SUSY-BASED VARIATIONAL METHOD FOR THE ANHARMONIC OSCILLATOR

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Abstract

Using a newly suggested algorithm of Gozzi, Reuter, and Thacker for calculating the excited states of one dimensional systems, we determine approximately the eigenvalues and eigenfunctions of the anharmonic oscillator, described by the Hamiltonian $H = p^2/2 + gx^4$. We use ground state post-gaussian trial wave functions of the form $\Psi(x) = N \exp[-b|x|^{2n}]$, where $n$ and $b$ are continuous variational parameters. This algorithm is based on the hierarchy of Hamiltonians related by supersymmetry (SUSY) and the factorization method. We find that our two parameter family of trial wave functions yields excellent energy eigenvalues and wave functions for the first few levels of the anharmonic oscillator.
The central idea of the factorization method for ordinary differential equations, introduced by Schrödinger [1] and by Infeld and Hull [2] to solve problems in quantum mechanics, is the recognition that once the ground state energy and wave function of a one-dimensional potential problem are known, then the potential is determined, as well as the factors of the Hamiltonian. Recently, Gozzi, Reuter, and Thacker [3] proposed a simple strategy for solving such one-dimensional potential problems approximately in a variational scheme, based on utilizing the hierarchy of Hamiltonians that are related by supersymmetry (SUSY) and factorization [4, 5, 6]. We apply their method here to the case of a one-dimensional anharmonic oscillator, using a simple variational wave function, and examine the results.

First let us review briefly the formalism for describing the hierarchy of isospectral Hamiltonians. Consider the Hamiltonian $H_1$ having $k$ bound states whose discrete eigenvalues and eigenvectors are denoted by $E_n^{(1)}$ and $\Psi_n^{(1)}$. Once we subtract the ground state energy, we can factorize the Hamiltonian as follows:

$$H_1 - E_0^{(1)} = \frac{1}{2} A_1^\dagger A_1 \equiv \frac{1}{2} \left[ -\frac{d}{dx} + W_1(x) \right] \left[ \frac{d}{dx} + W_1(x) \right]$$

$$= -\frac{1}{2} \frac{d^2}{dx^2} + V_1(x),$$

(1)

where the superpotential,

$$W_1(x) = -\frac{d}{dx} [\ln \Psi_0^{(1)} (x)],$$

(2)

and

$$V_1 \equiv (1/2)(W_1^2 - W_1').$$

(3)

The second Hamiltonian $H_2$ in the hierarchy, the SUSY partner of $H_1$,

$$H_2 = \frac{1}{2} A_1 A_1^\dagger + E_0^{(1)}$$

(4)

has the same spectrum as $H_1$, except that there is no state in $H_2$ corresponding to the ground state of $H_1$. Introduce the notation that in $E_n^{(m)}$, $n$ labels the energy level and $(m)$ refers to the m-th Hamiltonian $H_m$. 

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One can show that the energy eigenvalues and eigenfunctions of the two Hamiltonians $H_1$ and $H_2$ are related by

$$E_{n+1}^{(1)} = E_n^{(2)}, \quad \Psi_{n+1}^{(2)} = 2^{-1/2}(E_{n+1}^{(1)} - E_0^{(1)})^{-1/2}A_1\Psi_{n+1}^{(1)}$$

and in particular:

$$\Psi_{n+1}^{(1)} = 2^{-1/2}(E_{n+1}^{(1)} - E_0^{(1)})^{-1/2}A_1^\dagger\Psi_n^{(2)}$$

and

$$( -\frac{d}{dx} + W_1)\Psi_0^{(2)} = 2^{1/2}(E_1^{(1)} - E_0^{(1)})^{1/2}\Psi_1^{(1)}$$

so that the first excited state of the original Hamiltonian $H_1$ can be obtained from the ground state of the supersymmetric partner potential. If we determine the ground state wave function $\Psi_0^{(2)}$ and ground state energy ($=E_1^{(1)}$) for $H_2$, then we can repeat the above argument and determine a third Hamiltonian $H_3$ as the SUSY partner of $H_2$. Namely we can write

$$H_2 = \frac{1}{2}A_1A_1^\dagger + E_0^{(1)} = \frac{1}{2}A_1^\dagger A_2 + E_1^{(1)}$$

where

$$A_2 = \frac{d}{dx} + W_2(x).$$

Then

$$H_3 = \frac{1}{2}A_2A_2^\dagger + E_1^{(1)}.$$ 

We also notice that the Hamiltonian given by $\tilde{H}_2 = \frac{1}{2}A_1A_1^\dagger$ has a ground state energy which is the energy difference $E_1^{(1)} - E_0^{(1)}$. Furthermore we have the relationships:

$$E_{n+2}^{(1)} = E_{n+1}^{(2)} = E_n^{(3)},$$

$$\Psi_{n+1}^{(1)} = 2^{-1/2}(E_{n+1}^{(1)} - E_0^{(1)})^{-1/2}A_1^\dagger\Psi_n^{(2)}$$

$$= (1/2)(E_{n+1}^{(1)} - E_0^{(1)})^{-1/2}(E_{n+1}^{(1)} - E_0^{(1)})^{-1/2}A_1^\dagger A_2^\dagger\Psi_{n-1}^{(3)}.$$  

In particular, for $n = 1$ we determine the second excited state of $H_1$ from the ground state of $H_3$. Clearly this method can be generalized to obtain $k$ Hamiltonians of the hierarchy, where $k$ is the total number of bound states of $H_1$. 

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The scheme of Gozzi et al. [3] is to determine the ground state wave function $\Psi_0^{(1)}$ and energy $E_0^{(1)}$ of the original Hamiltonian $H_1$ using a variational method, then to approximately find the superpotential

$$W_1v(x) = -\frac{d}{dx} \left\{ \ln \Psi_0^{(1)}(x) \right\}.$$  \hfill (12)

This allows one to approximately determine the first SUSY partner potential corresponding to $\bar{H}_2$

$$V_{2v}(x) = \frac{1}{2} \left[ W_{1v}^2(x) + W_{1v}'(x) \right]$$  \hfill (13)

obtained from the approximate partner Hamiltonian $\bar{H}_{2v}$

$$\bar{H}_{2v} = \frac{1}{2} A_{1v} A_{1v}^\dagger, \quad A_{1v} = \frac{d}{dx} + W_{1v}.$$  \hfill (14)

whose ground state energy determines approximately the energy difference $E_1^{(1)} - E_0^{(1)}$ as discussed earlier. One next finds the variational ground state wave function and energy of the approximate SUSY partner Hamiltonian $\bar{H}_{2v}$ from which one can also calculate the approximate first excited state of the original Hamiltonian, and we can proceed as described above, using a new variational approximation for each ground state, until all the wave functions and energies of this approximate hierarchy of Hamiltonians are known.

The interesting question is how accurate is such a scheme? All the Hamiltonians of the variational hierarchy are not the real Hamiltonians of the hierarchy but approximate ones related to the variational approximation of the ground state wave function of the original problem. Thus we do not a priori know that we are calculating accurately the energy eigenvalues of the original Hamiltonian. We only know that we are accurately determining the energies of the approximate Hamiltonians of the hierarchy. Thus, for this scheme to work, one needs an extremely accurate method of finding the ground state wave function and energy of $H_1$. Also in this scheme the higher wave functions of $H_1$ are obtained by repeated derivatives of the ground state wave functions of the approximate hamiltonians. Thus we expect a loss in accuracy as we go to the higher wave functions.

In some recent work on soliton dynamics in various nonlinear systems including the nonlinear Schrödinger equation [10], we have demonstrated the...
efficacy of post-gaussian time dependent variational wave functions of the form
\[ u(x, t) = N(t) \exp[-b(t)|x - q(t)|^{2n}] . \] (15)

These wave functions, when used to minimize the action, gave excellent global fits to various solitons as well as very accurate determinations of the soliton energies. We found that these wave functions are globally accurate to a few percent or so, and give energy eigenvalues accurate to about 0.1%.

Thus, we propose to use as our trial wave functions for the ground state wave functions of the hierarchy of Hamiltonians,
\[ \Psi_0^{(k)} = N_k \exp[-\frac{1}{2}\frac{x^2}{\rho_k}^{n_k}] , \quad N_k = [2\sqrt{\rho_k} \Gamma(1 + \frac{1}{2n_k})]^{-1/2} . \] (16)

We first scale the Hamiltonian for the anharmonic oscillator,
\[ H = -\frac{1}{2} \frac{d^2}{dx^2} + gx^4 , \] (17)
by letting \( x \to x/g^{1/6} \) and \( H \to g^{1/3}H \). Then we find the ground state energy of the anharmonic oscillator and the variational parameters \( \rho_1 \) and \( n_1 \) by forming the functional
\[ E_0(\rho_1, n_1) = \langle \Psi_0 | -\frac{1}{2} \frac{d^2}{dx^2} + x^4 | \Psi_0 \rangle . \] (18)

We determine \( \rho_1 \) and \( n_1 \) by requiring
\[ \frac{\partial E_0}{\partial \rho_1} = 0 , \quad \frac{\partial E_0}{\partial n_1} = 0 . \] (19)

The equation for the energy functional for the anharmonic oscillator is:
\[ E_0(\rho_1, n_1) = \frac{n_1^2}{2\rho_1} \frac{\Gamma(2 - \frac{1}{2n_1})}{\Gamma(\frac{1}{2n_1})} + \rho_1^2 \frac{\Gamma(\frac{5}{2n_1})}{\Gamma(\frac{3}{2n_1})} . \] (20)

Minimizing this expression, we obtain the variational result
\[ E_0 = 0.66933 , \quad n_1 = 1.18346 , \quad \rho_1 = 0.666721 . \] (21)
This ground state energy is to be compared with a numerical evaluation which yields 0.667986, which is of the accuracy obtained in our soliton calculations. Since the trial wave function for all ground states is given by (10), the variational superpotential for all \( k \) is

\[
W_{k,v} = n_k |x|^{2n_k - 1} (\rho_k)^{-n_k}.
\]  

(22)

Since we are interested in the energy differences \( E_k - E_{k-1} \) of the anharmonic oscillator we will concentrate on the variational Hamiltonian

\[
\hat{H}_{k+1,v} = \frac{1}{2} A_{k,v} A_{k,v}^\dagger
\]

(23)

which approximately determines these energy differences as discussed above.

First, let us compare the exact potential \( x^4 - E_0 \) with the variational one obtained using the ground state variational wave function:

\[
V_{1,v}(x) = \frac{1}{2} \left[ W_{1,v}^2(x) - W_{1,v}'(x) \right].
\]

(24)

This is shown in the lower two curves of Fig. 1 for the most relevant range \( 0 \leq x \leq 1.5 \) for determining the ground state wave function. We see that the variational potential is quite different from the exact one, although it has almost the same ground state energy. It is also interesting to compare our variational “partner potential,”

\[
V_{2,v}(x) = \frac{1}{2} \left[ W_{1,v}^2(x) + W_{1,v}'(x) \right],
\]

(25)

with the exact one, obtained by first solving the Riccati equation for \( W_1 \),

\[
\frac{1}{2} \left[ W_1^2(x) - W_1'(x) \right] = x^4 - E_0,
\]

(26)

or equivalently solving the Schrödinger equation for

\[
\left[-\frac{1}{2} \frac{d^2}{dx^2} + x^4\right] \Psi_0 = E_0 \Psi_0
\]

(27)

for \( \Psi_0 \), and determining \( W_1 \) from the logarithmic derivative of \( \Psi_0 \). The result of this calculation of the exact partner potential and its variational approximation are shown in the upper two curves of Fig. 1.
We obtain the approximate energy splittings by minimizing the energy functional

\[
\Delta E_k(\rho_k, n_k) = \frac{1}{2} \langle \Psi_{0v}^{(k+1)} | \frac{d^2}{dx^2} + W_{k, v}^2 + W_{k, v}' | \Psi_{0v}^{(k+1)} \rangle = E_k^{(1)} - E_{k-1}^{(1)}. \tag{28}
\]

These integrals are trivial to carry out, and one obtains the simple recursion relation

\[
\Delta E_k(\rho_k, n_k) = \frac{n_k^2}{2\rho_k} \frac{\Gamma \left(2 - \frac{1}{2n_k} \right)}{\Gamma \left(\frac{1}{2n_k} \right)} + \frac{n_{k-1}^2}{2\rho_{k-1}} \left( \frac{\rho_k}{\rho_{k-1}} \right)^{2n_{k-1}} \frac{\Gamma \left(\frac{4n_{k-1}-1}{2n_k} \right)}{\Gamma \left(\frac{1}{2n_k} \right)}
\]

\[
+ \frac{n_{k-1}}{2\rho_k} \left(2n_{k-1} - 1 \right) \left( \frac{\rho_k}{\rho_{k-1}} \right)^{n_{k-1}} \frac{\Gamma \left(\frac{2n_{k-1}-1}{2n_k} \right)}{\Gamma \left(\frac{1}{2n_k} \right)}. \tag{29}
\]

One can perform the minimization in \( \rho \) analytically leaving one minimization to perform numerically.

The results for the variational parameters and for the energy differences are presented in Table 1 for the first five energy eigenvalues and compared with our numerical calculation, based on a shooting method, which essentially agrees with the results of Hioe and Montroll\[^{[1]}\], who made an exhaustive study of the anharmonic oscillator. For the ground state and first two excited states, we get excellent agreement with the numerical results. However, for the third excited state and higher, the variational approach relaxes to a Gaussian which leads to equal spacing with a \( \Delta E \) of around 2.3. Thus for the higher states our method fails to give the correct large \( n \) behavior, which from WKB results, is known to be \( 1.376(n + \frac{1}{2})^{4/3} \). So this method works where WKB fails and vice-versa. Of course, our results for the higher energy levels would be improved by using more variational parameters, which however would spoil the simplicity of the calculation presented here.

Finally, we have calculated the approximate excited states by repeated use of the approximate node insertion operators. The results for the first three variational wave functions are compared to the exact numerical results in Fig 2. We see that we are doing an excellent job in the regime \( 0 \leq x \leq 1.5 \), which is the most important region for determining the energy eigenvalues. The higher eigenvalues require more and more derivatives, and thus the accuracy of the results diminish for large \( x \) where the variational potential is not so accurate.
Table 1: Variational Parameters and Energies

| level | n     | $\rho$  | $E_n - E_{n-1}$ variation | exact     |
|-------|-------|---------|---------------------------|-----------|
| 0     | 1.183458 | 0.666721 | 0.669330                  | 0.667986  |
| 1     | 0.995834 | 0.429829 | 1.727582                  | 1.725658  |
| 2     | 1.000596 | 0.435604 | 2.316410                  | 2.303151  |
| 3     | 0.999917 | 0.434779 | 2.297082                  | 2.638935  |
| 4     | 1.000012 | 0.434894 | 2.299820                  | 2.908578  |

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FIGURE CAPTIONS

Fig. 1: Exact (solid line) and variational (dashed line) potentials for the anharmonic oscillator (lower curves) and its SUSY partner (upper curves).

Fig. 2: Exact (solid line) and variational (dashed line) wave functions for the lowest three levels of the anharmonic oscillator.