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## Variational method for approximating energy levels

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We present here a systematic scheme for improving the variational wave functions and corresponding energy levels for quantum systems. By expanding the wave function around a variational parameter value, a family of independent functions can be systematically generated. The eigenstates are then obtained by diagonalizing the Hamiltonian matrix within the basis and optimized with respect to the variational parameter. As a test, the ground state of the quartic anharmonic oscillator has been investigated, and it is found that this scheme converges more rapidly than the conventional Lanczos method and yields better approximations of the energy levels than other variational methods. The effectiveness of this scheme for larger systems remains to be seen.

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Recently Stubbins and Das [1] introduced a systematic scheme for improving any variational wave function. Their work is based on the introduction of a set of variational parameters in a trial wave function to form a family of independent functions. These functions are then used to construct a basis for the variational method. This scheme was applied to two models with great success: the quartic anharmonic oscillator [2–4] and the Mathieu equation [5]. It was found that, starting with the same trial wave function, this variational approach converges considerably faster than moments methods.

In this paper we wish to investigate this variational method in detail and propose an improved variational scheme which not only has the benefit of fast convergence, but also eliminates the possible numerical instabilities which may occur in the original work.

First we review briefly the Stubbins-Das (SD) method. As is well known [6] the variational method is based on the construction of a trial wave function from a linear combination of $N$ (independent) functions $\psi_j$

$$\Psi = \sum_{j=1}^{N} c_j \psi_j \tag{1}$$

with the expansion coefficients $c_j$ determined from the system of equations

$$\sum_{j=1}^{N} (\langle \psi_i | H | \psi_j \rangle - \varepsilon \langle \psi_i | \psi_j \rangle c_j) = 0, \quad i = 1, 2, ..., N. \tag{2}$$

Here the Dirac bra-ket notation is invoked and $H$ represents the Hamiltonian for the system. The vanishing of the secular determinant is a necessary and sufficient condition for a nontrivial solution

$$\det |H_{ij} - \Delta_{ij} \varepsilon| = 0 \tag{3}$$

with the notation

$$H_{ij} \equiv \langle \psi_i | H | \psi_j \rangle, \qquad \Delta_{ij} \equiv \langle \psi_i | \psi_j \rangle. \tag{4}$$

Accordingly these $N$ equations will generate upper bounds to the exact energies of the system. The trial wave function is usually chosen on physical grounds as well as calculational efficacy and is a crucial factor in determining the rate of convergence.

In the SD method, instead of using a single variational parameter $\beta$ in the trial wave function $\Psi = \Psi(\beta, x)$, a set of variational parameters $\{\beta_i\}$ is introduced to form a set of independent basis functions:

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$$\begin{aligned}\Psi_1 &= \Psi(\beta_1, x)\ ,\\ \Psi_2 &= \Psi(\beta_2, x)\ ,\\ &\vdots\\ \Psi_N &= \Psi(\beta_N, x)\end{aligned} \tag{5}$$

with $\beta_i \neq \beta_j$. Thus for a basis constructed of $N$ basis states there are $N$ variational parameters $\beta_1, \beta_2, \ldots, \beta_N$ that must be determined in order to obtain the energies of the system. This multidimensional minimization procedure is typically time consuming. A simplification introduced by Stubbins and Das is based on the observation that consecutive $\beta_i$'s are approximately evenly spaced, i.e., $\beta_{i+1} - \beta_i = \delta = \text{const}$. Therefore the problem can be reduced to minimizing the eigenvalues of $H$ with respect to $\beta_1$ and $\delta$. The SD method has been shown to be effective [1] in obtaining the solutions of the quartic anharmonic oscillator model and the Mathieu equation.

However, it has been noticed that as the basis set increases, a numerical instability develops [7, 8] in the SD method. This hampers its application to some other systems as the numerical problem may appear before a reasonable approximation to the energy levels can be reached. In order to achieve a better understanding of this instability, let us examine the second basis function $\Psi_2(\beta_2, x)$ constructed using the SD method:

$$\begin{aligned}\Psi_2(\beta_2, x) &= \Psi_1(\beta + \delta, x)\\ &= \Psi_1(\beta, x) + \frac{\partial \Psi_1(\beta, x)}{\partial \beta}\delta\\ &\quad + \frac{1}{2!}\frac{\partial^2 \Psi_1(\beta, x)}{\partial \beta^2}\delta^2 + \cdots\ ,\end{aligned} \tag{6}$$

where the subindex of $\beta_1$ has been omitted for simplicity. Since any trial wave function $\Psi_1$ chosen on physical grounds is already a good approximation, the true wave function should have little difference from $\Psi_1$. As a result, the value of $\delta \equiv \beta_2 - \beta$ is typically very small (which has been observed by Stubbins and Das); therefore in Eq. (6) $\Psi_2(\beta_2, x)$ is dominated by $\Psi_1(\beta, x)$. This implies that the basis vectors constructed in the SD method are almost linearly dependent on one another, which in turn gives rise to numerical instabilities in solving the secular equation of Eq. (3). Ironically, the problem becomes prominent if the initial trial wave function is chosen to be very close to the true wave function.

Close examination of Eq. (6) offers an efficient and numerically stable scheme of generating a set of variational basis functions:

$$\begin{aligned}\Psi_2(\beta, x) &= A_2(\beta)\frac{\partial \Psi_1(\beta, x)}{\partial \beta}\ ,\\ \Psi_3(\beta, x) &= A_3(\beta)\frac{\partial^2 \Psi_1(\beta, x)}{\partial \beta^2}\ ,\\ &\vdots\\ \Psi_N(\beta, x) &= A_N(\beta)\frac{\partial^{N-1} \Psi_1(\beta, x)}{\partial \beta^{N-1}}.\end{aligned} \tag{7}$$

As in the SD method, this basis set can be expanded systematically. However, the basis functions constructed in Eq. (7) have several important properties which are absent in the SD basis set. First of all, even though they do not form an orthogonal basis, the overlap of any two functions $\langle \Psi_i | \Psi_j \rangle (i \neq j)$ has a finite difference from 1 for any variational parameter value. Thus there is little risk of encountering numerical instabilities. Second, the second variational parameter $\delta$ in the SD scheme has been eliminated. This parameter $\delta$ was introduced *empirically* by Stubbins and Das based on the observation that optimized $\beta_i$'s are approximately evenly spaced for the couple of simple models which have been studied. However, there is no justification that this assumption is true for other quantum systems as well. In the basis set constructed using Eq. (7), there is no empirical parameter. Hence this offers a variational approach which is not model dependent. In addition, $\beta$ is the only variational parameter that remains, and thus the computational effort may be greatly reduced.

To illustrate this improved variational approach, we investigate the ground state energy of the quartic anharmonic oscillator system [2–4], which has been studied by Stubbins and Das [1]. The Hamiltonian of the system has the form

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 + \lambda x^4. \tag{8}$$

Here we use $\lambda = 1$ in order to make direct comparison. For even-parity states, the first trial wave function is chosen as

$$\Psi_1 = A_1 e^{-\beta^2 x^2/2} \tag{9}$$

with normalization constant

$$A_1 = \sqrt{\frac{\beta}{\sqrt{\pi}}}. \tag{10}$$

Following Eq. (7), the subsequent variational basis functions can be constructed by examining the derivatives of $\Psi_1$:

$$\begin{aligned}\frac{\partial \Psi_1(\beta, x)}{\partial \beta} &= -\beta x^2 \Psi_1 + \frac{\partial A_1}{\partial \beta}\Psi_1\ ,\\ \frac{\partial^2 \Psi_1(\beta, x)}{\partial \beta^2} &= -x^2 \Psi_1 + \beta^2 x^4 \Psi_1 + \frac{\partial^2 A_1}{\partial \beta^2}\Psi_1 + \frac{\partial A_1}{\partial \beta}\frac{\partial \Psi_1}{\partial \beta}\ ,\\ &\vdots\ .\end{aligned} \tag{11}$$

To further reduce the overlapping among the basis functions, the following basis set is conveniently chosen:

$$\begin{aligned}\Psi_1 &= A_1 e^{-\beta^2 x^2/2}\ ,\\ \Psi_2 &= A_2 x^2 e^{-\beta^2 x^2/2}\ ,\\ \Psi_3 &= A_3 x^4 e^{-\beta^2 x^2/2}\ ,\\ &\vdots\\ \Psi_i &= A_i x^{2(i-1)} e^{-\beta^2 x^2/2}\ ,\end{aligned} \tag{12}$$

where the normalization constants are

$$A_i = \sqrt{\frac{\beta}{\sqrt{\pi}}}\frac{(2\beta^2)^{i-1}}{\sqrt{(4i-5)!!}}, \qquad i = 1, 2, 3, \ldots \tag{13}$$

with the definition

$$(-1)!! = 0!! \equiv 1. \tag{14}$$

The overlap between any two functions in Eq. (12) has the simple expression

$$\langle \Psi_i | \Psi_j \rangle = \frac{[2(i+j)-5]!!}{\sqrt{(4i-5)!!(4j-5)!!}}, \qquad i \neq j. \tag{15}$$

The Hamiltonian matrix can be derived as

$$\begin{aligned}\langle \Psi_i | H | \Psi_j \rangle = & \frac{[2(i+j)-5]!!}{\sqrt{(4i-5)!!(4j-5)!!}} \\ & \times \left\{ \frac{\beta^2}{2} + \frac{4(i-1)(j-1)\beta^2}{[2(i+j)-5]} \right. \\ & + [2(i+j)-3] \frac{(1-\beta^4)}{4\beta^2} \\ & \left. + [2(i+j)-1][2(i+j)-3] \frac{\lambda}{4\beta^4} \right\}. \end{aligned} \tag{16}$$

The energy levels are then obtained by solving Eqs. (3), (15) and (16). The calculations have been carried out for different numbers of wave functions. In Table I the optimized $\beta$ and the ground state energy are listed, along with the energies from SD variational scheme and the Lanczos method [1]. It is seen that in general, the energy convergence rate using the improved variational scheme is about the same as that for SD and significantly faster than the Lanczos method.

TABLE I. The optimized variational parameter $\beta$ and the ground state energy calculated with $N$ basis functions using the improved variational scheme, the SD variational scheme, and the Lanczos method ($\lambda = 1$).

| $N$ | $\beta$ | Energy | SD [1] | Lanczos [1] |
|---|---|---|---|---|
| 1 | $\sqrt{2}$ | 0.8125 | 0.8125 | 0.8125 |
| 2 | 1.20373208 | 0.80741457 | 0.80417482 | 0.8049 |
| 3 | 1.54020553 | 0.80383857 | 0.80380029 | 0.80405 |
| 4 | 1.74680518 | 0.80377315 | 0.80377316 | 0.803803 |
| 5 | 1.89253322 | 0.80377078 | 0.80377080 | 0.803774 |
| 6 | 1.78599534 | 0.80377066 | 0.80377067 | 0.803771 |
| Exact | | 0.80377065 | | |

In summary, we have developed a scheme to construct systematically a set of variational basis functions. Compared with the method introduced by Stubbins and Das, in this approach it is not necessary to introduce any empirical parameter. As a result, possible numerical instabilities have been eliminated and the computational effort is reduced. For the test model it is seen that the improved variational scheme yields a faster energy convergence rate than using the Lanczos method.

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