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Convergent Rayleigh–Schrödinger perturbation expansions for low-lying eigenstates and eigenenergies of anharmonic oscillators in intermediate basis states

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Abstract

With suitably chosen unperturbed Hamiltonians, we show numerical evidence of convergence of Rayleigh–Schrödinger perturbation expansions for low-lying eigenstates and the corresponding eigenenergies of the quartic, sextic, and octic anharmonic oscillators, when the anharmonic terms are not very strong. In obtaining the perturbation expansions, unperturbed Hamiltonians are taken as the diagonal parts of the Hamiltonian matrices of the anharmonic oscillators in intermediate basis states and perturbations are taken as the off-diagonal parts. Intermediate basis states are calculated by part diagonalization of the total Hamiltonians in small subspaces of the underlying Hilbert space. In some strong-coupling regimes of the quartic and sextic anharmonic oscillators, the very simple approach of this Letter gives much more accurate results than previously used techniques.

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In Rayleigh–Schrödinger (RS) perturbation theory, an eigenvalue of a Hamiltonian H is expressed in a perturbation expansion in power of some perturbation parameter λ. In most cases, perturbation expansions give divergent results [1]. Various summation methods, e.g., the Borel and Padé methods which are suitable to cases of not large λ, have been developed to extract physically meaningful results from divergent expansions [2,3]. In recent years, techniques such as δ expansion [4], variational perturbation theory [5], and renormalized strong coupling expansion [6,7], have been developed for large λ. For the quartic, sextic, and octic anharmonic oscillators, which are well suited to illustrate the problem of divergent expansions, these techniques give results with impressive accuracy for ground-state energies. The techniques can also be generalized to calculate ground-state eigenfunctions [8], but, the accuracy of the results obtained is much lower than for ground-state energies. Recently, both the ordinary [9,10] and the renormalized strong coupling expansion methods have been made use of in the investigation of low-lying excited-states of anharmonic oscillators [11,12].

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Various partition methods have been used in summation techniques in separating a Hamiltonian H into a solvable part H_0 and a perturbation V, $H = H_0 + V$. For example, V may be chosen by the principle of minimal sensitivity [13]. It is also possible for H_0 to be chosen to have a tri-diagonal matrix form, which has been shown to be useful in the study of the sextic anharmonic oscillators with double-well shapes [14]. Usually, H_0 is chosen to be analytically solvable. However, the analytical solvability of H_0 is in fact unnecessary for the purpose of summation techniques, which is to calculate eigenenergies and eigenfunctions (if applicable) as accurate as possible. Indeed, in both the ordinary and the renormalized strong coupling expansion methods, the most singular part of the total Hamiltonian H is included in the unperturbed Hamiltonian H_0, which makes it possible to construct convergent perturbation expansions, guaranteed by Kato boundedness [15,16]. In such divisions of the total Hamiltonian, the most difficult problem is the calculation of the expanding coefficients, since even numerical solution of the eigenenergies and eigenvectors of H_0 is usually quite difficult. For the case of anharmonic oscillators, efficient techniques for the evaluation of the coefficients have been developed in recent years, which have confirmed the convergence of the expansions numerically [11,12,17].

The purpose of this Letter is to investigate the possibility of constructing convergent perturbation expansions, for which numerical solution of H_0 can be carried out easily. For this purpose, the unperturbed Hamiltonian H_0 is obtained by part diagonalization of the total Hamiltonian H in finite dimensional subspaces of the underlying Hilbert space. Suppose H has a partition $(H_0^{(a)}, V^{(a)})$, with $H_0^{(a)}$ being analytically solvable. A new partition (H_0, V) can be achieved by part diagonalization of H in small subspaces of the Hilbert space, each of which is spanned by a small number of the eigenstates of $H_0^{(a)}$. At least in some cases, the geometric mean of $|f_{kk'}|$ associated with H_0 and V, where $f_{kk'} = V_{kk'}/(E_0^0 - E_k^0)$ with E_k^0 being eigenenergies of H_0 and $V_{kk'}$ being couplings, can be smaller than that of $|f_{nn'}^{(a)}|$ associated with $H_0^{(a)}$ and $V^{(a)}$, and the sign of $f_{kk'}$ can be more irregular than the sign of $f_{nn'}^{(a)}$. Since RS perturbation expansions are mainly composed of products of factors like $f_{kk'}$, it is of interest to investigate whether the partition (H_0, V) could be better than $(H_0^{(a)}, V^{(a)})$, in giving useful perturbation expansions.

In this Letter, for the quartic, sextic, and octic anharmonic oscillators, we will show numerically that, with suitably chosen H_0 by part diagonalization of the total Hamiltonians, it is possible for the RS perturbation expansions to give convergent results for low-lying eigenenergies and eigenstates, when the anharmonic terms are not very strong. The method used here is easier to be carried out numerically than the methods such as the variational perturbation theory and the renormalized strong coupling expansions. Another advantage of the method is that it gives eigenstates with an accuracy similar to that of the eigenenergies.

Let us first discuss the quartic anharmonic oscillator with a Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}x^2 + \mu x^4, \tag{1}$$

or written in terms of creation and annihilation operators, $a^+ = (x - ip)/\sqrt{2}$ and $a = (x + ip)/\sqrt{2}$,

$$H = a^+a + \frac{1}{2} + \frac{3}{4}\mu\left(2\left(a^+a\right)^2 + 2a^+a + 1\right) + \mu\left[\frac{3}{2}\left(a^+\right)^2 + \left(a^+\right)^3 a + \frac{1}{4}\left(a^+\right)^4 + \text{H.c.}\right]. \tag{2}$$

Since the eigenstates of the harmonic oscillator $H_h = p^2/2 + x^2/2$ with eigenenergies $(2n + 1/2)$ $(n = 0, 1, 2, \ldots)$ are not coupled to those with eigenenergies $(2n + 3/2)$ by the term μx^4, here we discuss the former states only, denoted by $|n\rangle$. The elements $\langle n|H|n'\rangle$ are denoted by $H_{nn'}$. As is known, RS perturbation theory gives expanding coefficients C_m growing as $m!$ for the ground-state energy, when H_h is taken as the unperturbed Hamiltonian [18]. If the diagonal and off-diagonal parts of H in the H_h-representation are taken as the unperturbed Hamiltonian and the perturbation, respectively, expanding terms in the resulting divergent RS perturbation expansion for the ground-state energy will grow much slower than $m!$, usually exponentially with increasing m, since H_{nn} has a n^2-term (see Eq. (2)).

The critical step of our approach is to employ *intermediate basis states*, denoted by $|k\rangle$, which are obtained by part diagonalization of H in a series of small subspaces of the Hilbert space, denoted by $\mathcal{G}_l$,

with the label l being integers $0, 1, 2\ldots$. Concretely, the first subspace $\mathcal{G}_0$ is spanned by states $|0\rangle, |1\rangle, \ldots, |n_i - 1\rangle$; $\mathcal{G}_1$ is spanned by states $|n_i\rangle, |n_i + 1\rangle, \ldots, |2n_i - 1\rangle; \ldots$; $\mathcal{G}_l$ is spanned by states $|n_i l\rangle, |n_i l + 1\rangle, \ldots, |n_i l + n_i - 1\rangle; \ldots$, where n_i is a small positive integer for the dimension of the subspaces. The intermediate basis states $|k\rangle$ in the subspace $\mathcal{G}_l$, with $k = n_i l, n_i l + 1, \ldots, n_i l + n_i - 1$, are just the eigenstates of H in the subspace in energy order, respectively. Note that E_k^0 are in energy order only within a subspace $\mathcal{G}_l$. In our partition of H, H_0 and V are taken as

$$H_0 = \sum_k |k\rangle E_k^0 \langle k|, \tag{3}$$

$$V = \sum_{k,k'} |k\rangle V_{kk'} \langle k'|, \tag{4}$$

respectively, where $E_k^0 = \langle k|H|k\rangle$, $V_{kk'} = \langle k|H|k'\rangle$ for $k \neq k'$ and $V_{kk'} = 0$ for $k = k'$. That is, H_0 is the diagonal part of the matrix of H in states $|k\rangle$ and V is the off-diagonal part. In cases of $n_i \geqslant 5$, although there is generally no analytical expression for the nonzero elements of H_0 and V, their numerical calculation is quite easy, when n_i is not large. Denoting the eigenstates and eigenenergies of the Hamiltonian H by $|\alpha\rangle$ ($\alpha = 0, 1, 2, \ldots$) and E_α, respectively, we use the following form of the RS perturbation theory for $\alpha = k$ in the low-energy region.

$$E_\alpha = E_k^0 + \sum_{m=1}^{\infty} \varepsilon_m, \qquad |\alpha\rangle = |k\rangle + \sum_{m=1}^{\infty} |\phi_m\rangle, \tag{5}$$

where $\varepsilon_m = \langle k|V|\phi_{m-1}\rangle$, $|\phi_0\rangle = |k\rangle$, $|\phi_1\rangle = Q_k(V - \varepsilon_1)|k\rangle$ and

$$|\phi_m\rangle = Q_k \left[(V - \varepsilon_1)|\phi_{m-1}\rangle - \sum_{m'=1}^{m-2} \varepsilon_{m-m'} |\phi_{m'}\rangle \right] \tag{6}$$

for $m > 1$. Here $Q_k = \sum_{k' \neq k} |k'\rangle\langle k'|/(E_k^0 - E_{k'}^0)$.

For ground states of the quartic anharmonic oscillator, we have studied the parameter regime of $\mu \leqslant 2$. Numerically it has been found that $|\varepsilon_m|$ decrease rapidly with increasing m (Fig. 1) and partial sums of the two expansions in Eq. (5) approach to finite limits, respectively, when $n_i = 2$ is taken. With the m-axis in Fig. (1) changed to logarithm scale as well, it has been found that $|\varepsilon_m|$ decrease faster than power decay. Table 1 shows some values of E_0 calculated by partial sums in Eq. (5). m_s are the values of m after which the summation of ε_m does not change in numerical calculation, where double-double precision was used for data. For μ between 0.1 and 2.0, results of this Letter are much more accurate than those of Vinette and Čížek [6] and of Janke and Kleinert [19]. Calculation of the eigenfunctions of ground states by

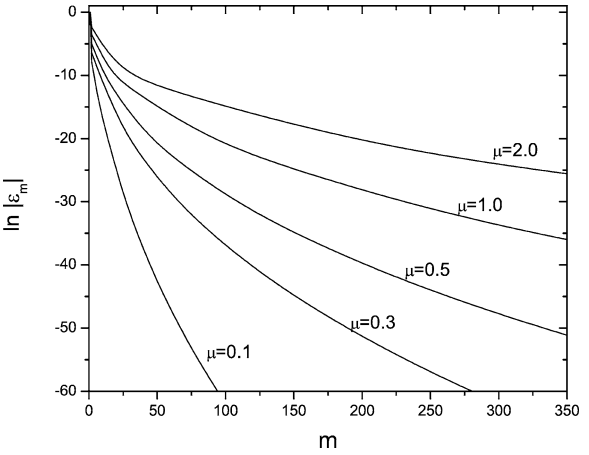

Fig. 1. Values of $|\varepsilon_m|$ in logarithm scale for some ground states of the quartic anharmonic oscillator. (Half of the ε_m, which are equal to zero, are not plotted.) $n_i = 2$ for intermediate basis states.

Table 1
Ground-state energies E_0 calculated by Rayleigh–Schrödinger perturbation expansions in intermediate basis states with $n_i = 2$. The expansions are truncated at m_s numerically. The lines labeled "JK" are results of Ref. [19]. The lines labeled "lb" and "ub" are the lower and upper bounds of Ref. [6]

μ	m_s	E_0
0.1	152	0.559 146 327 183 519 576 715 406 576 920
	JK	0.559 146 344 373 873 126 9
	lb	0.559 146 327 183 519 576 3
	ub	0.559 146 327 183 519 576 7
0.3	500	0.637 991 783 171 278 529 452 523 197 990
	JK	0.637 991 783 171 280 381 8
	lb	0.637 991 783 171 278 528 3
	ub	0.637 991 783 171 278 529 6
0.5	922	0.696 175 820 765 145 927 828 753 938 305
	JK	0.696 175 820 765 145 928 8
	lb	0.696 175 820 765 145 925 1
	ub	0.696 175 820 765 145 928 5
2.0	5268	0.951 568 472 729 500 011 146 925 361 101
	JK	0.951 568 472 729 500 011 146 930 52
	lb	0.951 568 472 729 499 9
	ub	0.951 568 472 729 500 1

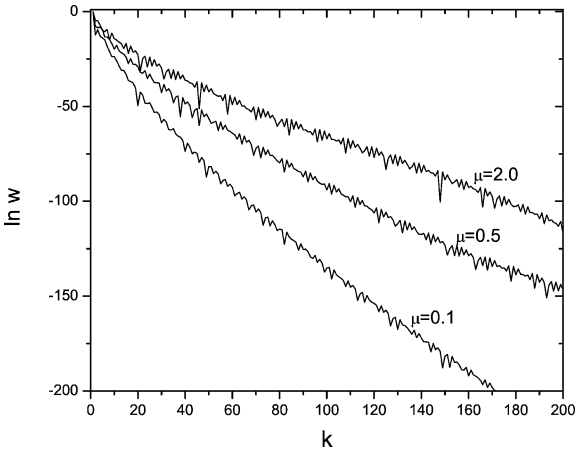

Fig. 2. Shapes of the eigenfunctions of some ground states of the quartic anharmonic oscillator in logarithm scale, $w = |\langle k|\alpha\rangle|^2$. $n_i = 2$ for intermediate basis states.

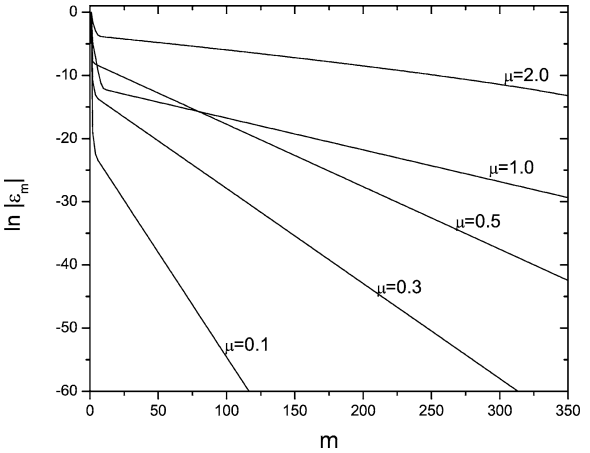

Fig. 3. Same as in Fig. 1, for the 4th excited states of even parity, with $n_i = 20$.

making use of Eq. (5) is as accurate as for the energies, which is much easier and more accurate than the method of Hatsuda, Kunihiro, and Tanaka [8]. Shapes of the eigenfunctions of some ground states are plotted in Fig. 2, where $w_{\alpha k} = |\langle k|\alpha\rangle|^2$. Note that such eigenfunctions are localized, therefore, approximate results can in fact be obtained by numerical diagonalization of sub-matrices of the total Hamiltonian in states $|n\rangle$ of n below some values n_m.

In the calculations discussed above, only states $|k\rangle$ of not large k are involved. When $n_i = 2$, part diagonalization of H in subspaces $\mathcal{G}_l$ can be done analytically and it is possible to discuss the influence of quite large k on the summation of ε_m. When n is large enough, only n^2 terms in $H_{nn'}$ are of interest, which are $H_{nn} \approx 6\mu n^2$, $H_{n,n+1} \approx 4\mu n^2$ and $H_{n,n+2} \approx \mu n^2$. For states $|k\rangle$ and $|k+1\rangle$ with large k in a subspace $\mathcal{G}_l$ spanned by two states $|n\rangle$ and $|n+1\rangle$,

$$E_k^0 \approx 2\mu n^2, \quad E_{k+1}^0 \approx 10\mu n^2, \qquad V_{k,k+2} \approx -\mu n^2, \tag{7}$$

$$V_{k,k+3} \approx -2\mu n^2, \quad V_{k+1,k+2} \approx 2\mu n^2, \qquad V_{k+1,k+3} \approx 3\mu n^2, \tag{8}$$

as a result, the dependence of the related factors $f_{kk'} = V_{kk'}/(E_0^0 - E_k^0)$ on n and μ is negligible. An advantage of taking intermediate basis states is that, for factors in a non-zero product $f_{k_1k_2} f_{k_2k_3} f_{k_3k_4} \cdots$, the limit of the largest geometric mean of $|f_{kk'}|$ is 0.5, smaller than that of $|f_{nn'}| = |H_{nn'}/(H_{00} - H_{nn})|$ with $n \neq n'$, which is $2/3$. Another advantage is that $V_{kk'}$ have both positive and negative signs and $H_{nn'}$ have positive sign only. We have studied RS perturbation expansion for the ground-state energy of a Hamiltonian $\widetilde{H}$ whose non-zero elements are exactly those on the right-hand sides of the approximations in (7) and (8), with the unperturbed Hamiltonian and perturbation taken as the diagonal and off-diagonal parts of $\widetilde{H}$, respectively. It has been found that non-zero $|\varepsilon_m|$ for the ground state of $\widetilde{H}$ has an exponential-type decay, which is close to $(3/4)^m$.

Numerically, partial sums of the expansions in Eq. (5) have been found to converge for low-lying excited states of the quartic anharmonic oscillator as well, when $\mu \leqslant 2$. As an example, Fig. 3 shows $\ln|\varepsilon_m|$ for the 4th excited states of some values of μ, calculated with $n_i = 20$, where the decrease of $|\varepsilon_m|$ is quite close to exponential decay. Similar to the case of ground states, exponential-type decay with increasing k has also been found for the eigenfunctions of low-lying excited states. Relatively high excited states usually need relatively large values of n_i, when μ is fixed.

For the sextic anharmonic oscillator with the term μx^4 in Eq. (1) replaced by μx^6, similar results have also been obtained numerically for both low-lying states and their energies. The convergence of partial sums of the expansions in Eq. (5) for the sextic anharmonic oscillator has been found much slower

Table 2
Same as in Table 1, for $2E_0$ of the sextic and octic anharmonic oscillators, with $n_i = 10$. The lines labeled "W" are results of Ref. [7]

	μ	m_s	$2E_0$
sextic	0.1	18000	1.173 889 345 125 433 152 981 850 087 81
		W	1.173 889 345
		lb	1.173 889 345 117
		ub	1.173 889 345 130
sextic	0.5	18000	1.435 624 619 003 392 316
		W	1.435 624 619
		lb	1.435 624 618 9
		ub	1.435 624 619 1
sextic	2.0	30000	1.830 437 343 750
		W	1.830 437 344
		lb	1.830 437 343 6
		ub	1.830 437 344 4
octic	0.1	30000	1.241 027 91
		W	1.241 03
		lb	1.241 027 88
		ub	1.241 027 94

than in the case of the quartic anharmonic oscillator. Table 2 shows that results of the method here are more accurate than the results of Weniger [7] for ground-state energies of the sextic anharmonic oscillator. The values of m_s in Table 2 were not determined in the same way as in Table 1, but, were taken to be 15000, 18000, and 30000, respectively, due to the slow decay of $|\varepsilon_m|$. (For $\mu = 2.0$, double precision was used for data in the calculation.) Calculation of low-lying states and their energies of the octic anharmonic oscillator, with μx^4 in Eq. (1) replaced by μx^8, can be carried out as well, with results obtained less accurate than for the sextic anharmonic oscillator, due to the even slower decay of $|\varepsilon_m|$. When μ is not large, e.g., $\mu = 0.1$, it is still possible to obtain results a little better than those in Ref. [7], with the summation of ε_m truncated at $m_s = 30000$. Generally to say, when the values of μ are large enough for the three anharmonic oscillators, respectively, methods in Refs. [7,19] should be better than the one here in the calculation of eigenenergies, since the convergence of the expansions there becomes faster, but, the decrease of $|\varepsilon_m|$ here becomes slower (see Figs. 1 and 3), with increasing μ.

In summary, for the quartic, sextic, and octic anharmonic oscillators with not very strong anharmonic terms, we have shown numerical evidence of convergence of the simple Rayleigh–Schrödinger (RS) perturbation expansions for both low-lying eigenstates and the corresponding eigenenergies, when unperturbed Hamiltonians and perturbations are taken as the diagonal and off-diagonal parts of the total Hamiltonians, respectively, in the representation of suitably chosen intermediate basis states. Unperturbed Hamiltonians used here for RS perturbation expansions may be unsolvable analytically, but, numerical calculation can be carried out easily for the elements of both the unperturbed Hamiltonians and the perturbations in intermediate basis states. Rigorous proof of the results found numerically in this Letter is still absent. It should also be worth investigating whether the method used here could be useful in other models where RS quantum mechanical perturbation theory gives divergent expansions.

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