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Energy Levels for the Pure λx^{2m} Potentials

M. Jafarpour* and D. Afshar

Department of Physics, Shahid Chamran University, Ahvaz, Islamic Republic of Iran

Abstract

We used Wick's normal-ordering technique, squeezed creation and annihilation operators, and a variation method, to find the eigenvalues of the general pure λx^{2m} potential. Numerical results for low-lying energy levels of pure quadratic, quartic, sextic, octic and decatic potentials, for different values of λ were obtained. Some interesting features of these energy levels are explained.

Keywords: Anharmonic oscillator; Squeezed state; Wick's normal ordered

1. Introduction

Anharmonic oscillators are approximate models to describe many phenomena in physics and chemistry. The Hamiltonian for an important class of such systems may be expressed by $\frac{p^2}{2}+\frac{x^2}{2}+\sum_m \lambda x^{2m}$, where m is a positive integer and the polynomial represents the perturbation potential to the harmonic oscillator. The anharmonic oscillators with only one perturbation term have been studied extensively in the past [1-5]. They not only are tools to explain the molecular vibrational data [6,7], but also they are a testing ground for several approximation and computational techniques [8,9], that can be applied to other problems [10]. If the quadratic term is also absent, one is left with the Hamiltonian $\frac{P^2}{2m}+\lambda x^{2m}$, with only a one-term potential, which may not look like an anharmonic oscillator in the customary sense. This potential model has been used to study the chaotic systems in recent years [11-14]. Moreover it may also be considered the strong coupling limit of the Hamiltonian $\frac{p^2}{2}+\frac{x^2}{2}+\lambda x^{2m}$, and thus may be a useful tool to compare the results obtained by different computational techniques [15-20]. A general solution for this problem, for arbitrary values of m and λ, is lacking. Only some special cases, in particular the pure quartic oscillator, the case $m=2$, has been studied [21-23].

The aim of this work is to obtain a general solution for the potential λx^{2m} for arbitrary values of λ and m. Then we shall apply our general results, to obtain energy eigenvalues for the pure quadratic, quartic, sextic, octic and decatic potentials with several different values of λ.

Considering the Hamiltonian $\frac{P^2}{2m}+\lambda x^{2m}$, it seems that we are not dealing with an anharmonic oscillator here; but we may write

$$H=\frac{P^2}{2}+\frac{x^2}{2}+(-\frac{x^2}{2}+\lambda x^{2m}), \qquad (1)$$

which characterizes a harmonic oscillator, with two perturbation terms. However, the first perturbation term is not small, and the second one also may not be necessarily small, compared to the unperturbed Hamiltonian. Therefore, usual perturbation techniques may not be applicable here.

We have developed a method based on Wick's

*E-mail: mojtaba_jafarpour@hotmail.com

normal-ordering of the field operators, squeezed states, and a variation technique [24], which has been applied to different problems by us and others [25,26], with success. This method is also well suited to solve the problem at hand. We shall give only a brief account of this method in Section 2 to prepare the necessary tools and relations we need in this work. The reader may consult reference [24] for more details.

We organize our paper as follows. The generalized number states and a theorem regarding the Wick's normal-ordered product of the creation and annihilation operators are discussed in Section 2. Our approach to variation method and the optimal generalized number states, which we use to write down the Hamiltonian and its matrix elements, are presented in Section 3. Our numerical results and discussion are presented in Section 4.

2. Generalized Number States and the Normal Ordering of the Operators

The Hamiltonian H_0 may be given in terms of the creation and annihilation operators as follows

$$H_0 = a^+ a + \frac{1}{2}, \tag{2}$$

where

$$\left[a, a^+\right] = 1, \tag{3}$$

and

$$x = \frac{\left(a + a^+\right)}{\sqrt{2}}. \tag{4}$$

We now introduce the generalized number states briefly [27-30]. We define the squeezed annihilation and creation operators b and b^+, by the following transformations

$$a = \frac{b + tb^+}{\sqrt{1-t^2}}, \tag{5}$$

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

These squeezed operators have the properties

$$\left[b, b^+\right] = 1, \tag{7}$$

and

$$b\left|0,t\right\rangle = 0, \tag{8}$$

where

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

is the normalized squeezed vacuum state. The generalized number states $\left|n,t\right\rangle$, which form a complete orthonormal set, are given by

$$\left|n,t\right\rangle = \frac{\left(b^+\right)^n}{\sqrt{n!}}\left|0,t\right\rangle. \tag{10}$$

We also write down the Wick's normal-ordered form of the operator $\left(b + b^+\right)^{2m}$ in which, using the commutator (7), all the creation operators stand to the left of the annihilation operators [24]

$$\left(b + b^+\right)^{2m} = \sum_{k=0}^{m} \frac{2m!}{2^k k!} \sum_{j=0}^{2m-2k} \frac{\left(b^+\right)^{2m-2k-j} b^j}{j!(2m-2k-j)!}. \tag{11}$$

This ordered form would help us to set up our matrix representation in the next section.

3. Variational Method and the Hamiltonian Matrix

We write the Hamiltonian H in the form

$$H = \frac{1}{2} + a^+ a - \frac{1}{4}\left(a + a^+\right)^2 + \lambda\left(\frac{a + a^+}{\sqrt{2}}\right)^{2m}, \tag{12}$$

where, we have used equations (2)and(4) **.** We may also use equations (5,6) and (11) to write the Hamiltonian H in terms of the squeezed operators b and b^+, in a Wick's normal-ordered form. We find

$$\begin{aligned} H &= \frac{1+\Omega^2}{4\Omega} + \frac{1+\Omega^2}{2\Omega} b^+ b \infty \\ &+ \frac{1-\Omega^2}{4\Omega}\left(b^2 + b^{+2}\right) - \frac{1}{4\Omega}\left(b + b^+\right)^2 \\ &+ \frac{\lambda}{(2\Omega)^m} \\ &\sum_{k=0}^{m} \sum_{n=0}^{2m-2k} \frac{(2m)!}{2^k k! n! (2m-2k-n)!} \left(b^+\right)^{2m-2k-n} b^n, \end{aligned} \tag{13}$$

where, the new real parameter $\Omega = \frac{1-t}{1+t}$ has been defined.

Now, we calculate the expectation value of the

Hamiltonian (13) in the squeezed vacuum state $|0,\Omega\rangle$; we find

$$\varepsilon(\Omega)=\langle 0,\Omega|H\,|0,\Omega\rangle=\frac{\Omega}{4}+\frac{\lambda(2m)!}{2^{2m}\Omega^m m!}. \qquad (14)$$

Considering Ω as a variation parameter, we may minimize $\varepsilon(\Omega)$ to find the following equation, which provides us with Ω_o, the optimal value of Ω

$$1-\frac{\lambda(2m)!}{2^{2m-2}\Omega_o^{m+1}(m-1)!}=0. \qquad (15)$$

We have solved this simple equation for several values of m and λ numerically. The pertinent data is presented in Table 1.

Having obtained the Ω_o values, we now use $\{|n,\Omega_o\rangle\}$, the optimal orthonormal set, to construct the Hamiltonian matrix as follows

$$\begin{aligned}H_{ij}=&\frac{\lambda}{(2\Omega_o)^m}\\ &\sum_{k=0}^{m}\sum_{n=0}^{2m-2k}\frac{(2m)!\sqrt{j!(j+2m-2k-2n)!}}{2^k\,k!\,n!(2m-2k-n)!(j-n)!}\\ &\qquad\delta_{i,j+2m-2k-2n}\\ &+\left[\frac{\Omega_o}{4}+\frac{\Omega_o}{2}j\right]\delta_{ij}\\ &-\frac{\Omega_o}{4}\Big[\sqrt{j(j-1)}\,\delta_{i,j-2}\\ &\qquad+\sqrt{(j+1)(j+2)}\,\delta_{i,j+2}\Big],\end{aligned} \qquad (16)$$

where we have used the relation

$$\langle n',t\,|(b^+)^q\,b^p\,|n,t\rangle=\frac{\sqrt{n!(n-p+q)!}}{(n-p)!}\delta_{n',n-p+q}, \qquad (17)$$

which can be proved, using

$$b^p\,|n,t\rangle=\sqrt{\frac{n!}{(n-p)!}}\,|n-p,t\rangle, \qquad (18)$$

and

$$(b^+)^q\,|n,t\rangle=\sqrt{\frac{(n+q)!}{n!}}\,|n+q,t\rangle. \qquad (19)$$

The Hamiltonian matrix given by (16) is an infinite dimensional one; we truncate the basis to $n\le N-1$, and diagonalize the N-dimensional matrix we obtain, to calculate the eigenvalues.

4. Numerical Results and Discussion

Our numerical results for the quadratic, quartic, sextic, octic and decatic potentials, with values of λ equal to 0.01, 1 and 100, are presented in Tables 2 through 6. We used Matlab® to diagonalize our matrices. A few remarks on the properties of the energy levels are in order now.

a) The values obtained for each energy level converge fast as N increases, but the convergence is faster for smaller values of m.

b) For a specific value of m, the energy of each level, say the ground state, increases as λ increases. This can be explained by the uncertainty principle. In fact, by increasing λ, the particle is confined in a smaller interval; therefore, Δx decreases and Δp and ΔE increase, and higher ground state energies are required. We can also show this mathematically: Using the uncertainty criterion

$$xp\approx 1, \qquad (20)$$

we minimize the Hamiltonian

$$H=\frac{p^2}{2}+\lambda x^{2m}, \qquad (21)$$

Table 1. Ω_o values

λ	m	Ω_o
0.1	1	0.14142135623731
	2	1.02874841323592
	3	1.09050558806661
	4	1.24344277610831
	5	1.48649144164618
1	1	1.41421356237310
	2	2.00000000000000
	3	2.29558184499807
	4	2.61781187492896
	5	2.95585750501681
100	1	14.1421356237309
	2	8.17384740184630
	3	6.92364066519287
	4	6.40298854588826
	5	6.26736854650948

Table 2. Energy eigenvalues for $H_1 = \frac{p^2}{2} + \lambda x^2$

λ	N	E_0	E_1	E_2	E_3
0.01	10	0.07071067811865	0.21213203435596	0.35355339059327	0.49497474683058
	30	0.07071067811865	0.21213203435596	0.35355339059327	0.49497474683058
	50	0.07071067811865	0.21213203435596	0.35355339059327	0.49497474683058
1	10	0.70710678118655	2.12132034355964	3.53553390593274	4.94974746830584
	30	0.70710678118655	2.12132034355964	3.53553390593274	4.94974746830584
	50	0.70710678118655	2.12132034355964	3.53553390593274	4.94974746830583
100	10	7.071067811865	21.213203435596	35.355339059327	49.497474683058
	30	7.071067811865	21.213203435596	35.355339059327	49.497474683058
	50	7.071067811865	21.213203435596	35.355339059327	49.497474683058

Table 3. Energy levels for $H_2 = \frac{p^2}{2} + \lambda x^4$

λ	N	E_0	E_1	E_2	E_3
0.01	10	0.14391704489909	0.51569839928336	1.01243909569983	1.58099788524579
	30	0.14391327691899	0.51569497046968	1.01189389134408	1.58043511784247
	50	0.14391327691898	0.51569497046967	1.01189389134408	1.58043511784246
1	10	0.66803082044435	2.39375845846577	4.69907761771126	7.34618456481051
	30	0.667986259157	2.393644016519	4.696795387828	7.335729996331
	50	0.66798625916	2.39364401648	4.69679538686	7.33572999523
100	10	3.100775109649	11.110612198112	21.830550961077	34.129854106880
	30	3.10051756166	11.11031134003	21.80059302827	34.04944255861
	50	3.1005175615	11.1103113385	21.8005930214	34.0494424322

Table 4. Energy levels of $H_3 = \frac{p^2}{2} + \lambda x^6$

λ	N	E_0	E_1	E_2	E_3
0.01	10	0.21533492074829	0.81588564726505	1.70954771636700	2.81256162040836
	30	0.215257383368	0.815787389080	1.706013532460	2.808262366572
	50	0.21525738244	0.81578738671	1.70601349318	2.80826225625
1	10	0.682110583773	2.582604795031	5.437062336587	8.982619063466
	30	0.6807036816	2.5797472862	5.3948912174	8.8805279747
	50	0.6807036117	2.5797462294	5.3948883601	8.8805050258
100	10	2.157480246480	8.165751386078	17.233254372881	28.398059072183
	30	2.1525744655	8.1578791456	17.0601536997	28.0827798057
	50	2.152573825	8.157873872	17.060134966	28.082622757

Table 5. Energy levels for $H_4 = \frac{p^2}{2} + \lambda x^8$

λ	N	E_0	E_1	E_2	E_3
0.01	10	0.281237715134	1.093396064172	2.358780746216	4.038317590703
	30	0.2802882338	1.0874457159	2.3425682962	3.9656022860
	50	0.280286871	1.087442714	2.342533151	3.965541208
1	10	0.71047070549	2.74477160886	6.02910676433	10.21013306103
	30	0.704055268	2.731591545	5.884320286	9.961868057
	50	0.70404885	2.73153297	5.88417853	9.96099591
100	10	1.78531670901	6.89322223007	15.18041460803	25.61791690883
	30	1.768515656	6.861470144	14.780915594	25.023663878
	50	1.76849086	6.86130061	14.78039124	25.02089224

Table 6. Energy levels for $H_5 = \frac{p^2}{2} + \lambda x^{10}$

λ	N	E_0	E_1	E_2	E_3
0.01	10	0.3442095955	1.34671448380	3.00389872942	5.22402896976
	30	0.338369271	1.328118262	2.906120435	4.999819205
	50	0.33834961	1.32800157	2.90571109	4.99872180
1	10	0.74501564181	2.89611635322	6.56194234442	11.2151993706
	30	0.72902579	2.86161666	6.26143237	10.77507149
	50	0.7289539	2.8610968	6.2601944	10.7694829
100	10	1.60580303313	6.23844181646	14.1647771159	24.1370250439
	30	1.57067472	6.16523646	13.49043013	23.21538423
	50	1.5704848	6.1640458	13.4872061	23.2021484

Table 7. Energy levels for the Hamiltonian $H_6 = p^2 + x^4$ with $N = 50$

	E_0	E_1	E_2	E_3
Upper limit by Chhajlany *et al.*	0.53018104545	1.899836516	3.727848973	5.822372765
Our results	0.53018104525	1.89983651490	3.72784896899	5.82237275569
Lower limit by Chhajlany *et al.*	0.53018085	1.8998356	3.72784675	5.8223685

with respect to one of the variables x or p. We find

$$H_{m,\min} \approx (m+1)(2m)^{-\frac{m}{m+1}} \lambda^{\frac{1}{m+1}}. \qquad (22)$$

It is apparent from this result that for any positive integer value of m, that we are concerned with, the function $H_{m,\min}$ is an increasing function of λ; in agreement with the data.

c) As λ decreases, the energy levels are pushed together for any specific value of m; this seems reasonable, because one expects a free particle with a continuous spectrum, at the $\lambda \to 0$ limit.

d) Table 1 shows that for the higher values of m and λ, the Ω_o values deviate from 1 substantially. Now, $\Omega_o = 1$ is realized when $t = 0$ and it is seen from equations (5-6) that this condition transforms the squeezed creation and annihilation operators b and b^+ to the corresponding normal operators, and the squeezed number states to the corresponding normal ones. These facts then imply that for the small values of λ and m, one obtains good results by using the normal number states instead of the squeezed ones. However, for larger values of λ and m, Ω_o departs from the value unity considerably and the squeezed number states deviate from the normal ones substantially ; therefore, squeezed number states yield more accurate results in such cases.

The value of the ground state energy of the quartic oscillator (n = 2), calculated based on other methods, is given by $0.667986259\ \lambda^{1/3}$ [15,31] .This result is compatible with ours, given in Table 3.

Finally, Chhajlany et al [32] have obtained numerical results for the energy levels of the Hamiltonian $H_6 = p^2 + x^4$, using "auxiliary potential" approach. This Hamiltonian is just equivalent to $2H$ with λ and m equal to $\frac{1}{2}$ and 2, respectively. It is therefore appropriate that we calculate the energy eigenvalues for this Hamiltonian and compare our results with theirs. Both data are presented in Table 7. It is clear that the values we have obtained for the levels are within the bounds given by Chhajlany et al; hence, the two methods are in good agreement for the quartic potential.

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