Accurate energy spectrum for power-law potentials with trigonometric basis: The optimal length

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We propose an optimal length for accurate calculation of eigenvalues and eigenfunctions of power-law potentials with trigonometric basis functions. We show that, this proposal make us free from using the variational procedure which promotes this method as one of the most accurate and efficient techniques for finding the energy spectrum of anharmonic oscillators.

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I. INTRODUCTION

Eighty years after the birth of quantum mechanics, the Schrödinger's famous equation

$$\mathcal{H}\Psi = E\Psi, \tag{1}$$

still remains a subject for numerous studies, aiming at extending its field of applications and at developing more efficient analytic and approximation methods for obtaining its energy eigenvalues and its stationary states. The interest in this subject ranges from various branches of physics to chemistry.

This has been the driving force behind the development of perturbative and non-perturbative methods for this kind of problems. Among them are the semiclassical approximation [1], finite-difference technique [2], hypervirial recurrence relation scheme [3], renormalized hypervirial-Padè scheme [4], variational matrix solution [5], Rayleigh-Ritz variational method supplemented by the Lanczos algorithm [6], Brillouin-Wigner perturbation theory based on shifted oscillator variational functions [7], instanton method [8, 9], transfer matrix method [10], uniform approximation of the logarithmic derivative of the ground state eigenfunction [11], and many other specific methods.

Various variational methods are usually used in quantum mechanics, statistical mechanics and field theory. In quantum mechanics, variational parameters are incorporated into trial wave functions and trial Hamiltonians. The *Rayleigh-Ritz* method is the minimization of the ground state energy with respect to these variational parameters. The applications of this formalism using various set of basis such as harmonic-oscillator [12], Chebyshev polynomials [13], hypervirial theorems [14], and the coherent states [15], have been already appeared in the literature.

In Refs. [16, 17], it was shown by numerical results that the trigonometric basis functions which obey Dirichlet boundary condition $\Psi(-L) = \Psi(L) = 0$, where L is the domain of the basis set, can be effectively used to find the spectrum of an unbounded problem. They showed that, the low lying energy levels $E_n(L)$ are equal to those of $L = \infty$ with high accuracy, if the boundedness parameter L is in near vicinity of the optimal length L_{op}. In fact, they have employed the *Rayleigh-Ritz* variational method with the particle-in-a-box basis set in order to find the optimal lengths related to the anharmonic oscillators. They showed that the trigonometric functions are a suitable basis set in variational calculations which result in the highly accurate results. Moreover, the model is simple, fast-convergent, and works for various kind of potentials.

Recently, it was shown that the usage of trigonometric basis functions which obeying periodic boundary condition $\Psi(-L) = \Psi(L)$ results in more accurate solutions with respect to Dirichlet boundary condition [18]. This is due to the fact that the Dirichlet boundary condition enforces the wave function to vanish at $x = \pm L$, but the periodic boundary condition lets the wave function to fit itself more closer to the exact solution which is not necessarily zero at the boundaries. Therefore, using the periodic boundary condition, the same accuracy can be obtained with the smaller number of the basis functions.

In this paper, first we diagonalize the Hamiltonian of the anharmonic oscillators using the trigonometric basis functions obeying Dirichlet boundary condition. Then, we propose an analytic relation between the optimal length and the number of the basis functions. Therefore, we do not need the variational procedure and we obtain a simple, efficient, and accurate method for solving anharmonic oscillators.

II. DIAGONALIZATION OF THE HAMILTONIAN

Let us consider the following dimensionless time-independent one-dimensional Schrödinger equation

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\Psi(x) = E\Psi(x), \tag{2}$$

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where $V(x)=\sum_{i=1}^{M} a_{2i}x^{2i}$. Since the potential is an even function of x, to avoid large matrices, we can use even and odd basis functions separately

$$\phi_m(x)=\sqrt{\frac{1}{L}}\cos\left[\left(m-\frac{1}{2}\right)\frac{\pi x}{L}\right],\ m=1,2,3,... \quad (3)$$

and

$$\phi_m(x)=\sqrt{\frac{1}{L}}\sin\left(\frac{m\pi x}{L}\right), \qquad m=1,2,3,... \quad (4)$$

for even and odd parity solutions, respectively. Now, we can expand the solution using these orthonormal basis sets

$$\Psi(x)=\sum_m A_m\phi_m(x), \quad (5)$$

where the wave function satisfies the Dirichlet boundary condition $\Psi(L)=\Psi(-L)=0$. Moreover, the wave function should be the solution of the Schrödinger equation which results to the secular equations

$$\sum_{n=1}^{\infty}(H_{mn}-E\delta_{mn})A_n=0, \qquad m=1,2,3,... \quad (6)$$

where δ_{mn} is the Kronecker's delta and H_{mn} are the matrix elements defined by

$$H_{mn}=-\left\langle\phi_n,\frac{d^2\phi_m}{dx^2}\right\rangle+\sum_{i=1}^{M}a_{2i}\left\langle\phi_m,x^{2i}\phi_n\right\rangle. \quad (7)$$

We can evaluate the inner products using the basis functions (3,4)

$$H_{mn}=\left(m-\frac{1}{2}\right)^2\frac{\pi^2}{L^2}\delta_{mn} + \sum_{i=1}^{M}a_{2i}\left(\frac{L}{\pi}\right)^{2i}\left(D^{(i)}_{m+n-1}+D^{(i)}_{m-n}\right), \quad (8)$$

for even states and

$$H_{mn}=\frac{m^2\pi^2}{L^2}\delta_{mn} + \sum_{i=1}^{M}a_{2i}\left(\frac{L}{\pi}\right)^{2i}\left(D^{(i)}_{m-n}-D^{(i)}_{m+n}\right), \quad (9)$$

for odd states, where $D_k^{(i)}$ is defined by

$$D_k^{(i)}=\frac{1}{\pi}\int_0^{\pi}x^{2i}\cos(kx)dx, \quad (10)$$

which explicitly takes the following form

$$D_k^{(i)}=\sum_{p=0}^{i-1}\frac{(-1)^{p+k}}{k^{p+1}}\begin{pmatrix}2i\\2p+1\end{pmatrix} \times(2p+1)!\,\pi^{2(i-1-p)},\ k>0, \quad (11)$$

$$D_k^{(i)}=\frac{\pi^{2i}}{2i+1}, \qquad k=0. \quad (12)$$

Therefore, the eigenvalues and eigenfunctions of the Schrödinger equation (2) are equal to the corresponding quantities of the matrix H.

In practice, we choose $2N$ (N even and N odd) basis functions to obtain the desired accuracy. On the other hand, the accuracy crucially depends on the domain of the basis functions L. In fact, we need to look for the optimal length L_{op} which results in the maximum accuracy for each N. So, we should repeat the diagonalization procedure many times (variational procedure) to find the optimal length which minimizes the energy eigenvalues. However, the variational part is much time consuming especially for large values of N which prevents this method from being considered as a popular differential equation solver. In the next section, for the case of power-law potentials, we propose an analytic relation between the optimal length and the number of the basis function which makes us free from the variational part of the method.

III. THE OPTIMAL LENGTH

From Eqs. (3,4) is apparent that there should exist an optimal length which minimizes the Hamiltonian. This is due to the fact that the average potential energy goes to infinity as $L\to\infty$. Also, the average kinetic energy behaves in the same manner as $L\to 0$. So, a balanced finite estimate of each of these quantities would require a nonzero finite L.

The usage of the trigonometric basis functions is equivalent with putting the potentials in an infinite potential well *i.e.* $V(x)=\sum_{i=1}^{M}a_{2i}x^{2i}$ for $|x|<L$ and $V(x)=\infty$ elsewhere. Since for $|x|\geq L$ this model is not identical with the original one, the particle-in-a-box basis functions with energies larger than $V(L)$ would not have a useful contribution to the sought-after solutions. So, we propose a rough criterion between the cut-off N and the optimal domain of the basis functions L_{op}

$$V(L_{op})=\alpha\frac{N^2\pi^2}{L_{op}^2}, \quad (13)$$

where α only depends on the form of the potential. Calculations show that the actual optimal length for various power-law potentials agrees well with the above relation. In fact, for the potential in the form $V(x)=\beta x^{2M}$ we obtain

$$L_{op}=\frac{\sqrt{2\pi}}{\beta^{\frac{1}{2(M+1)}}}\left(\frac{N}{2^M}\right)^{\frac{1}{M+1}}, \quad (14)$$

which corresponds to $\alpha=(\pi/2)^{M-1}$ in Eq. (13). In figure 1, we have shown the calculated optimal lengths for $M=1,2,3,4$. As the figure shows there is a complete correspondence between the calculated ones using the variational procedure and using relation (14).

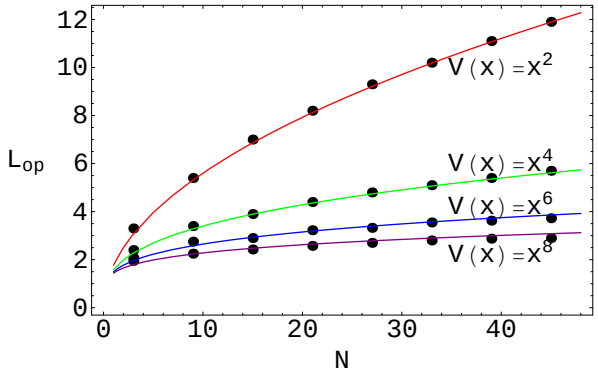

FIG. 1. The optimal length versus the number of basis using the variational procedure (circles), and using Eq. (14) for $i = 1, 2, 3, 4$.

Now, consider a general polynomial potential $V(x) = \sum_{i=1}^{M} a_{2i} x^{2i}$. Since α depends on i, we cannot simply use Eq. (13) for the polynomial potential. However, for large values of N, its energy spectrum approximately coincides with $V(x) = a_{2M} x^{2M}$. So, for the general polynomial potential, the relation (14) is valid for $N \gg 1$ with $\beta = a_{2M}$. On the other hand, since the variational part is inefficient and too much time consuming for large N, the validness of (14) is so useful.

Note that, for the case of the periodic boundary condition, there is not exists a true minimum value in the graph of the energy versus the domain of basis functions [18]. In fact, because of the nature of the boundary condition, we observe an inflection point instead of a minimum value at the optimal length. On the other hand, contrary to the Dirichlet boundary condition, the wave function is not forced to vanish at the boundaries. Since for the large values of the optimal length the exact wave function is almost zero at the boundaries, we expect that the difference between the results of these two boundary conditions would not be significant for large L_{op}. So, we can also use the relation (14) for the periodic boundary condition with large N.

Now, to find the validness limit of equation (14), let us consider the particle in a box with size 2 as an extreme exact solvable case. This potential is equivalent with $V(x) = \beta x^{2M}$ where $M = \infty$. It is obvious that the actual optimal length for this problem is $L_{op} = 1$ for all N. However, the predicted length using Eq. (14) is $\sqrt{\pi/2} = 1.25331$. Therefore, the relation (14) is not accurate for the potentials with large exponent ($M \gg 1$).

IV. CONCLUSIONS

We proposed a prescription for finding the optimal length in order to accurately calculate the eigenvalues and eigenfunctions of power-law potentials using the trigonometric basis functions. We showed that, using this prescription, the highly accurate results can be obtained at the first run of the diagonalization scheme without using the variational procedure. Also, it is shown that, the proposed optimal length relation is not valid for the potentials with large exponent.

[1] S. Y. Slavyanov, *Asymptotic Solutions of the One-Dimensional Schrödinger Equation* (American Mathematical Society, Providence, 1996).
[2] M. R. M. Witwit, J. Phys. A **25**, 503 (1992).
[3] R. J. Hodgsonand and Y. P. Varshni J. Phys. A **22**, 61 (1989).
[4] M. Bansal, S. Srivastava, and Vishwamittar, Phys. Lett. A **44**, 8012 (1991).
[5] R. Balsa, M. Plo, J. Esteveand and A. Pacheco, Phys. Rev. D **28**, 1945 (1983).
[6] R. Bishop, M. Flynn, M. Bosca and R. Guardiola, Phys. Rev. A **40**, 6154 (1989).
[7] F. Arias de Saavedra and E. Buendia, Phys. Rev. A **42**, 5073 (1990).
[8] H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics* (World Scientific, Singapore, 1990), Chap. 17.
[9] E. Gildener and A. Patrascioiu, Phys. Rev. D **16**, 423 (1977); S. Coleman, Phys. Rev. D **15**, 2929 (1977); G. Álvarez, J. Math. Phys. **45**, 3095 (2004).
[10] Z. Cao, Q. Shen, and F. Zhou, Phys. Rev. A **67**, 062112 (2003).
[11] A. Turbiner, Lett. Math. Phys. **74**, 169 (2005).
[12] J. Killingbeck, Phys. Lett. A **84**, 95 (1981).
[13] J. P. Boyd, J. Math. Phys. **19**, 1445 (1978).
[14] R. J. Swenson and S. H. Danforth, J. Chem. Phys. **57**, 1734 (1972).
[15] C. S. Hsue and J. L. Chern, Phys. Rev. D **29**, 643 (1984).
[16] H. Taşeli, J. Comput. Phys. **101**, 252 (1992); Int. J. Quantum Chem. **46**, 319 (1993).
[17] A. Chandra and K. Bhattacharyya, Pramana J. Phys. **43**, 117 (1994); R. K. Pathak and K. Bhattacharyya, Int. J. Quantum Chem. **54**, 13 (1995); Chem. Phys. Lett. **230**, 437 (1994); R. K. Pathak, A. K. Chandra, and K. Bhattacharyya, Phys. Rev. A **48**, 4097 (1993); Phys. Lett. A **188**, 300 (1994); K. Bhattacharyya and R. K. Pathak, Int. J. Quantum Chem. **59**, 219 (1996).
[18] P. Pedram, M. Mirzaei, and S. S. Gousheh, Molecular Physics **108**, 1949 (2010).