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2007 J. Phys. A: Math. Theor. 40 14457

(http://iopscience.iop.org/1751-8121/40/48/011)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **40** (2007) 14457–14469 doi:10.1088/1751-8113/40/48/011

The multistate Rayleigh–Ritz variational method with the principle of minimal sensitivity for anharmonic oscillators

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Received 12 August 2007, in final form 9 October 2007
Published 14 November 2007
Online at stacks.iop.org/JPhysA/40/14457

Abstract

A theoretical scheme to employ the principle of minimal sensitivity for choosing the optimal values of nonlinear parameters is proposed for the multistate Rayleigh–Ritz variational method. Anharmonic oscillators are particularly considered in this paper. Applications of the present scheme to the one-dimensional Morse and two double-well potentials indicate that it provides much more accurate and faster convergent approximations to the exact energy eigenvalues than several schemes existing in the literatures.

PACS number: 03.65.Ge

1. Introduction

The multistate Rayleigh–Ritz variational method (MSRRVM) [1] is one of the most basic and widely used methods for approximately solving the time-independent Schrödinger equation. Originally, it was proposed and used by Rayleigh in 1873 and Ritz in 1908 for non-perturbatively solving eigenvalue problems of linear differential equations. Naturally, the MSRRVM was applied to quantum systems shortly after quantum mechanics was born [2]. Since then, the MSRRVM has been applied to a great variety of quantum systems with success.

Nevertheless, a perfect and more complete scheme for determining the values of the nonlinear parameters assigned in the MSRRVM is still needed, though the MSRRVM has been being used successfully in quantum theory for about 80 years. This need can be seen from the importance of the nonlinear parameters in the procedure of the MSRRVM and the particularities of those schemes used in the applications of the MSRRVM.

In performing the procedure of the MSRRVM, determination of the value of the nonlinear parameter is an important step. (Here, we are restricted to the single-parameter case for

simplicity.) The nonlinear parameter is contained in the N functions, ϕ_ns, which are extracted by truncating some complete infinite orthonormal set $\{\phi_n\} \equiv \{\phi_0, \phi_1, \phi_2, \ldots\}$. (One can consider a more general set also.) Usually, the nonlinear parameter exists in the functions, ϕ_ns and, in the MSRRVM, is artificially regarded as a parameter to be determined. The N functions, ϕ_ns, are linearly combined to construct a normalized trial wavefunction Ψ:

$$\Psi = \sum_{n=0}^{N-1} C_n \phi_n \tag{1}$$

for a system with a Hamiltonian operator $\hat{H}$, where the coefficients C_n are the linear superposition coefficients. The coefficients C_n can be determined by minimizing $\langle \Psi | \hat{H} | \Psi \rangle$ with respect to C_n, and satisfy the following set of N homogeneous linear equations:

$$\sum_{n=0}^{N-1} (H_{mn} - E^{(N)} \delta_{mn}) C_n = 0, \qquad m = 0, 1, 2, \ldots, N-1 \tag{2}$$

with $H_{mn} \equiv \langle \phi_m | \hat{H} | \phi_n \rangle$, δ_{mn} is the Kronecker symbol and $E^{(N)}$ is the Lagrange undetermined multiplier. It is $E^{(N)}$ that the MSRRVM takes as an approximation to the exact energy eigenvalue of the system. All H_{mn} with $m, n < N$ form a matrix H_N and equation (2) is nothing but its eigenvalue equation with $E^{(N)}$ being the eigenvalue. For non-degenerate cases, the N eigenvalues of H_N, $E_k^{(N)}$s ($k = 0, 1, \ldots, < N$), provide approximate values to the lowest lying N exact energy eigenvalues $E_k^{(\mathrm{exact})}$ ($k < N$) [3]. (When $N = 1$, the MSRRVM approximates the ground-state energy and is the variational method introduced in the textbooks on quantum mechanics.) Obviously, approximations to the exact energies provided by the MSRRVM depend upon the value of the nonlinear parameter. In fact, nontrivial solutions of equation (2) lead to $E^{(N)}$ satisfying the secular equation

$$\mathrm{Det}(H_{mn} - E^{(N)} \delta_{mn}) = 0, \tag{3}$$

where the symbol $\mathrm{Det}(A)$ represents the determinant of the matrix A, and accordingly equation (3) gives the dependence of $E^{(N)}$ on the nonlinear parameter. Therefore, the value of the nonlinear parameter is closely related to the accuracy of the approximations. Furthermore, the MSRRVM can be performed at any N, and a different N gives rise to different approximations $E_k^{(N)}$s. Those successive approximations with various N compose the sequence $\left\{E_k^{(N)}\right\} \equiv \left\{E_k^{(0)}, E_k^{(1)}, E_k^{(2)}, \ldots\right\}$ for every k. $E_k^{(N)}$ in the sequence approaches the kth exact energy eigenvalue $E_k^{(\mathrm{exact})}$ when N tends to the infinity (the interlace theorem) [3, 4]. So the value of the nonlinear parameter is crucial to the convergent speed of the sequence $\left\{E_k^{(N)}\right\}$ to $E_k^{(\mathrm{exact})}$. In a word, the value of the nonlinear parameter greatly affects both the accuracy of the MSRRVM approximations at any given N and the convergent speed of the sequence $\left\{E_k^{(N)}\right\}$ to $E_k^{(\mathrm{exact})}$.

Generally, for any given N, the nonlinear parameter can take any value in its own domain and a different value of it will yield an approximation for $E_k^{(\mathrm{exact})}$ with a different accuracy. It is presumed that, for a given N, there should exist a value, $\mu_{k,\mathrm{exact}}^{(N)}$, of the nonlinear parameter for the MSRRVM which gives rise to $E_k^{(\mathrm{exact})}$, although it cannot be determined exactly. But one can manage to establish a criterion for choosing a value for the nonlinear parameter which approaches $\mu_{k,\mathrm{exact}}^{(N)}$ most closely. Such a chosen value of the nonlinear parameter is called the optimal value. It is believed that, for any given N, the optimal value of the nonlinear parameter will give rise to the best approximation and the fastest convergency to $E_k^{(\mathrm{exact})}$.

In the present paper, we intend to concentrate our attention only on one-dimensional anharmonic oscillators to show the criterion for choosing the optimal value of the nonlinear

parameter more clearly. Various anharmonic oscillators have been investigated with the MSRRVM in the literatures [5–12]. In the context, the aforementioned complete set $\{\phi_n\}$ is usually chosen as the following energy eigenfunctions of a harmonic oscillator:

$$\phi_n(x) = A_n \, \mathrm{e}^{-\mu x^2/2} H_n(\sqrt{\mu}x), \qquad n = 0, 1, 2, \ldots, \tag{4}$$

where $A_n = (\mu/\pi)^{1/4}/\sqrt{2^n n!}$ and $H_n(x)$ the nth-order Hermitian polynomial. In equation (4), the parameter μ is assigned as the aforementioned nonlinear parameter to be determined. We will also be concerned only for this choice, equation (4), in the present paper. In the investigations to anharmonic oscillators with the MSRRVM, in order to choose the optimal value μ_{O} for μ, several criterions or schemes were proposed by employing diagonal elements H_{nn} [5–12]. Among the schemes, the first scheme is to determine μ_{O} by minimizing H_{00} with respect to μ and uses the resultant value of μ_{O} for every dimension N [5]. This scheme of fixing μ_{O} from H_{00} is almost always feasible and has provided good approximate results to the exact energy eigenvalues for symmetrical single-well anharmonic-oscillator potentials [6]. Noticing that the scheme of fixing μ_{O} from H_{00} is not appropriate to the double-well anharmonic-oscillator potential, Balsa *et al* proposed another scheme of minimizing the expectation value H_{nn} $(n < N)$ with respect to both μ and the quantum number n, and consequently produced a good approximation for the double-well anharmonic oscillator [6]. The quantum number n is not a continuously varying quantity, and so Quick and Miller proposed yet another scheme of minimizing the sum of some diagonal elements H_{nn} $(n < N)$ with respect to μ and the scheme provided better approximations than Balsa's scheme [8]. Later in 1989, Bishop *et al* modified Balsa's scheme through minimization of H_{nn} only with respect to μ and by directly fixing $n = N - 1$. The scheme also yielded better approximations than Balsa's scheme [9]. In 2002, Jafarpour and Afshar proposed an optimal squeezed state scheme (similar to the aforementioned scheme of fixing μ_{O} from H_{00}) and provided good approximations [11]. Recently, Van der Straeten and Naudts adopted Bishops' scheme successfully to investigate a double-well anharmonic oscillator in an external field [12]. The above schemes of determining μ_{O} have, with their own peculiarities, played an important role in the successful applications of the MSRRVM.

However, the nonlinear parameter is contained not only in the diagonal elements H_{nn} but also in the off-diagonal elements $H_{mn}(m \neq n)$. Moreover, the final object of the MSRRVM calculation is not the diagonal elements H_{nn}, but $E_k^{(N)}$. Thus, we feel that a more appropriate criterion or scheme is needed in choosing μ_{O}. Such a new scheme is expected to provide more accurate and faster convergent approximations than those schemes existing in the literatures.

Here, in order to choose μ_{O}, we suggest to use the principle of minimal sensitivity (PMS) [13], which has extensively been used in the variational perturbation theory [14, 15]. Based on the PMS, we shall propose a scheme which directly considers the dependence of $E^{(N)}$ upon μ, in which not only the diagonal elements H_{nn} but also the off-diagonal elements H_{mn} $(m \neq n)$ are involved. For checking the accuracy and convergency to $E_k^{(\mathrm{exact})}$, we shall consider the one-dimensional Morse and two double-well anharmonic-oscillator potentials using our scheme. It will be shown that the MSRRVM with the PMS produces much more accurate and faster convergent approximations than the several schemes existing in the literatures.

In the following section, we describe the scheme for determining μ_{O} with the PMS. In section 3, we calculate the matrix elements H_{mn} for a relatively general anharmonic oscillator. H_{mn} for such an anharmonic oscillator has been given by employing creation and annihilation operators in [14], but here we adopt the coordinate representation of the Schrödinger picture. In section 4, energy eigenvalues for some concrete anharmonic oscillators will be calculated using the MSRRVM with the PMS, and their comparisons with the results in [6, 9, 11] will be made for checking the accuracy of the approximations. A conclusion will be made at the end.

2. The scheme of determining μ_{O} based on the PMS

The main spirit of the PMS is that, for an approximation scheme which breaks down the known invariance of the exact result, the 'optimum' approximant is the one that is least sensitive to variations in the unphysical parameters [13]. It was proposed originally for solving the difficulty of the dependency of perturbative results in quantum field theory upon the renormalization schemes [13], and has now been used to determine optimal value of an artificial parameter in the variational perturbation theory [14]. With the aid of the PMS, the variational perturbation theory can provide a good approximation and a fast convergency to the exact quantity and has been applied in quantum field theory, statistical physics, condensed matter physics, quantum mechanics (of course, including the quantum anharmonic oscillators) and quantum chemistry [14–16]. Although the MSRRVM is not a series-expansion technique on the exact energy as the variational perturbation theory is, it still possesses characteristics similar to the series-expansion technique. That is, an approximation from the MSRRVM depends upon the value of the parameter μ which is to be determined. For a different dimension N it provides a different approximation to $E_k^{(\mathrm{exact})}$, and successive approximations produced by it tend to the exact energy which is independent of the parameter μ. So, we expect that the PMS can be employed to choose μ_{O} in the MSRRVM. Actually, the fact that the exact energies for an anharmonic oscillator are invariant with a varying μ can be regarded as 'the known invariance of the exact result' in the PMS. Such an invariance is broken down by the approximation to the exact energies produced by the MSRRVM at any given N. Hence, the parameter μ which does not have the invariance due to the approximation from the MSRRVM can be determined according to the PMS.

From the above brief analysis, the value of μ about which $E^{(N)}$ is most insensitive to variations in μ can be regarded as the optimal value, μ_{O}. As $E^{(N)}$ depends on the value of μ and equation (3) defines the concrete dependence relation at any given dimension N, the most insensitivity of $E^{(N)}$ to μ is expected to yield the most accurate approximations for the exact energy eigenvalues. The independence of $E_k^{(\mathrm{exact})}$s of μ means that all $E_k^{(\mathrm{exact})}$s are constants in the whole domain of μ, and the dependence of the approximation $E^{(N)}$ at any given N on μ implies that $E^{(N)}$ varies when μ varies in its domain. Generally, in the domain of μ, $E^{(N)}$ may vary rapidly at some points and slowly at some other points. Since $E_k^{(N)}$s tend to $E_k^{(\mathrm{exact})}$s eventually with the infinite increase of N and $E_k^{(N)}$s are multi-value solutions of equation (3) for $E^{(N)}$ with $\mu = \mu_{\mathrm{O}}$, $E^{(N)}$ should mimic $E_k^{(\mathrm{exact})}$s as possibly as it can in the aspects of the dependence upon μ. So the value of μ about which $E^{(N)}$ varies most slowly will give rise to the best approximation to $E_k^{(\mathrm{exact})}$s. Therefore, the value of μ determined at a given N according to the PMS should be μ_{O}, the optimal value of μ, which, presumably, gives rise to the most accurate and fastest convergent approximations at the given N to $E_k^{(\mathrm{exact})}$s.

Since μ_{O} is the value in the domain of μ where $E^{(N)}$ varies most slowly with μ, μ_{O} should generally come out of maxima, minima and may be knees of the function $E^{(N)}(\mu)$. Thus, in order to single out μ_{O}, the first step is to find the maxima and the minima, i.e., to find the stationary points μ_S of the function $E^{(N)}(\mu)$, that is to solve the following equation:

$$\left.\frac{\mathrm{d}E^{(N)}(\mu)}{\mathrm{d}\mu}\right|_{\mu=\mu_S} = 0. \tag{5}$$

Note that generally it is difficult to obtain an explicit form of the function $E^{(N)}(\mu)$ from equation (3), and so it is difficult to solve equation (5), too. Nevertheless, a simple derivation can show that equation (5) is equivalent to the condition

$$\left.\frac{\partial D_N(\mu, E^{(N)})}{\partial \mu}\right|_{\mu=\mu_S} = 0, \tag{6}$$

with $D_N(\mu, E^{(N)}) \equiv \mathrm{Det}(H_{mn} - E^{(N)}\delta_{mn})$. Actually, the function $D_N(\mu, E^{(N)})$ has two arguments μ and $E^{(N)}$, and equation (3) defines well the implicit function of μ, $E^{(N)} = E^{(N)}(\mu)$ (assumed). Thus, one has

$$\frac{\mathrm{d}D_N(\mu, E^{(N)})}{\mathrm{d}\mu} = \frac{\partial D_N(\mu, E^{(N)})}{\partial \mu} + \frac{\partial D_N(\mu, E^{(N)})}{\partial E^{(N)}}\frac{\mathrm{d}E^{(N)}}{\mathrm{d}\mu} = 0.$$

Then, employing equation (5), one can handle equation (6). Equation (6) is a binary equation with the unknowns μ and $E^{(N)}$. Because μ and $E^{(N)}$ have to satisfy equation (3), equations (6) and (3) can be grouped into a consistent system of nonlinear equations to determine both μ_S and $E_S^{(N)} \equiv E^{(N)}(\mu_S)$. Now, we note that we can solve the problem by solving the system of equations (6) and (3) for both $E_S^{(N)}$ and μ_S instead of solving equation (5) for μ_S directly. As for solving the system of equations (6) and (3), one can do it with the help of computer application program packages.

The second step of singling out μ_O is to pick up μ_O from the stationary points μ_S. Generally, there exist many pairs of solutions of equations (6) and (3), $\left(E_{S1}^{(N)}, \mu_{S1}\right)$, $\left(E_{S2}^{(N)}, \mu_{S2}\right)$, ..., and every μ_{Sl} in the pairs $\left(E_{Sl}^{(N)}, \mu_{Sl}\right)$ ($l = 1, 2$, and so on) would be negative, positive or even complex. The optimal value μ_O of μ should be positive. Thus, if there is only one pair of solutions, for example $\left(E_{Sj}^{(N)}, \mu_{Sj}\right)$, with $\mu_{Sj} > 0$ among all the pairs of solutions $\left(E_{Sl}^{(N)}, \mu_{Sl}\right)$ ($l = 1, 2$, and so on), then the positive μ_{Sj} is really μ_O. If there exist many pairs of solutions $\left(E_{Si}^{(N)}, \mu_{Si}\right)$ with μ_{Si} ($i = 1, 2, \ldots$) positive, then one can pick up μ_O from them by using the second derivative of $E^{(N)}(\mu)$ with respect to μ, $\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}$. In the same way as done to get equation (6), one has

$$\frac{\mathrm{d}^2D_N(\mu, E^{(N)})}{\mathrm{d}\mu^2} = \left\{2\frac{\partial^2 D_N(\mu, E^{(N)})}{\partial E^{(N)}\partial\mu} + \frac{\partial}{\partial E^{(N)}}\left[\frac{\partial D_N(\mu, E^{(N)})}{\partial E^{(N)}}\frac{\mathrm{d}E^{(N)}}{\mathrm{d}\mu}\right]\right\}\frac{\mathrm{d}E^{(N)}}{\mathrm{d}\mu} + \frac{\partial^2 D_N(\mu, E^{(N)})}{\partial\mu^2} + \frac{\partial D_N(\mu, E^{(N)})}{\partial E^{(N)}}\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2} = 0.$$

Then, employing equation (5), one can obtain the following equation:

$$\left.\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}\right|_{\mu=\mu_S} = -\left.\frac{\partial^2 D_N(\mu, E^{(N)})/\partial\mu^2}{\partial D_N(\mu, E^{(N)})/\partial E^{(N)}}\right|_{\mu=\mu_S}. \tag{7}$$

Thus, one can calculate the value of $\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}$ at any stationary point by using equation (7). If one establishes a two-dimensional coordinate system with μ abscissa and $E^{(N)}$ ordinate, then $E^{(N)}(\mu)$ will be a curve in the coordinate plane $\{\mu, E^{(N)}\}$ and the absolute value of $\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}$ at $\mu = \mu_{Si}$ will be the reciprocal radius of curvature of the curve $E^{(N)}(\mu)$ at $\mu = \mu_{Si}$. Smaller the absolute value of $\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}$ at $\mu = \mu_{Si}$ is, bigger the corresponding radius of curvature is, and accordingly more slowly $E^{(N)}(\mu)$ varies about $\mu = \mu_{Si}$. Hence, for some number j of the positive integer set i with $i = 1, 2, \ldots$, if $\mu = \mu_{Sj}$ makes the absolute value of $\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}$ at $\mu = \mu_{Sj}$ smaller than the value at $\mu = \mu_{Si}$ for all $i \neq j$, then $\mu = \mu_{Sj}$ is the optimal value μ_O of μ. So, in the multi-roots case, one can substitute all the pairs of solutions $\left\{E_{Si}^{(N)}, \mu_{Si}\right\}$ with $\mu_{Si} > 0$ ($i = 1, 2, \ldots$) into equation (7) to calculate the value of $\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}$, and then singles out μ_{Sj} as the optimal value μ_O, where the fixed j satisfies the inequality $\left|\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}\right|_{\mu=\mu_{Sj}}\Big| \leqslant \left|\frac{\mathrm{d}^2E^{(N)}}{\mathrm{d}\mu^2}\right|_{\mu=\mu_{Si}}\Big|$ for all $i \neq j$. A concrete illustration for the procedure of determining μ_O will be given when we discuss the second anharmonic oscillator in section 4.

We want to point out that sometimes, one may encounter two special cases. One case is that there exist no pairs of solutions with μ_{Si} being positive for the system of equations (6) and (3). For this case, one can seek for knees, i.e., the optimal value of μ making $\frac{\mathrm{d}^2 E^{(N)}}{\mathrm{d}\mu^2}\big|_{\mu=\mu_{\mathrm{O}}} = 0$. Another case is that there exist neither stationary points with $\mu_{Si} > 0$ nor knees with $\mu_{Si} > 0$. When the case occurs, one will not be able to find any optimal value of μ at the dimension N in consideration, and have to continue the MSRRVM at the next higher N, a situation analogous to which was met when the principle of minimal sensitivity was applied in the variational perturbation theory of the non-extensive Tsallis statistics [16].

As an end of this section, we stress that the scheme of singling out μ_{O} with the PMS need not be a minimization procedure, which is used both in those schemes for the MSRRVM existed previously in the literatures and in the variational method.

3. The matrix element H_{mn} for an anharmonic oscillator

Anharmonic-oscillator potentials are usually polynomial or exponential functions. In this section, we intend to consider a relatively general anharmonic oscillator with a potential, $V(x)$, having a Fourier representation in a sense of tempered distributions [17]. That is, one can write $V(x)$ as

$$V(x) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega}{\sqrt{2\pi}} \tilde{V}(\Omega)\, \mathrm{e}^{\mathrm{i}\Omega x}. \tag{8}$$

Speaking roughly, this requires that the integral $\int_{-\infty}^{\infty} V(\alpha)\, \mathrm{e}^{-\alpha^2}\, \mathrm{d}\alpha$ is finite. Such a potential covers various polynomial and some exponential potentials. For such a general anharmonic oscillator, we will calculate $H_{mn} = \langle\phi_m|\frac{\hat{p}^2}{2M}|\phi_n\rangle + \langle\phi_m|V(x)|\phi_n\rangle$ in the Schrödinger picture with M, the mass of the oscillator.

For the dynamic part, one can easily get

$$\langle\phi_m|\frac{\hat{p}^2}{2M}|\phi_n\rangle = \frac{\hbar^2}{2M}\frac{\mu}{2}\big[(2n+1)\delta_{mn} - \sqrt{(n+1)(n+2)}\delta_{mn+2} - \sqrt{n(n-1)}\delta_{mn-2}\big]. \tag{9}$$

To calculate the potential part,

$$\langle\phi_m|V(x)|\phi_n\rangle = \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega}{\sqrt{2\pi}} \tilde{V}(\Omega) \int_{-\infty}^{\infty} \phi_m(x)\, \mathrm{e}^{\mathrm{i}\Omega x} \phi_n(x)\, \mathrm{d}x, \tag{10}$$

one can use [18, section 11.4, formula (19), p 198]

$$\int_{-\infty}^{\infty} \mathrm{e}^{-(x-\mathrm{i}a)^2} H_m(x) H_n(x)\, \mathrm{d}x = \sqrt{\pi} 2^m n! (\mathrm{i}a)^{m-n} L_n^{(m-n)}(2a^2) \tag{11}$$

for $m \geqslant n$. Here, the symbol $L_n^{(\alpha)}(x) = \frac{\Gamma(n+\alpha+1)}{n!\Gamma(\alpha+1)}\big[1 + \sum_{j=1}^{n}(-1)^j \frac{n(n-1)\cdots(n-j+1)}{(\alpha+1)(\alpha+2)\cdots(\alpha+j)}\frac{x^j}{j!}\big]$ is a generalized Laguerre polynomial. Actually, equation (11) can be obtained by directly performing the integration through the generating function of the Hermitian polynomials. From equation (11), the potential part can be expressed as

$$\langle\phi_m|V(x)|\phi_n\rangle = A_n A_m 2^m n! \sqrt{\frac{\pi}{\mu}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega}{\sqrt{2\pi}} \tilde{V}(\Omega)\, \mathrm{e}^{-\Omega^2/4\mu} \left(\mathrm{i}\frac{\Omega}{2\sqrt{\mu}}\right)^{m-n} L_n^{(m-n)}\left(\frac{\Omega^2}{2\mu}\right). \tag{12}$$

Substituting the series expression of the generalized Laguerre polynomial into the last equation, one has

$$\langle\phi_m|V(x)|\phi_n\rangle = \sum_{j=0}^{\mathrm{Min}\{m,n\}} \frac{C_n^j C_m^j j!}{\sqrt{m!n!}} (2\mu)^{-\frac{m+n-2j}{2}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega}{\sqrt{2\pi}} \tilde{V}(\Omega)\, \mathrm{e}^{-\frac{\Omega^2}{4\mu}} (\mathrm{i}\Omega)^{(m+n-2j)} \tag{13}$$

with $\mathrm{Min}\{m,n\}$ representing the smaller value between m and n. Finally, using the formula $\int_{-\infty}^{\infty} \mathrm{e}^{-a^2x^2 \pm qx}\,\mathrm{d}x = \mathrm{e}^{\frac{q^2}{4a^2}} \frac{\sqrt{\pi}}{a}$ to perform a Gaussian transform and noting that $V^{(n)}(x) \equiv \frac{\mathrm{d}^n V(x)}{\mathrm{d}x^n} = \int_{-\infty}^{\infty} \frac{\mathrm{d}\Omega}{\sqrt{2\pi}} \tilde{V}(\Omega)(\mathrm{i}\Omega)^n \mathrm{e}^{\mathrm{i}\Omega x}$, one obtains

$$\langle\phi_m|V(x)|\phi_n\rangle = \sum_{j=0}^{\mathrm{Min}\{m,n\}} \frac{C_n^j C_m^j j!}{\sqrt{m!n!}} (2\mu)^{-\frac{m+n-2j}{2}} \int_{-\infty}^{\infty} \frac{\mathrm{d}\alpha}{\sqrt{\pi}} V^{(m+n-2j)}\left(\frac{\alpha}{\sqrt{\mu}}\right) \mathrm{e}^{-\alpha^2}, \tag{14}$$

with C_n^j being the number of combinations.

The sum of equation (9) and equation (14) is H_{mn} for a relatively general anharmonic oscillator, which is consistent with that in [14]. Noticing the integrals $\int_{-\infty}^{\infty} \frac{\mathrm{d}\alpha}{\sqrt{\pi}} \alpha^m \mathrm{e}^{-\alpha^2} = \delta_{m,2n} 2^n (2n-1)!!$ for $m = 0, 1, 2, \ldots$, one can easily get H_{mn} for an anharmonic oscillator with any polynomial potential. For example, one can check that equations (9) and (14) here yield [11, equation (20)] with μ here corresponding to Ω_0 there and [12, equation (6)] with μ here to $\hbar^2/(mr_0^2)$ there. Moreover, for an anharmonic oscillator with the usual exponential potential, the integrals in equation (14) are only Gaussian integrals and are easily carried out. As a matter of fact, for any anharmonic oscillator, so long as the integration in equation (14) can be executed, one can get its H_{mn} from the formulae in this section.

4. Examples and comparisons

We adopt natural units with $\hbar = 1$ and $M = 1$ to carry out computations in this section. For the convenience of comparisons, we apply our scheme to the one-dimensional Morse and two double-well anharmonic oscillators which were discussed in [6, 9, 11, 19]. For every oscillator, at every N in considerations, one can first make Mathematica program according to the scheme stated in section 2 to determine μ_{O}, and then use the standard Mathematica program to compute the eigenvalues of the matrix H_N and get the N approximate energies $E_k^{(N)}$s ($k \leqslant N$). In practical computations on choosing μ_{O}, the number of solutions of equations (3) and (6) increases rapidly with the increase of the dimension N so that our PC (Pentium 4) takes a great deal of time to choose μ_{O}. Therefore, we choose to use the graphic method or some methods which consume less time for solving equations (3) and (6) and singling out μ_{O}, and consequently μ_{O}s singled out here are mostly not quite accurate. This is not a problem because $E_k^{(N)}$s are not sensitive to the variations of μ according to the PSM. Actually, we obtained good approximate results using the not quite accurate values for μ_{O}.

The first application we intend to consider here is to the one-dimensional Morse oscillator with the potential

$$V(x) = D_e(1 - \mathrm{e}^{-\alpha x})^2. \tag{15}$$

This is an asymmetrical single-well potential, and the exact energy eigenvalues for the system have been known. In [11], the Taylor series (equation (23) there) of the potential equation (15) was truncated and kept only the first 23 terms. Here, to get H_{mn}, we need not to truncate the potential as a polynomial. According to equations (9) and (14), performing easily the Gaussian integrals yields

Table 1. Comparison with [11, table 1]. The four lowest energy eigenvalues for the 1D Morse oscillator. For every energy eigenvalue, the first line represents the present calculation and the second line represents [11]. The right column gives the exact energies.

N	10	20	30	50	∞
$\mu_{\rm O}$	16.3832	16.269	14.735	19.699 065	
E_0	9.875 004 716 988 9.880 031 9140	9.875 000 000 061 9.875 001 8376	9.875 000 000 000 9.875 000 0037	9.875 000 000 0000 9.875 000 0000	9.875
E_1	28.875 057 290 915 28.918 707 977	28.875 000 001 217 28.875 033 730	28.875 000 000 000 28.875 000 083	28.875 000 000 0000 28.875 000 000	28.875
E_2	46.878 317 697 654 47.052 872 4878	46.875 000 076 082 46.875 450 6843	46.875 000 000 009 46.875 000 6713	46.875 000 000 0000 46.875 000 0000	46.875
E_3	63.923 569 523 16 64.806 109 6161	63.875 004 736 89 63.877 855 3192	63.875 000 000 05 63.875 003 3686	63.875 000 000 000 63.875 000 0000	63.875

$$H_{mn} = \frac{\hbar^2}{2M}\frac{\mu}{2}[(2n+1)\delta_{mn} - \sqrt{(n+1)(n+2)}\delta_{mn+2} - \sqrt{n(n-1)}\delta_{mn-2}]$$
$$+ D_e\delta_{mn} - 2D_e\sqrt{m!n!}\sum_{j=0}^{\mathrm{Min}\{m,n\}}\frac{(-\alpha)^{m+n-2j}}{j!(m-j)!(n-j)!}(2\mu)^{-\frac{m+n-2j}{2}}\,\mathrm{e}^{\frac{\alpha^2}{4\mu}}$$
$$+ D_e\sqrt{m!n!}\sum_{j=0}^{\mathrm{Min}\{m,n\}}\frac{(-2\alpha)^{m+n-2j}}{j!(m-j)!(n-j)!}(2\mu)^{-\frac{m+n-2j}{2}}\,\mathrm{e}^{\frac{\alpha^2}{\mu}}. \qquad (16)$$

A direct calculation can also give the last equation.

With the help of Mathematica (Version 5.0), taking $\alpha = 1$ and $D_e = 200$, we obtained $E_k^{(N)}$s at various dimensions N for the Morse oscillator with equation (15). The numerical study indicates that at a different N, there exists a different $\mu_{\rm O}$, and generally the accuracy of the results increases with the increase of N. Furthermore, at any given N, the approximate results for the lower lying states are generally more accurate than those for the higher lying states. These characteristics exist also in the approximate results for the other oscillators we will consider later. Table 1 gives the comparison of our results for the four lowest energy eigenvalues with [11, table 1]. In table 1, the right column is the exact energy eigenvalues ($N \to \infty$), and for every energy eigenvalue, the first and second lines correspond to ours and [11, table 1], respectively. Table 1 shows that our approximate results only at $N = 30$ have been at least as accurate as the results at $N = 50$ in [11], and at $N = 20$ and 30, our scheme provides at least three significant figures more accurate results than those in [11]. For example, the relative errors of $E_0^{(20)}$, $E_1^{(20)}$, $E_2^{(20)}$ and $E_3^{(20)}$ produced by our scheme to the corresponding exact energies are 6.2×10^{-12}, 4.2×10^{-11}, 1.6×10^{-9} and 7.4×10^{-8}, respectively, whereas those at $N = 20$ in [11] are 1.86×10^{-7}, 1.168×10^{-6}, 9.6×10^{-6} and 4.47×10^{-5}, respectively. Additionally, we repeated calculations in table 1 of [11] to give more digits. The results indicate that although our result at $N = 50$ is more accurate than the corresponding results in [11]; the differences between them are not big at all. This implies that our method has a fast convergency than the method in [11] and will provide similar accuracy to the method in [11] with a larger N. This characteristic also exists in the next comparisons, tables 2 and 3, for the other potential in [11] and with the method in [9].

Before continuing to the second system, we check the dependence of our approximations in table 1 on the variations of μ. Taking the approximations to the ground-state energy

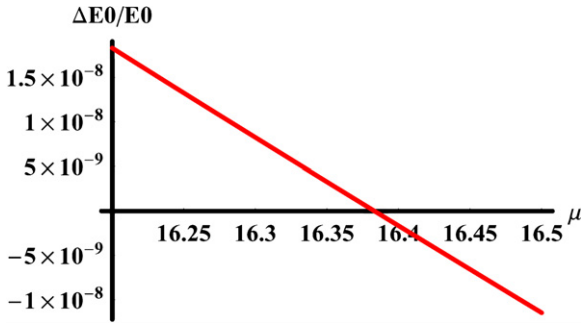

Figure 1. The dependence of the relative error $\frac{E_0^{(N)}(\mu)-E_0^{(N)}(\mu_O)}{E_0^{(N)}(\mu_O)}$ with $N = 10$ upon μ. $\mu_O = 16.3832$. In the figure, $\Delta E0/E0$ represents the relative error.

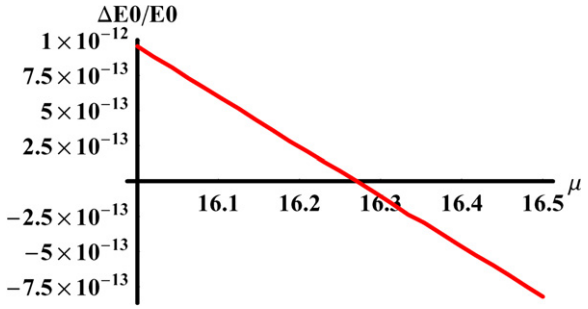

Figure 2. Similar to figure 1 but with $N = 20$ and $\mu_O = 16.269$.

E_0 at $N = 10$ and 20 as examples, we depict the dependence of the relative errors to the approximations $\frac{E_0^{(N)}(\mu)-E_0^{(N)}(\mu_O)}{E_0^{(N)}(\mu_O)}$ upon μ at $N = 10$ and 20 in figures 1 and 2, respectively. In these two figures, $\Delta E0/E0$ represents the relative error. Figure 1 indicates that when μ varies from 16.2 to 16.5, the relative error to $E_0^{(10)}(\mu_O)$ is of the order of 10^{-8} or less. Figure 2 indicates that when μ varies from 16. to 16.5, the relative error to $E_0^{(20)}(\mu_O)$ is of the order of 10^{-13}. Because the relative error of $E_0^{(10)}(\mu_O)$ and $E_0^{(10)}(\mu_O)$ to $E_0^{(\text{exact})}$ is of the order of 10^{-7} and 10^{-12}, respectively, deviation of the value of μ from the true optimal value of μ used in the practical computation is not enough to affect the significant figures of the approximations at the dimensions $N = 10$ and 20 to the two lowest lying energy eigenvalues for the one-dimensional Morse oscillator. This point should be valid for approximations at all dimensions of N to all energy eigenvalues of the one-dimensional Morse oscillator and of other oscillators, so long as the PMS is adopted. So, hereafter we will not discuss the dependence of the approximations upon μ. This insensitivity of the approximations to μ lightens greatly the labor on choosing the optimal value of μ. (One has may be noted that, in figures 1 and 2, the geometrical forms of the curves are not wells and accordingly the values of μ_O we singled out there do not make $E_0^{(10)}$ and $E_0^{(20)}$ minimized. This is understandable, because μ_O is the value of μ, where $E^{(N)}$ is most insensitive to μ, but need not to be the value where $E_0^{(N)}$ is a minimum.)

Table 2. Comparisons with [11, table 2]. The four lowest energy eigenvalues for the double-well oscillator equation (17). For every energy eigenvalue, the first line is for ours and the second line for [11].

N	10	20	30	50	100
μ_O	3.1504	3.7176	4.7453	5.1663	7.011
E_0	1.804 035 016 8424	1.800 813 526 4598	1.800 813 494 6236	1.800 813 494 6206	1.800 813 494 6206
	1.808 714 77	1.800 821 70	1.800 813 51	1.800 813 49	1.800 813 49
E_1	1.899 192 175 1201	1.896 505 447 3860	1.896 505 382 3335	1.896 505 382 3333	1.896 505 382 3333
	1.900 771 31	1.896 507 20	1.896 505 39	1.896 505 38	1.896 505 38
E_2	4.375 442 249 0606	4.370 466 955 4131	4.370 466 726 2303	4.370 466 726 2086	4.370 466 726 2086
	4.385 255 38	4.370 514 70	4.370 466 78	4.370 466 73	4.370 466 73
E_3	5.589 061 669 75	5.573 350 565 91	5.573 350 204 76	5.573 350 204 75	5.573 350 204 75
	5.616 193 58	5.573 382 97	5.573 350 43	5.573 350 20	5.573 350 20

Now we consider the following double-well potential:

$$V(x) = (x^2 - 2)^2, \tag{17}$$

which was also treated in [11].

Before reporting our results for the present potential, in order to illustrate the procedure of determining μ_O in section 2, here we first state how to determine μ_O at the dimension $N = 2$ for the potential equation (17). In this case, equations (3) and (6) yield

$$45 - 192\mu_S + (480 - 72E^{(2)})\mu_S^2 + 8(-61 + 16E^{(2)})\mu_S^3 + 16(13 - 8E^{(2)} + (E^{(2)})^2)\mu_S^4 - 16(-4 + E^{(2)})\mu_S^5 + 3\mu_S^6 = 0$$

and

$$-90 + 288\mu_S + 24(-20 + 3E^{(2)})\mu_S^2 + (244 - 64E^{(2)})\mu_S^3 - 8(-4 + E^{(2)})\mu_S^5 + 3\mu_S^6 = 0,$$

respectively. With the help of Mathematica program, one can find that there are seven pairs of solutions for the system of last two equations, $\left(E_{Sl}^{(2)}, \mu_{Sl}\right)$ $(l = 1, 2, \ldots, 7)$. Among them, there exist four pairs of solutions with μ_{Si} positive $(\{i\} = \{1, 2, \ldots, 4\})$. Then one can substitute the four pairs of solutions $\left\{E_{Si}^{(N)}, \mu_{Si}\right\}$ $(i = 1, 2, 3, 4)$ into equation (7) for the calculation of the value of $\frac{\mathrm{d}^2 E^{(2)}}{\mathrm{d}\mu^2}$, and will find that $\left\{E_{Sj}^{(N)}, \mu_{Sj}\right\} = \{2.469\,207\,154\,862\,0063, 1.088\,699\,919\,167\,7311\}$ gives rise to the smallest value among $\left|\frac{\mathrm{d}^2 E^{(2)}}{\mathrm{d}\mu^2}\right|_{\mu=\mu_{Si}}$|s with $i = 1, 2, 3, 4$. Hence, $\mu_O = 1.088\,699\,919\,167\,7311$, which yields two approximate energies $E_1^{(2)} = 2.469\,207\,154\,864\,083$ and $E_2^{(2)} = 3.067\,890\,021\,771\,4844$ to $E_1^{(\mathrm{exact})}$ and $E_2^{(\mathrm{exact})}$, respectively.

The comparison of our results for the potential equation (7) with [11, table 2] is made in table 2. (In fact, the authors did not use their scheme relevant to H_{00} for choosing μ_O for [11, table 2], as was pointed out in [12].) In table 2, for every energy eigenvalue, the first and second lines correspond to ours and [11, table 2], respectively. In table 2 all the approximations at a given N produced by the present scheme are more accurate than those in [11, table 2] at the same N, only except for $E_3^{(10)}$. Moreover, our approximate results only at $N = 30$ have been as accurate as the results at $N = 50$ in [11, table 2]. Thus, the above two comparisons imply that the scheme with the PMS is effective and appropriate to both the single-well and the double-well oscillators, and can give rise to much more accurate and faster convergent approximations to the exact energy eigenvalues than the scheme of minimizing the diagonal element H_{00}.

Table 3. Comparisons with [9, table 1]. The two energy eigenvalues E_0, E_{38} for the deep double-well potential equation (18). The data of odd columns are from [9, table 1], and in the bottom line, our results are obtained for $N = 201$ and [9]'s for $N = 199$.

N	μ_O	E_0		E_{38}	
1	0.059 995 6809	0.059 995 6809	208.348 332 793 41	208.348 332 793	
19	0.8500	0.567 915 5728	7.377 020 917 0415	8.859 927 521	
39	1.7404	1.141 055 937	5.026 580 037 9050	5.037 280 168	350.550 618 3360	567.110 592 768
59	2.2963	1.676 300 880	4.989 998 032 7601	4.990 015 387	251.113 888 8782	276.881 099 043
79	2.6260	2.166 890 7091	4.989 954 551 2080	4.989 954 561	209.654 744 7627	213.766 610 789
99	3.2664	2.613 343 2046	4.989 954 548 6212	4.989 954 548	184.455 411 5988	187.145 654 479
159	4.5269	3.731 245 9255	4.989 954 548 6210	4.989 954 548	181.943 599 5015	181.943 599 502
201	5.216	4.337 755 7125	4.989 954 548 6210	4.989 954 548	181.943 599 5015	181.943 599 501

Table 4. Comparisons with [19, table 4]. The four lowest energy eigenvalues for the 1D Morse oscillator. In our computations, $N = 31$ and $\mu = 31.8$. For every energy eigenvalue, the left data are for ours and the right data for [19]. The four lowest lying exact energy eigenvalues are 19.75, 57.75, 93.75 and 127.72, respectively.

E_0		E_1	
19.750 000 000 000 018	19.750 000 000 00	57.750 000 000 000 03	57.750 000 000 00
E_2		E_3	
93.750 000 000 000 67	93.750 000 000 00	127.750 000 000 4998	127.750 000 00

The third anharmonic oscillator we consider here is a deep double-well oscillator

$$V(x) = (x^2 - 25)^2. \tag{18}$$

As was introduced in section 1, [9] used a different scheme of choosing μ_O, which modified the scheme in [6], and provided more accurate approximations for the anharmonic oscillator equation (18) than [6]. Here, table 3 gives the comparison of our results with the results in [9, table 1]. In table 3, the data of the even columns are our results and those of the odd columns (except for the first column) come from [9, table 1]. Additionally, in the bottom line of the table, our results are obtained for $N = 201$ (of course, one can consider $N = 199$), and [9]'s for $N = 199$. As it should be, for $N = 1$, our result is identical to that in [9]. At higher dimensions $N \neq 1$, our results are more accurate than those in [9] and accordingly than those in [6]. As mentioned in the first example, our scheme provides much more accurate results than [9] for not a too big N and similar accurate results to [9] for a larger N. This characteristic indicates a fast convergence of our approximation. So, this comparison implies that our scheme can provide better approximations than the scheme of minimizing the diagonal element H_{nn} with $n = N - 1$ in [9].

In the above, we have compared our scheme of determining μ with various schemes in [6, 9, 11]. We noted that for the Morse oscillator, [19] also considered its energy eigenvalues for $\alpha = \sqrt{2}$ and $D_e = 400$ (in terms of notations here) by substituting powers for ϕ_ns in equation (1) and requiring the vanishing finite-boundary condition for Ψ in equation (1). Using the MSRRVM with the PMS, we also compute its four lowest energy eigenvalues for $\alpha = \sqrt{2}$ and $D_e = 400$. Our results are compared with those in [19, table 4]. In table 4, for every energy eigenvalue, the left data are ours and the right are those in [19]. Table 4 indicates that our computation at $N = 31$ provides approximations at least as accurate as those in [19] to the four lowest lying exact energy eigenvalues 19.75,57.75,93.75 and 127.72, respectively.

5. Conclusion

In this paper, by considering anharmonic oscillators, we have proposed a scheme of singling out the optimal value of the nonlinear parameter appeared in the MSRRVM according to the PMS. Through the MSRRVM with the PMS, in which the trial state is expanded in terms of the energy eigenfunctions for a harmonic oscillator, we have approximated the lowest lying energy eigenvalues for the one-dimensional Morse and two double-well oscillators, and compared the resultant approximations with those given by the MSRRVM with other schemes of determining μ_{O} in [6, 9, 11]. Although we have not used μ_{O} with a high accuracy, the comparisons have shown that the MSRRVM with the PMS can provide much more accurate and faster convergent approximations to the exact energy eigenvalues than the MSRRVM does with the schemes of determining μ_{O} relevant to the diagonal elements H_{nn} [6, 9, 11]. Although the schemes of determining μ_{O} relevant to the diagonal elements H_{nn}s are easier to be performed than our scheme based on the PMS which is relevant to all elements H_{mn}s with $m, n \leqslant N$, the insensitivity to μ and the higher accuracy and the faster convergency of our scheme can compensate for it and save labor. Moreover, it is not too difficult to employ high speed computers nowadays, and hence the MSRRVM with the PMS should be helpful and effective for approximating energy eigenvalues of a system.

It seems to us that the PMS is a very useful principle. It has been employed in variational perturbation theory for two decades or so, and now played an effective role in solving the problem of how to determine the value of μ in the MSRRVM for anharmonic oscillators. We feel that for other systems and the general trial wavefunctions equation (1), the PMS can also be employed to determine the values of nonlinear parameters in MSRRVM. Perhaps, for any approximate scheme in which parameters to be determined exist, the PMS can play a role in singling out the values of the parameters.

Acknowledgments

Lu's interest on the present work dates back to his visit in Professor H Kleinert's group at The Institute for Theoretical Physics, Department of Physics, Free University of Berlin and The Institute for Physics and Applied Physics, Department of Physics, Yonsei University in 2002. CKK acknowledges partial support from Korea Science and Engineering Foundation (R01-2006-000-10083-0).

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