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Optimized basis expansion as an extremely accurate technique for solving time-independent Schrödinger equation

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Abstract

We use the optimized trigonometric finite basis method to find energy eigenvalues and eigenfunctions of the time-independent Schrödinger equation with high accuracy. We apply this method to the quartic anharmonic oscillator and the harmonic oscillator perturbed by a trigonometric anharmonic term as not exactly solvable cases and obtain the nearly exact solutions.

Keywords: Schrödinger equation; Anharmonic oscillator; Finite basis method; Variational scheme

Background

Eighty years after the birth of quantum mechanics, the Schrödinger's famous equation still remains a subject of numerous studies, aiming at extending its field of applications and at developing more efficient analytic and approximation methods to obtain its solutions. There has always been a remarkable interest in studying exactly solvable Schrödinger equations. In this sense, the exact solubility has been found for only a very limited number of potentials, most of them being classified already by Infeld and Hull [1] on the basis of the Schrödinger factorization method [2-4]. However, a vast majority of the problems of physical interest do not fall in the above category, and we have to resort to approximation techniques.

The need for such methods have stimulated the development of more sophisticated integration approaches such as embedded exponentially fitted Runge-Kutta [5], dissipative Numerov-type method [6], relaxational approach [7] based on the Henyey algorithm [8], an adaptive basis set using a hierarchical finite element method [9], and an approach based on microgenetic algorithm [10], which is a variation of a global optimization strategy proposed by Holland [11]. We can also mention the variational sinc collocation method [12] and the instanton method [13].

In this paper, we expand the wave function in terms of an orthonormal set of the eigenfunctions of a Hermitian operator, namely, the basis-set expansion method. Indeed, we use the trigonometric basis functions obeying periodic boundary condition. The accuracy of the solutions strongly depends on the domain of the wave function. So, we implement the Rayleigh-Ritz variational method to find the domain's optimal value. The application of this method for the Dirichlet boundary condition is also discussed in [14,15]. Note that an analytic relation for this optimal length is recently presented in [16] which is only applicable for the power low potentials. A two-dimensional application of this method is also discussed in the context of quantum cosmology [17].

The remainder of this paper is organized as follows. In 'The trigonometric basis-set expansion method' Section, we present the underlying theoretical bases for the formulation of the trigonometric basis-set expansion method and the optimization procedures. In Section 'Applications', to illustrate the method, we apply this method for the simple harmonic oscillator (SHO). We then solve two perturbed harmonic oscillators that are not exactly solvable, the first with a quartic anharmonic term, and second with a rapidly oscillating trigonometric anharmonic term. We present our conclusions in the 'Conclusions' Section.

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The trigonometric basis-set expansion method

Let us consider the time-independent one-dimensional Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{1}$$

where m, $V(x)$, and E stand for the reduced mass, potential, and energy, respectively. This equation can be written in the form

$$-\frac{d^2\psi(x)}{dx^2} + \hat{f}(x)\psi(x) = \epsilon\,\psi(x), \tag{2}$$

where

$$\hat{f}(x) = \frac{2m}{\hbar^2}\,V(x), \qquad \epsilon = \frac{2m}{\hbar^2}\,E. \tag{3}$$

As mentioned before, we use the trigonometric basis set to find the energy spectrum. Since we need to choose a finite subspace of a countably infinite basis, we restrict ourselves to the finite region $-L < x < L$. This means that we can expand the solution as

$$\psi(x) = \sum_{i=1}^{2}\sum_{m=0}^{\infty} A_{m,i}\; g_i\left(\frac{m\pi x}{L}\right), \tag{4}$$

where

$$\begin{cases} g_1\left(\frac{m\pi x}{L}\right) = \frac{1}{\sqrt{LR_m}}\sin\left(\frac{m\pi x}{L}\right), \\ g_2\left(\frac{m\pi x}{L}\right) = \frac{1}{\sqrt{LR_m}}\cos\left(\frac{m\pi x}{L}\right), \end{cases} \quad R_m = \begin{cases} 2 & m = 0, \\ 1 & \text{otherwise.} \end{cases} \tag{5}$$

In the above choice of the basis, we are implicitly assuming periodic boundary condition. We can also make the following expansion:

$$\hat{f}(x)\psi(x) = \sum_{i}\sum_{m} B_{m,i}\; g_i\left(\frac{m\pi x}{L}\right), \tag{6}$$

where $B_{m,i}$ are coefficients that can be determined once $\hat{f}(x)$ is specified. By substituting Equations (4) and (6) into Equation (2) we obtain

$$\begin{aligned} \sum_{m,i}&\left[\left(\frac{m\pi}{L}\right)^2 A_{m,i} + B_{m,i}\right] g_i\left(\frac{m\pi x}{L}\right) \\ &= \epsilon \sum_{m,i} A_{m,i}\, g_i\left(\frac{m\pi x}{L}\right). \end{aligned} \tag{7}$$

Because of the linear independence of $g_i(\frac{m\pi x}{L})$, every term in the summation must satisfy

$$\left(\frac{m\pi}{L}\right)^2 A_{m,i} + B_{m,i} = \epsilon\, A_{m,i}. \tag{8}$$

It only remains to determine the matrix B. Using Equations (6) and (4), we have

$$\sum_{m,i} B_{m,i} g_i\left(\frac{m\pi x}{L}\right) = \sum_{m,i} A_{m,i}\hat{f}(x) g_i\left(\frac{m\pi x}{L}\right). \tag{9}$$

By multiplying both sides of the above equation by $g_{i'}(\frac{m'\pi x}{L})$ and integrating over the x-space and using the orthonormality condition of the basis functions, one finds

$$\begin{aligned} B_{m,i} &= \sum_{m',i'} A_{m',i'} \int_{-L}^{L} g_i\left(\frac{m\pi x}{L}\right)\; \hat{f}(x)\; g_{i'}\left(\frac{m'\pi x}{L}\right) \\ dx &= \sum_{m',i'} A_{m',i'} C_{m,m',i,i'}. \end{aligned} \tag{10}$$

Therefore, we can rewrite Equation (8) as

$$\left(\frac{m\pi}{L}\right)^2 A_{m,i} + \sum_{m',i'} C_{m,m',i,i'}\, A_{m',i'} = \epsilon\, A_{m,i}, \tag{11}$$
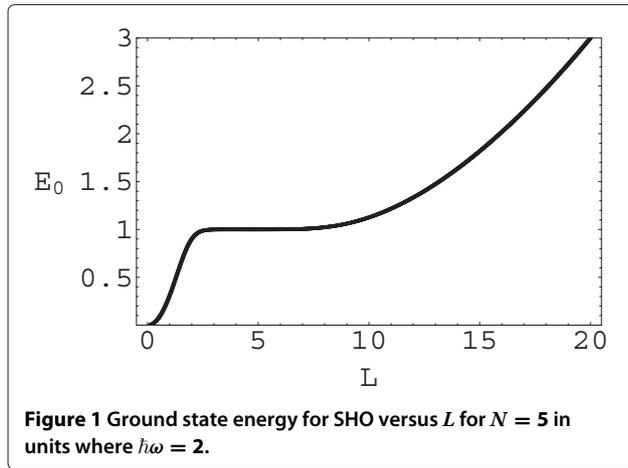
where the coefficients $C_{m,m',i,i'}$ are defined by Equation (10). It is obvious that the presence of the operator $\hat{f}(x)$ in Equation (2) leads to nonzero coefficients $C_{m,m',i,i'}$ in Equation (11), which in principle could couple all of the matrix elements of A. It is easy to see that the more basis functions we include, the closer our solution will be to the exact one. By selecting a finite subset of the basis functions, e.g., choosing the first $2N$ which could be accomplished by letting the index m run from 1 to N in the summations, Equation (11) can be written as

$$DA = \epsilon\, A, \tag{12}$$

where D is a square matrix with $(2N) \times (2N)$ elements. The eigenvalues and eigenfunctions of the Schrödinger equation are approximately equal to the corresponding quantities of the matrix D, that is, the solution to this matrix equation simultaneously yields $2N$ sought after eigenstates and eigenvalues. We are free to adjust two parameters: $2N$ (the number of basis elements used) and $2L$ (the length of the spatial region). This length should be preferably larger than spatial spreading of all the sought-after wave functions. However, if $2L$ is chosen to be too large, we loose overall accuracy. It is important to note that for each N, L has to be properly adjusted. This is in fact the optimization procedure, and we denote this optimal quantity by $\hat{L}(N)$: for a few values of N, we compute $\epsilon(N, L)$ which invariably has an inflection point in the periodic boundary condition. Therefore, all we have to do is to compute the position of this inflection point and compute an interpolating function for obtaining $\hat{L}(N)$.

Applications

In this section, for illustrative purposes, we first apply the optimization procedure to find the bound states of a SHO which is an exactly solvable case. We then apply this method to two perturbed harmonic oscillators, the first with a quartic anharmonic term, and the second with a rapidly oscillating trigonometric anharmonic term.

Figure 1 Ground state energy for SHO versus L for $N = 5$ in units where $\hbar\omega = 2$.

Table 1 The results for the first ten eigenvalues and eigenfunctions of the SHO with $N = 100$

n	ϵ_n^{exact}	Error
0	1	2.6×10^{-139}
1	3	1.1×10^{-133}
2	5	5.9×10^{-134}
3	7	7.5×10^{-129}
4	9	2.2×10^{-129}
5	11	1.5×10^{-124}
6	13	3.1×10^{-125}
7	15	1.3×10^{-120}
8	17	2.4×10^{-121}
9	19	7.1×10^{-117}

Simple harmonic oscillator

The Schrödinger equation for SHO is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi(x) = E\psi(x), \tag{13}$$

where ω is the natural frequency of the oscillator. The dimensionless equation now reads

$$-\frac{d^2\psi(x)}{dx^2} + x^2\psi(x) = \epsilon\psi(x), \qquad \text{where} \qquad \epsilon = \frac{2E}{\hbar\omega}. \tag{14}$$
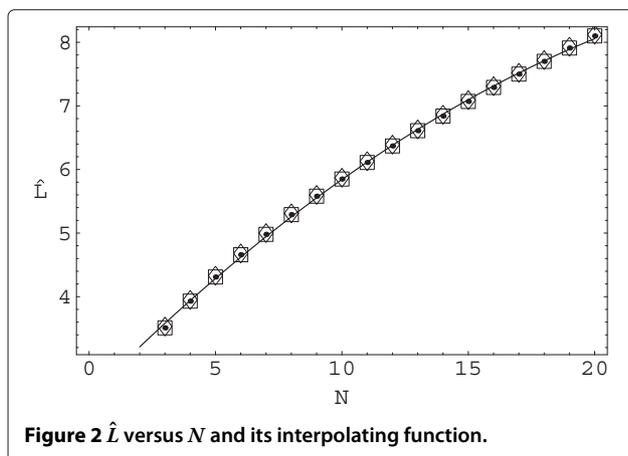
The exact solutions are

$$\psi_n(x) = \left(\frac{\omega}{\pi}\right)^{1/4}\frac{H_n(\sqrt{\omega}x)}{\sqrt{2^n n!}}e^{-\omega x^2/2},$$

$$\epsilon_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, ..., \tag{15}$$

where $H_n(x)$ denote the Hermite polynomials.

In Figure 1, we showed the ground state energy computed for $N = 5$ as a function of L using periodic boundary condition. Note the existence of the inflection point that determines $\hat{L}(5)$. We repeat this procedure for

a few other values of N. After plotting these values, we can obtain an interpolating function $\hat{L}(N)$. In Figure 2, we show our results for $\hat{L}(N)$ and its interpolating function. Having determined $\hat{L}(N)$, we can proceed to compute the bound states. Table 1 shows the results for the first ten energy eigenvalues for $N = 100$. Figure 3 shows the exact and approximate ground state wave functions for $N = \{1, 2\}$ with optimized length $\hat{L} = \{2.52479, 3.04635\}$, respectively.

Anharmonic oscillator with a quartic term

Now, we apply this method to an anharmonic oscillator which has a quartic term. The Schrödinger equation for this not exactly solvable model is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \left(\frac{1}{2}m\omega^2 x^2 + \gamma x^4\right)\psi(x) = E\psi(x). \tag{16}$$

The results that we have obtained using $N = 100$ are extremely accurate (see Table 2). This problem is also

Figure 2 $\hat{L}$ versus N and its interpolating function.

Figure 3 Exact and approximate ground state wave functions of SHO for $N = 1, 2$ with optimized $\hat{L} = \{2.52479, 3.04635\}$, respectively.
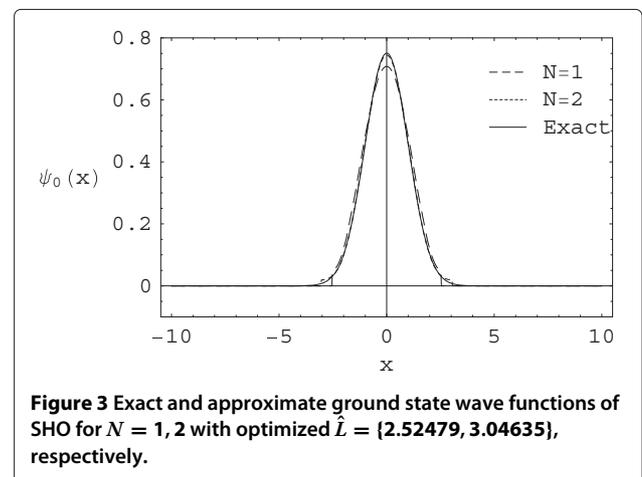
Table 2 First ten energy levels of anharmonic oscillator, the dimensionless form of which is $(-d^2/dx^2 + x^2 + \bar{\gamma}x^4)$ $\psi(x) = \epsilon\psi(x)$, where $\bar{\gamma} = 4\gamma/(m\omega^4) = 0.1$

n	ϵ_n	SD
0	1.06528550954371768885709162878909308430448641781 89	124
1	3.3068720131529135071281216846928690495946552097 516	121
2	5.7479592688335633047335031184771312788809760663 913	120
3	8.3526778257857547121552577346436977053951052605 059	118
4	11.098595622633043011086458749297403250621831282 348	118
5	13.969926197742799300973433956842133961140713634 295	116
6	16.954794686144151337692616508817134375549987258 361	114
7	20.043863604188461233641421107385111570572266905 826	115
8	23.229552179939289070647087434323318243534938599 487	112
9	26.505554752536617417469503006738723676057932189 542	110

We used $N = 100$ basis functions. SD denotes the number of significant digits.

approximately solved using the zero, first, and second order variational Sturmian approximations [18]. Moreover, in [19], the highly accurate results are obtained with 90 significant digits.

Harmonic oscillator perturbed by a rapid oscillation

A rather interesting example is the harmonic oscillator perturbed by a rapid oscillation, the Schrödinger equation of which is given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \left(\frac{1}{2}m\omega^2 x^2 + \alpha\cos(\beta\pi x)\right)\psi(x) = E\psi(x),$$

(17)

where ω is the natural frequency of the oscillator, and α and β are arbitrary constants. This differential equation is not exactly solvable. For large β, the behavior of the potential is very oscillatory and centered around the curve $\frac{1}{2}m\omega x^2$. The results for the ground state are shown in the Figure 4. In the left part of the figure, we showed the full

potential, the ground state wave function, and a zoomed area highlighting the fine structural behavior of the wave function. In the right part of the figure, we showed the ground state energy E_0 versus N. Note that for N smaller than $\beta\hat{L}$ (100 here), this method is not sensitive enough to respond to the rapidly oscillating part of the potential and the results are very close to those of the (unperturbed) SHO. As is apparent from the figure, for N slightly larger than $\beta\hat{L}$, the energy eigenvalue approaches the exact energy eigenvalue as N increases.

It is now worth mentioning the two main advantages of this technique with respect to [16]: First, the method of [16] is only applicable for the bounded power low potentials, but this method works for the general class of the bounded C^∞ potentials. Second, in our method, the potentials do not have to be symmetric. Note that we can obtain arbitrary accuracy by increasing the number of the basis functions. But, the speed of the calculation decreases due to the presence of large matrices. Indeed, one of the time consuming parts of the algorithm is finding the coefficients $C_{m,m',i,i'}$ that are defined by Equation (10). One advantage of our method with respect to other spectral methods such as Chebyshev spectral method is that these coefficients can be obtained analytically before numerical diagonalization of the Hamiltonian for a large class of potentials.

Conclusions

We have used the optimized trigonometric finite basis method as an extremely accurate technique to obtain energy eigenvalues and eigenfunctions of the bound states of the time-independent Schrödinger equation. The optimization procedure is based on the presence of an inflection point in the plot of the energy eigenvalue versus the domain of the basis. We applied this method to the quartic anharmonic oscillator case which is not exactly solvable and found the solutions with high accuracy. Also, we solved the problem of SHO perturbed by a trigonometric anharmonic term and showed how the
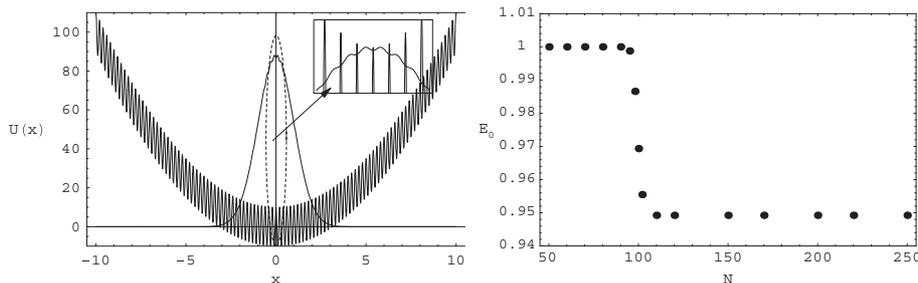
Figure 4 Potential of harmonic oscillator perturbed by rapid oscillations and ground state energy versus *N*. (left) Potential of the harmonic oscillator perturbed by rapid oscillations, the dimensionless Schrödinger equation of which is $(-d^2/dx^{2y} + x^2 + \alpha'\cos(\beta'\pi x))\psi(x) = E'\psi(x)$. We have chosen the parameters $\beta' = \sqrt{2/m}\beta/\omega = 10$ and $\alpha' = (2/\hbar\omega)\alpha = 10$. Superimposed on the same graph is the ground state wave function calculated with $N = 150$. (right) The ground state energy versus N.

optimization scheme properly handles problems involving potentials with rapid oscillations.

Authors' contributions

PP and SSG developed the theoretical part. PP and MM carried out the computational part and performed the calculations. All authors read and approved the final manuscript.

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