INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) 87–92 PII: S0305-4470(02)25801-1

Calculation of energy eigenvalues for the quantum anharmonic oscillator with a polynomial potential

Mojtaba Jafarpour and Davood Afshar

Physics Department, Shahid Chamran University, Ahwaz, Iran

Received 30 May 2001, in final form 26 September 2001
Published 21 December 2001
Online at stacks.iop.org/JPhysA/35/87

Abstract

We choose the squeezed vacuum state as a one-parameter trial wavefunction, to minimize the energy of an anharmonic oscillator, with a polynomial perturbation potential. Using the optimal vacuum state obtained, we generate the optimal generalized number state basis, and set up the Hamiltonian in the normal-ordered form. Then, truncating the basis, we produce finite-dimensional matrices in a simple manner, and find their eigenvalues by standard methods. We will apply our method to the Morse potential, whose exact eigenvalues are known, as a check on the accuracy of the results that we have derived. Two models of the double well and the quartic potential are considered as examples.

PACS number: 03.65.Ge

1. Introduction

The anharmonic oscillator is an important model in the study of many problems in physics. However, in contrast to the harmonic oscillator, it cannot be solved analytically, and thus one has to resort to approximation methods for its solution. The anharmonic quantum oscillator with quartic perturbation has been studied extensively in the past [1–10]. The quantum anharmonic oscillator with sextic, octic, and the general one-perturbation term, λx^m, has also been studied more recently [11–17]. The aim of this work is to calculate the energy eigenvalues of the quantum anharmonic oscillator, with a polynomial perturbation potential, whose Hamiltonian is given by

$$H = \frac{p^2}{2} + \frac{x^2}{2} + \sum_{m=0}^{M} \lambda_m x^m = H_0 + \sum_{m=0}^{M} \lambda_m x^m \tag{1}$$

where H_0 is the Hamiltonian for a harmonic oscillator with the mass and the angular frequency assumed equal to unity. In fact, we may cast any Hamiltonian

$$H = \frac{p^2}{2} + V(x) = H_0 - \frac{1}{2}x^2 + V(x) \tag{2}$$

in the form (1) if the potential $V(x)$ is a polynomial, or if it can be expanded in a series and truncated into a polynomial as an acceptable approximation. Thus, our work covers a wide range of Hamiltonians, and not just the ones traditionally called 'anharmonic oscillators'.

We shall follow a two-step approach to solve the Hamiltonian (1). First, we choose a squeezed vacuum state as a one-parameter trial wavefunction, and minimize the energy of the system by variation [4]. Then, using the optimal vacuum obtained, we construct the optimal generalized number states basis, and use it to set up the Hamiltonian in terms of the generalized creation and annihilation operators in normal-ordered form [14]. Finally, considering a truncated basis, we produce a finite-dimensional matrix, whose eigenvalues we obtain by standard methods.

The organization of the paper is as follows. We introduce the generalized number states and a theorem regarding the normal-ordered form of a function of the second-quantized operators in section 2. The normal-ordered form of the Hamiltonian, and its matrix representation, are derived in section 3. We specialize our work to the famous Morse oscillator, whose exact solutions are known, as a check on the general results that we have derived, in section 4. Two models, of the double well and the quartic potential, are also considered as examples in this section.

2. Generalized number states

The ordinary annihilation and creation operators for the harmonic oscillator with the Hamiltonian H_0 are defined by

$$a = \frac{x + \mathrm{i}p}{\sqrt{2}} \tag{3}$$

$$a^+ = \frac{x - \mathrm{i}p}{\sqrt{2}} \tag{4}$$

where they satisfy the commutation relation

$$[a, a^+] = 1. \tag{5}$$

We now perform a Bogoliubov transformation [4], to define the generalized annihilation and creation operators b and b^+:

$$b = \frac{a - ta^+}{\sqrt{1 - t^2}} \tag{6}$$

$$b^+ = \frac{a^+ - ta}{\sqrt{1 - t^2}} \tag{7}$$

where t is a real number which satisfies $|t| < 1$, and the commutation relation

$$\left[b, b^+\right] = 1 \tag{8}$$

holds.

We now define the normalized squeezed vacuum state $|0, t\rangle$ by

$$|0, t\rangle = (1 - t^2)^{(1/4)} \mathrm{e}^{(t/2)a^{+2}} |0\rangle \tag{9}$$

where b is its annihilation operator, and we have

$$b|0, t\rangle = 0. \tag{10}$$

The generalized number states, $|n, t\rangle$, may be generated by application of the operator b^+, n times, to the squeezed vacuum state $|0, t\rangle$; we write

$$|n, t\rangle = \frac{(b^+)^n}{\sqrt{n!}} |0, t\rangle \tag{11}$$

where $\{|n, t\rangle\}$ is a complete set and will be used to set up the Hamiltonian matrix later.

It is worthwhile to make a parenthetical but interesting observation at this point: constructing the generalized number operator b^+b, using equations (3)–(7), we find

$$H_\Omega = b^+b + \frac{1}{2} = \frac{p^2}{2\Omega} + \frac{\Omega x^2}{2} \tag{12}$$

where we have defined the real parameter $\Omega = \frac{1-t}{1+t}$. Now, comparing the above result with H_0, we conclude that the transformation that we have used is mathematically equivalent to rescaling the Hamiltonian H_0, according to the ansatz $x \to \sqrt{\Omega}x$. Thus, the parameter Ω gains a central role in our subsequent calculations, although we are not concerned with the rescaling aspects in our work. Using the eigenfunctions of the rescaled harmonic oscillator Hamiltonian is a standard method and helps to simplify some calculations [18, 19].

We also need to prove a theorem regarding the normal-ordered form. Let $f(b, b^+)$ be an operator function of the generalized creation and annihilation operators b and b^+; we may use the commutation relation (8) to write this function in the so-called ordered form, in which all the powers of b stand to the right of all the powers of b^+. We also define the operator function $: f(b, b^+) :$, which is obtained from $f(b, b^+)$ by moving all powers of the annihilation operator b to the right, without application of the commutation relation (8). Using the Baker–Hausdorff formula, we write

$$\exp[\alpha(b + b^+)] = \exp\left[\frac{\alpha^2}{2}\right]\exp(\alpha b^+)\exp(\alpha b) = \exp\left[\frac{\alpha^2}{2}\right] :\exp[\alpha(b + b^+)]:. \tag{13}$$

Now expanding both sides of the above equation in powers of α, and equating the coefficients, we find

$$\begin{aligned}(b + b^+)^m &= \sum_{k=0}^{[m/2]} \frac{m!}{2^k k!\,(m-2k)!} :(b + b^+)^{m-2k}: \\ &= \sum_{k=0}^{[m/2]} \frac{m!}{2^k k!} \sum_{j=0}^{m-2k} \frac{(b^+)^{m-2k-j} b^j}{j!\,(m-2k-j)!}.\end{aligned} \tag{14}$$

This gives the normal-ordered form of the function $(b + b^+)^m$, which has also been derived by iteration methods in [16]. We will use this result later, to construct the Hamiltonian matrix elements, in the generalized number state basis.

3. Hamiltonian matrix and variational method

Using equations (3) and (4), the second-quantized form of the Hamiltonian (1) is given by

$$H = \frac{1}{2} + a^+a + \sum_m \lambda_m \left(\frac{a + a^+}{\sqrt{2}}\right)^m. \tag{15}$$

Now, using equations (6), (7) and (14), and expanding the binomial coefficient in the last, we write H in terms of the normal-ordered product of the operators b and b^+ as follows:

$$\begin{aligned}H = \frac{1}{2} + \frac{(1-\Omega)^2}{4\Omega} + \frac{1+\Omega^2}{2\Omega} b^+b + \frac{1-\Omega^2}{4\Omega}(b^2 + b^{+2}) \\ + \sum_{m=0}^{M} \frac{\lambda_m}{(2\Omega)^{(m/2)}} \sum_{k=0}^{[m/2]} \sum_{n=0}^{m-2k} \frac{m!(b^+)^{m-2k-n} b^n}{2^k k! n!\,(m-2k-n)!}\end{aligned} \tag{16}$$

where the parameter $\Omega = \frac{1-t}{1+t}$ has already been defined after equation (12).

Now, we use the squeezed vacuum state as a one-parameter trial wavefunction to find the expectation value of the Hamiltonian H. We obtain

$$\varepsilon\,(\Omega) = \langle 0, \Omega|H|0, \Omega\rangle = \frac{1}{2} + \frac{(1-\Omega)^2}{4\Omega} + \sum_{m=0,2,4,\ldots}^{\{M\}} \frac{\lambda_m m!}{2^m \Omega^{(m/2)}\,(m/2)!} \tag{17}$$

where $\{M\}$ denotes the largest even number which is equal to or less than M. Minimizing $\varepsilon(\Omega)$, we find the equation

$$1 - \frac{1}{\Omega_o^2} - \sum_{m=2,4,\ldots}^{\{M\}} \frac{\lambda_m m!}{2^{m-2}\Omega_o^{(m/2+1)}[(m/2)-1]!} = 0 \tag{18}$$

which we solve numerically to obtain the value of Ω_o, the optimal value of Ω.

Having found Ω_o, we now use the optimal generalized number states

$$|n, \Omega_o\rangle = \frac{(b^+)^n}{\sqrt{n!}}|0, \Omega_o\rangle \tag{19}$$

to set up the matrix representation for H given by equation (16). We find

$$\begin{aligned} H_{ij} = {} & \left[\frac{1+\Omega_o^2}{4\Omega_o} + \frac{1+\Omega_o^2}{2\Omega_o} j\right]\delta_{ij} + \frac{1-\Omega_o^2}{4\Omega_o}\left\{[j(j-1)]^{\frac{1}{2}}\delta_{i,j-2} + [(j+1)(j+2)]^{\frac{1}{2}}\delta_{i,j+2}\right\} \\ & + \sum_{m=0}^{M}\sum_{k=0}^{[m/2]}\sum_{n=0}^{m-2k} \frac{\lambda_m m!\big[j!\,(j+m-2k-2n)!\big]^{\frac{1}{2}}}{(2\Omega_o)^{(m/2)}2^k k! n!\,(j-n)!\,(m-2k-n)!}\delta_{i,j+m-2k-2n}. \end{aligned} \tag{20}$$

This is an infinite-dimensional matrix, but we can deal with an N-dimensional one, if we truncate the basis by limiting the value of n in equation (20) to $n \leqslant N-1$. Then, we use a diagonalization method or appropriate software to find the low-lying eigenvalues of the oscillator. We have used Matlab® to obtain our numerical results.

4. Accuracy check and examples

We first apply our method to the one-dimensional Morse oscillator with the Hamiltonian

$$H_1 = \frac{p^2}{2} + D_e(1 - \mathrm{e}^{-\alpha x})^2 \tag{21}$$

where D_e and α are the depth and the range parameter, respectively, and the mass of the oscillator is put equal to unity [20, 21]. Assuming $\hbar$ also equal to unity, the exact energy eigenvalues are given by

$$E_n = \alpha\sqrt{2D_e}\left[\left(n+\frac{1}{2}\right) - \left(n+\frac{1}{2}\right)^2\frac{\alpha}{\sqrt{8D_e}}\right]. \tag{22}$$

We can also expand H_1 in the following form:

$$H_1 = H_0 + \sum_{m=2}^{\infty}\lambda_m\,(\alpha, D_e)x^m \tag{23}$$

where

$$\sum_{m=2}^{\infty}\lambda_m\,(\alpha, D_e)\,x^m = \big[D_e\alpha^2 - \tfrac{1}{2}\big]x^2 + D_e\big[-(\alpha x)^3 + \tfrac{7}{12}(\alpha x)^4 - \tfrac{1}{4}(\alpha x)^5 + \tfrac{31}{360}(\alpha x)^6 - \cdots\big]. \tag{24}$$

Table 1. Energy eigenvalues for the Morse oscillator with $\alpha = 1$, $D_e = 200$, $\Omega_o = 9.099\,025\,893\,345\,88$ and 23 perturbation terms.

N	E_0	E_1	E_2	E_3
10	9.880 031 9140	28.918 707 977	47.052 872 4878	64.806 109 6161
20	9.875 001 8376	28.875 033 730	46.875 450 6843	63.877 855 3192
30	9.875 000 0037	28.875 000 083	46.875 000 6713	63.875 003 3686
50	9.875 000 0000	28.875 000 000	46.875 000 0000	63.875 000 0000
Exact	9.875	28.875	46.875	63.875

Table 2. Energy eigenvalues for the Hamiltonian H_2 with $\Omega_o = 2.000\,000\,000\,000$.

N	E_0	E_1	E_2	E_3
10	1.808 714 77	1.900 771 31	4.385 255 38	5.616 193 58
20	1.800 821 70	1.896 507 20	4.370 514 70	5.573 382 97
30	1.800 813 51	1.896 505 39	4.370 466 78	5.573 350 43
50	1.800 813 49	1.896 505 38	4.370 466 73	5.573 350 20
100	1.800 813 49	1.896 505 38	4.370 466 73	5.573 350 20

The Hamiltonian (21) is now cast in a form suited to our method. We just have to provide the values of α, D_e, Ω_o, the number of perturbation terms that we want to use and the dimension of the Hamiltonian matrix to the computer program to find the eigenvalues. We have compared our numerical results with the exact values computed from equation (22) in table 1. As the data in table 1 reveal, increasing the dimension of the Hamiltonian matrix increases the accuracy of the results. Moreover, the method yields results that are more accurate for the lowest-lying states. The convergence and the accuracy are very good in general; although we have truncated the series in equation (24) and only 23 perturbation terms are considered, the relative error for all the energy entries is of the order of 10^{-12} or less for $N = 50$.

Encouraged by the above results, we now consider the following Hamiltonians as useful examples:

$$\begin{aligned}
H_2 &= \frac{p^2}{2} + (x^2 - 2)^2 = H_0 + x^4 - \tfrac{9}{2}x^2 + 4 \\
H_3 &= \frac{p^2}{2} + (x^2 - 2)^4 = H_0 + x^8 - 8x^6 + 24x^4 - \tfrac{65}{2}x^2 + 16 \qquad (25) \\
H_4 &= \frac{p^2}{2} + \lambda x^4 = H_0 - \tfrac{1}{2}x^2 + \lambda x^4.
\end{aligned}$$

H_2 and H_3 are both double-well Hamiltonians, and their eigenvalues are shown in tables 2 and 3 respectively. Obviously, H_3 provides a higher potential barrier than H_2, and this fact is reflected in the much smaller values for $E_1 - E_0$ and $E_3 - E_2$ in H_3 than in H_2. The relative errors for all the entries in table 2 with $N = 50$ are of the order of 10^{-9} or less, and they are of the order of 10^{-6} or less in table 3 with the same N. The Hamiltonian H_4 represents a quartic potential well and its energy eigenvalues are shown in table 4. The convergences of the eigenvalues in this table are faster than in the previous two, and with $N = 50$ the relative error for all the entries is of the order of 10^{-9} or less.

Finally, considering the convergence and the accuracy of the results, our work may be considered as a simple and reliable method for obtaining the eigenvalues of any Hamiltonian represented by equation (1).

Table 3. Energy eigenvalues for the Hamiltonian H_3 with $\Omega_o = 4.882\,928\,426\,153$.

N	E_0	E_1	E_2	E_3
10	2.517 422 46	2.585 969 28	8.614 019 68	8.882 024 49
20	2.449 174 45	2.452 622 41	8.244 231 87	8.329 536 37
30	2.446 807 90	2.449 915 01	8.234 083 45	8.316 594 35
50	2.446 745 06	2.449 838 32	8.233 745 67	8.316 211 76
100	2.446 744 74	2.449 838 16	8.233 743 94	8.316 210 73

Table 4. Energy eigenvalues for the Hamiltonian H_4 with $\lambda = 1$ and $\Omega_o = 2.000\,000\,000\,000$.

N	E_0	E_1	E_2	E_3
10	0.668 030 82	2.393 758 46	4.699 077 62	7.346 184 56
20	0.667 986 26	2.393 644 10	4.696 795 74	7.335 732 08
30	0.667 986 26	2.393 644 02	4.696 795 39	7.335 730 00
50	0.667 986 26	2.393 644 02	4.696 795 39	7.335 730 00
100	0.667 986 26	2.393 644 02	4.696 795 39	7.335 730 00

Acknowledgment

We thank a referee for very useful comments.

References

[1] Bender C M and Wu T M 1969 *Phys. Rev.* **184** 1231
[2] Bhaumik K and Dutta-Roy B 1975 *J. Math. Phys.* **16** 1131
[3] Hioe F T, MacMillen D and Montroll E W 1978 *Phys. Rep.* **43** 305
[4] Hsue C S and Chern J L 1984 *Phys. Rev.* D **29** 643
[5] Chahjlany S C, Letov D A and Malney V N 1991 *J. Phys. A: Math. Gen.* **24** 2731
[6] Muñoz-Tapia R 1993 *Am. J. Phys.* **61** 1005
[7] Bacus B, Meurice Y and Soemadi A 1995 *J. Phys. A: Math. Gen.* **28** L381
[8] McRae S M and Vrscay 1997 *J. Math. Phys.* **38** 2899
[9] Mandal S 1998 *J. Phys. A: Math. Gen.* **31** L501
[10] Ivanov I A 1998 *J. Phys. A: Math. Gen.* **31** 6995
[11] Fernández F M and Guardiola 1993 *J. Phys. A: Math. Gen.* **26 7169**
[12] Ivanov I A 1998 *J. Phys. A: Math. Gen.* **31** 5697
[13] Skála L, Čížek J and Zamastil J 1999 *J. Phys. A: Math. Gen.* **32 L123**
[14] Sharma L K and Fiase J O 2000 *Eur. J. Phys.* **21** 167
[15] Speliotopoulos A D 2000 *J. Phys. A: Math. Gen.* **33** 3809
[16] Pathak A 2000 *J. Phys. A: Math. Gen.* **33** 5607
[17] Skála L, Čížek J, Weniger E J and Zamastil J 1999 *Phys. Rev.* A **59** 102
[18] Killingbeck J P, Scott T and Rath B 2000 *J. Phys. A: Math. Gen.* **33** 6999
[19] Basla R, Plo M, Esteve J G and Pacheco A F 1983 *Phys. Rev.* D **28** 1945
[20] Cooper I L 1992 *J. Phys. A: Math. Gen.* **25** 1671
[21] Avram N M, Drăgănescu Gh E and Avram C N 2000 *J. Opt. B: Quantum Semiclass. Opt.* **2** 214