABLE IV. Anharmonic oscillator (6.1) with $\mu=\nu=l+1=1$ and convergence of its MRS energies ($E^{\text{exact}}\doteq 1.392\,352$ and $E_0=1$).

γ	0	0.25	0.50	0.75
$E^{(1)}$	1.75	1.61	1.50	1.44
$E^{(2)}$	1.384	1.406	1.401	1.400
$E^{(3)}$	1.48	1.42	1.401	1.396
$E^{(4)}$	1.36	1.394	1.394	1.3935
$E^{(5)}$	1.45	1.402	1.394	1.3929
$E^{(6)}$	1.35	1.392 24	1.3931	1.3926
$E^{(7)}$	1.45	1.396	1.3929	1.3925
$E^{(8)}$	1.33	1.3920	1.3927	1.392 40
$E^{(9)}$	1.47	1.394	1.3926	1.392 38
$E^{(10)}$	1.30	1.3920	1.3925	1.392 366

is a standard testing ground for the various computational techniques. In particular, its RS perturbative divergence[8] is assumed to be a good model of divergences encountered in the quantum field theory.[9] Its various standard resummation representations (for a review, see, e.g., Ref. 10) start from the divergent RS series, therefore.

In the present MRS resummation framework, the pentadiagonal[11] matrix representation of (6.1) seems to be a good test of our method in a "realistic" situation since the trivial choice of $H=H_t$ ceases to be possible, and the matrix elements of $H-H_t$ are not small. Thus, the example (6.1) need not give the convergent MRS expansions *a priori,* and an application of the present formulas to (6.1) is a problem with an open solution.

In the first step we may try to choose some "safe" small $E_0=1$ and incorporate the different portions of H into the approximant H_t. In Table IV a sample of the results is displayed, based on the definition

$$\langle m\,|\,H_t\,|\,m\rangle=\langle m\,|\,H\,|\,m\rangle\ ,$$
$$\langle m\,|\,H_t\,|\,m+1\rangle=\langle m+1\,|\,H_t\,|\,m\rangle=\gamma\langle m\,|\,H\,|\,m+1\rangle\ , \tag{6.2}$$

of H_t. We may observe the following.

(a) For $\gamma=0$, the energies seem to diverge. This choice of the diagonal H_t corresponds to a degeneracy of our continued-fraction MRS formalism to the simple RS one.

(b) For $0<\gamma\leq 0.75$, the convergent MRS results are obtained. The rate of convergence of this resummation increases with the increasing value of γ. Beyond $\gamma=0.75$, our auxiliary continued fractions cease to converge[4]—the operators H_t become too "off diagonal" from the present point of view.

For the excited states, the convergence pattern of the MRS formalism remains similar to the ground-state calculations. For the particular first excited state of our anharmonic oscillator, this is demonstrated in Fig. 2. Again, the convergence deteriorates beyond some critical values, while between them a flat dependence of the precision $N(E_0)$ on E_0 is accompanied by the random fluctuations.

The higher-order corrections seem to improve the lower-order results in a systematic way. For the same set of couplings, energies E_0 and unperturbed operator H_t with $\gamma=0.75$, this is illustrated in Table V. The magnitude of both the kth order corrections E_k and total errors $E-E^{\text{exact}}$, decreases with the increasing MRS perturbation order k steadily.

VII. SUMMARY

In the very background of the standard RS perturbative formalism, we may find a decision to use a diagonal un-

TABLE V. An acceleration of the MRS anharmonic oscillator convergence (the last column describes the first excited state) for a better choice of E_0.

k	$E^{(k)}-E^{\text{exact}}$			
0	2.1	2.6	3.1	1.9
1	5.1×10^{-2}	6.1×10^{-2}	7.7×10^{-2}	3.6×10^{-1}
2	6.0×10^{-3}	3.1×10^{-3}	3.8×10^{-3}	1.2×10^{-1}
3	2.2×10^{-3}	2.5×10^{-3}	4.3×10^{-3}	3.3×10^{-2}
4	7.9×10^{-4}	6.3×10^{-4}	1.2×10^{-4}	2.3×10^{-2}
5	3.3×10^{-4}	3.2×10^{-4}	5.3×10^{-4}	7.3×10^{-3}
6	1.4×10^{-4}	1.2×10^{-4}	2.8×10^{-5}	4.4×10^{-3}
7	6.7×10^{-5}	6.3×10^{-5}	8.5×10^{-5}	2.2×10^{-3}
8	3.2×10^{-5}	2.8×10^{-5}	1.5×10^{-5}	1.4×10^{-3}
9	1.6×10^{-5}	1.5×10^{-5}	1.7×10^{-5}	7.6×10^{-4}
10	8.6×10^{-6}	7.5×10^{-6}	5.6×10^{-6}	4.2×10^{-4}

perturbed propagator R_0. This becomes a pure convention in the slowly convergent cases. Indeed, an inclusion of the higher-order corrections makes the formulas complicated in any case. Often, this forces us to omit the nonnegligible contributions in the complicated (say, many-body) calculations just because of the purely technical reasons. Hence, a minimalization of the perturbation $H-H_0$ becomes the most important task there.

Within the standard RS limitations, a choice of a good approximant $H \approx H_t$ is complicated by its direct connection with the choice of the working basis $|\chi_n\rangle$. This has inspired our present proposal—we choose the trial state $|0\rangle$, the trial energy E_0, and a very flexible (tridiagonal) form of the unperturbed matrix as input in the perturbative formalism. This improves our chance to minimize the difference $H-H_t$ up to a level necessary for a good convergence of the expansions (2.1).

Our decision to use the unperturbed propagator R, defined in terms of the analytic continued fractions, extends the scope of perturbative calculations to the tridiagonal forms of the unperturbed Hamiltonian. Formally, we may return to a diagonal-matrix case simply by a formal limit $H_t \to H_0$, i.e., $b_n \to 0$, $c_{n+1} \to 0$, and $a_n \to \varepsilon_n$. We would get $|n\rangle \to |\chi_n\rangle$ and $f_n \to 1/(E_0-\varepsilon_n)$, i.e., just a smooth transition to the RS perturbation formalism. Vice versa, the RS→MRS transition may be characterized briefly as a rearrangement of some "uncomfortable" perturbation components in the propagator $R(E_0)$. Technically, the continued fractions f_n represent, then, simply a "compression" of the three diagonals of H_t into an array f_n generalizing the RS unperturbed energies.

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