

Correct bound states of the non-linear oscillator through non-variational method: Failure of the variational method

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Abstract. A method for obtaining correct bound states of the non-linear oscillator $H = P^2 + X^2 + X^2\langle X^2 \rangle$ is described. It is shown that the variational method fails to yield correct ground state energy.

Keywords. Non-linear oscillator; ground state energy; variational method.

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Non-linear effective Hamiltonians are useful in several branches of physics and chemistry. In particular the non-linear Schrodinger equation

$$H|\psi\rangle = E|\psi\rangle \quad (1)$$

with

$$H = H_0 + \sum_1^N \lambda_i \langle A_i \rangle B_i \quad (2)$$

where

$$\langle A_i \rangle = \langle \psi | A_i | \psi \rangle \quad (3)$$

and λ_i are respective coupling constants, describe the molecular solvent interactions [1–3] and therefore of great interest in physical chemistry. However from the physics point of view this type of non-linear oscillator has not been able to draw much attention. In the one-dimensional system a simple non-linear Hamiltonian of this system can be written as [4]

$$H = P^2 + X^2 + X^2\langle X^2 \rangle. \quad (4)$$

An interesting point in eq. (4) is that its ground state energy and wave function are exactly calculated but not the higher bound states. Perhaps its exact solvability nature on the ground state will find some place in generating squeezed states [5]. Further this exact ground state is the guiding factor for testing an arbitrary approximation for higher bound states provided the arbitrary approximation yields the exact ground state. Some methods

like connected moments [6], perturbation theory [7] and Hankel–Hamdard determinants [4] have been tested for the ground state. Even for the ground state, connected moments yield a poor state of convergency [6] in the lower order. The same conclusion is also valid for the Hankel–Hamdard determinants [4]. However the perturbation series raises a problem of convergency in the large order [7]. In this letter we give a simple matrix diagonalisation method for calculating higher bound states and simultaneously find that the variational method fails to reproduce the correct ground state of this system. The Hamiltonian in eq (4) is rewritten in terms of creation operator a^+ and annihilation operator a using the following transformations.

$$X = \frac{(a + a^+)}{\sqrt{(2W)}}, P = i(a^+ - a)\sqrt{(W/2)}; a|0\rangle = 0. \quad (5)$$

The Hamiltonian after normal ordering reads as

$$H = [2a^+a + 1] \left[\frac{W}{2} + \frac{1}{2W} + \frac{\langle(2a^+a + 1)\rangle}{4W^2} \right] + \left[\frac{-W^3 + W + 0.5}{2W^2} + \frac{n}{2W^2} \right] [a^2 + (a^+)^2]. \quad (6)$$

Further the parameter W is determined [8,9] from the condition $\langle 0|H|2\rangle = 0$ and this leads to

$$W^3 = W + 0.5. \quad (7)$$

Hence for the ground state, the system yields the exact energy and is $E_0 = W$. However for the excited states, the system as such cannot yield the exact energy because $\langle n|H|n+2\rangle \neq 0$. However using the function $|n\rangle W$ one can get higher bound states on solving the eigenvalue relation

$$H|\psi\rangle = E|\psi\rangle$$

by expressing

$$\psi = \sum_m A_m |m\rangle w. \quad (8)$$

Now substituting eq (8) with eq (1) we get the following three term relation in A_m as

$$A_{m+2}P_m + A_m Q_m + A_{m-2}R_m = 0 \quad (9)$$

where

$$Q_m = (2m + 1)W + \frac{m(2m + 1)}{2W^2} - E, \quad (10)$$

$$P_m = m + \frac{\sqrt{(m + 2)(m + 1)}}{2W^2} \quad (11)$$

and

$$R_m = P_{m-2}. \quad (12)$$

Now eq (10) is solved using the matrix diagonalisation technique and the bound states are tabulated in table 1. In this method the direct matrix diagonalisation technique is

Correct bound states of non-linear oscillator

Table 1. Bound states of the $H = P^2 + X^2 + \langle X^2 \rangle X^2$.

| Energy level | Matrix size | | |
|--------------|-------------|------------|------------|
| | 45 × 45 | 95 × 95 | 145 × 145 |
| 0 | 1.191 487 | 1.191 487 | 1.191 487 |
| 1 | 4.551 966 | 4.551 966 | 4.551 966 |
| 2 | 8.397 330 | 8.397 330 | 8.397 330 |
| 3 | 14.805 017 | 14.805 017 | 14.805 017 |
| 4 | 20.219 187 | 20.219 187 | 20.219 187 |
| 5 | 26.808 112 | 26.808 112 | 26.808 112 |
| 6 | 33.956 148 | 33.956 147 | 33.956 147 |
| 7 | 41.679 338 | 41.679 324 | 41.679 324 |
| 8 | 49.922 208 | 49.922 127 | 49.922 127 |
| 9 | 58.664 871 | 58.664 102 | 58.664 102 |
| 10 | 67.887 269 | 67.884 185 | 67.884 185 |
| *0 | 1.176 580 | 1.176 580 | 1.176 580 |

* Variational approach.

Table 2. Bound states of the $H = P^2 + X^2 + \langle X^4 \rangle X^2$.

| Energy level | Matrix size | | |
|--------------|-------------|-------------|-------------|
| | 45 × 45 | 95 × 95 | 145 × 145 |
| 0 | 1.224 744 | 1.224 744 | 1.224 744 |
| 5 | 114.968 475 | 114.968 473 | 114.968 473 |
| 10 | 619.687 187 | 619.676 542 | 619.676 531 |

Table 3. Bound states of the $H = P^2 + X^2 + X^2 \langle X^2 \rangle + \langle X^4 \rangle X^2$.

| Energy level | Matrix size | | |
|--------------|-------------|-------------|-------------|
| | 45 × 45 | 95 × 95 | 145 × 145 |
| 0 | 1.338 665 | 1.338 665 | 1.338 665 |
| 5 | 102.972 853 | 102.972 851 | 102.972 851 |
| 10 | 516.508 034 | 516.497 696 | 516.497 697 |

adopted. For the higher bounds one has to diagonalise a large matrix. Further in this approach if the parameter W is determined using the variational technique [10] then it satisfies the relation

$$W^3 = W + 1. \quad (13)$$

The ground state energy using the variational parameter is also tabulated in table 1. It is observed that the variational method [10] fails to yield the correct ground state for this oscillator. The worst part of the variational method is that it converges to a wrong value. Hence this paper adds to the existing exposition on the failure of the variational based approximation methods like the Hill determinant method [11] and the super symmetric WKB approximation [12] in bound state calculation. Further we find that the method presented here can be extended to non-linear oscillators of the form

$$H = P^2 + X^2 + X^2 \langle X^4 \rangle \quad (14)$$

and

$$H = P^2 + X^2 + X^2\langle X^2 \rangle + X^2\langle X^4 \rangle. \quad (15)$$

In table 2 and table 3 we show only bound states for eqs (14) and (15) respectively. Details of calculation for the eqs (14,15) will be published elsewhere. One question that arises, is of the practical utility of this type of non-linear oscillator. Even though it is difficult to answer immediately, one can initiate a problem in generating squeezed states as stated in the beginning [5]. For generating squeezed states correct information can be gathered using the parameter in eq (7) for the Hamiltonian eq (4). However if one uses the variational parameter eq (13) then it is obvious that variational approximation can lead to wrong information.

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