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Energy eigenvalues of a quantum anharmonic oscillator from supersymmetry: the concept of conditional shape-invariance symmetry

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Abstract
The eigenvalues for oscillators with quartic and sextic anharmonicities $\left(V(r) = \frac{l(l+1)}{r^2} + ar^2 + br^4 + cr^6\right)$ have been calculated for a restricted set of parameters by supersymmetric quantum mechanics. We show that energies of at most a few levels can be obtained algebraically for a severely restricted set of parameters resulting from the satisfaction of a few constraint conditions. We present how conditional shape-invariance symmetry of supersymmetric partner potentials leads to the conditional exact solution. We also indicate its generalization in N dimensions.

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Double-well anharmonic oscillators with a quartic term $\left(V(x) = -\frac{1}{2}m\omega^2x^2 + \beta x^4\right)$ are widely used as theoretical models in molecular spectroscopy, quantum field theory, nuclear physics and also in solid-state physics [1–4]. This potential is interesting as it defines the quantum tunneling through the double-well barrier [5]. The bistable potential is also widely used to describe superconducting Josephson devices. Some recently discovered phenomena such as structural phase transition and polaron formation in solids, are well described by an anharmonic potential with more higher-order terms [6]. Nataurally, the addition of a sextic term in the above potential $\left[V(x) = -\frac{1}{2}m\omega^2x^2 + \beta x^4 + \gamma x^6\right]$ will improve the required high precision description of quantum bistable systems. Thus, the accurate knowledge of energy eigenvalues of the sextic anharmonic potential (SAHO) is essential. These have been studied extensively by a number of authors, and we have the Hill determinant and modified Hill determinant method [7–9], Pade approximation [10, 11], perturbation method [12], Borel summation technique [13] and supersymmetric quantum mechanics (SSQM) [14–16]. It is still a challenging problem in the search for an analytic solution for this potential. SAHO is basically a quasi and conditionally exactly solvable (CES) potential; i.e., a few eigenvalues can be determined at a time if the potential parameters obey certain constraint conditions. So apart from its wide applicability the problem is itself intrinsically important.

In this paper, we want to review the problem in the light of supersymmetric quantum mechanics [17] together with the shape-invariance condition [18]. Most of the earlier methods have used the one-dimensional problem with different anharmonic terms. We choose the SAHO in 3D as

$$V(r) = ar^2 + br^4 + cr^6 + \frac{l(l+1)}{r^2}, \qquad c > 0, \tag{1}$$

where the centrifugal term $\frac{l(l+1)}{r^2}$ will make the problem more complicated. We also prescribe its generalization to N-dimensional space. In [9], Chaudhuri and Mondal have used supersymmetry (SUSY) formalism for the SAHO, for the ground state only; but they neither presented the calculation and the results for excited states nor did they discuss the inherent symmetry for quasi conditional exactness. In [19], the wavefunction ansatz technique was presented to get low-lying excited states for the one-dimensional sextic potential $[V(x) = Ax^6 + Bx^2]$. However, there remains the question of convergence in the power series expansion and the choice of the ansatz is parity dependent.

Our technique is a 'superpotential ansatz', as the superpotential W is directly related to the potential $V(r)$ through the Riccati equation [17] (in units such that $\frac{\hbar}{\sqrt{2m}} = 1$)

$$V_1(r) = W^2 - W', \tag{2}$$

where $V_1(r)$ is the original potential $V(r)$ in the shifted energy scale. So just by looking at the form of the potential one can choose the form of W. This form remains unchanged for all states as the excited levels are calculated by SUSY level degeneracy relation $E_{n+1}^{(1)} = E_n^{(2)}$ [17]. One just has to repeat the SUSY transformation in each step, calculate partner potentials in the hierarchy to get the ground states of each partner, which are the different excited states of the original potential, according to the level degeneracy relation of the hierarchy of Hamiltonians. It is well known that SUSY shape-invariance condition [18] is sufficient to get exact analytic solutions for all the states. In the case of SAHO, we will show that it is basically shape invariant, only it requires a new set of constraint conditions for each passage from one member to the next one in the hierarchy of partner potentials. It implies that the shape invariance is satisfied in a single step when the corresponding constraints are satisfied, in the process of the construction of the hierarchy of partner potentials. Each step has a different set of constraint conditions and energies of at most a few levels can be obtained algebraically depending on the possibility of simultaneous satisfaction of such sets of constraint conditions.

For the potential given in equation (1), we start with the superpotential ansatz

$$W(r) = Ar + Br^3 - \frac{D}{r}, \qquad B > 0, \quad D > 0. \tag{3}$$

Let E_0 be the ground-state energy of the lth partial wave in $V(r)$, then the effective potential in the shifted energy scale (such that the ground state of $V_1(r)$ lies at zero energy) is

$$\begin{aligned} V_1 &= V(r) - E_0 \\ &= ar^2 + br^4 + cr^6 + \frac{l(l+1)}{r^2} - E_0. \end{aligned} \tag{4}$$

According to SSQM

$$V_1 = W^2 - W'. \tag{5}$$

From equations (3), (4) and (5), the unknowns A, B and D satisfy

$$\begin{aligned} &D^2 - D = l(l+1) \\ &A^2 - 2BD - 3B = a \\ &2AB = b \\ &B^2 = c \\ &2AD + A = E_0. \end{aligned} \tag{6}$$

The solution of the last four equations of (6) is

$$B = \sqrt{c}, \qquad A = \frac{b}{2\sqrt{c}}, \qquad D = \frac{b^2}{8c\sqrt{c}} - \frac{3}{2} - \frac{a}{2\sqrt{c}} \tag{7}$$

and the ground-state energy is given by

$$E_0 = -\frac{b}{2\sqrt{c}}\left[2 + \frac{a}{\sqrt{c}} - \frac{b^2}{4c\sqrt{c}}\right], \tag{8}$$

together with a constraint condition on the angular momentum

$$\left(\frac{b^2}{8c\sqrt{c}} - \frac{a}{2\sqrt{c}} - 2\right)^2 - \frac{1}{4} = l(l+1). \tag{9}$$

The ground-state wavefunction is

$$\begin{aligned}\Psi_0(b,c,l) &= N_0\,\mathrm{e}^{-\int W\mathrm{d}r}\\ &= N_0 r^{l+1}\exp\left[-\frac{\sqrt{c}}{4}r^4 - \frac{b}{4\sqrt{c}}r^2\right].\end{aligned} \tag{10}$$

To investigate if the potential V_1 is shape invariant, we contruct its supersymmetric partner [17]

$$\begin{aligned}V_2 &= W^2 + W'\\ &= [A^2 - 2BD + 3B]r^2 + 2ABr^4 + B^2r^6 + \frac{(D^2+D)}{r^2} - 2AD + A\\ &= a'r^2 + br^4 + cr^6 + \frac{l'(l'+1)}{r^2} + R',\end{aligned} \tag{11}$$

where the new parameters (l', a', R) are related to the old parameters (using equation (6)) by translation as

$$\begin{aligned}&l'(l'+1) = D^2 + D = l(l+1) + 2D\\ &a' = A^2 - 2BD + 3B = a + 6\sqrt{c}\\ &R' = -2AD + A = -E_0 + \frac{b}{\sqrt{c}}.\end{aligned} \tag{12}$$

The condition for shape-invariance symmetry between two partner potentials V_1 and V_2 is mathematically expressed as

$$V_2(x, a_1) = V_1(x, a_2) + R(a_1), \qquad a_2 = f(a_1), \tag{13}$$

where a_1 and a_2 are parameters appearing in the potentials. So, SAHO (V_1) is basically shape invariant with translation of parameters (equation (12)). But this shape invariance is not unconditional, since constraint condition (9) must be satisfied. So, the potential admits conditional shape invariance between the first two partners, which is responsible for the conditional exact analytic solution for the ground state. But this shape invariance is not unconditionally valid in successive steps. To see, we repeat our procedure with $V_2(r)$ as the new starting potential, defining $V'(r) = V_2(r)$.

Let E_0' be the ground-state energy in $V'(r)$, then in a new shifted energy scale

$$\begin{aligned}V_1'(r) &= V'(r) + E_0 - E_0'\\ &= a'r^2 + br^4 + cr^6 + \frac{l'(l'+1)}{r^2} + R' + E_0 - E_0'.\end{aligned} \tag{14}$$

Starting with a similar ansatz for its superpotential

$$\hat{W}(r) = A'r + B'r^3 - \frac{D'}{r}, \qquad B' > 0, \quad D' > 0, \tag{15}$$

when the new parameters are as in equation (7):

$$B' = \sqrt{c}, \qquad A' = \frac{b}{2\sqrt{c}}, \qquad D' = \frac{b^2}{8c\sqrt{c}} - \frac{9}{2} - \frac{a}{2\sqrt{c}}. \tag{16}$$

The ground-state energy E_0' (by which SSQM is the first excited state (E_1) of the original V_1) is given by

$$E_0' = E_1 = -\frac{b}{2\sqrt{c}}\left[6 + \frac{a}{\sqrt{c}} - \frac{b^2}{4c\sqrt{c}}\right] \tag{17}$$

subject to the constraint condition (as before)

$$\left(\frac{b^2}{8c\sqrt{c}} - \frac{a}{2\sqrt{c}} - 5\right)^2 - 2\left(\frac{b^2}{8c\sqrt{c}} - \frac{a}{2\sqrt{c}}\right) + \frac{11}{4} = l(l+1). \tag{18}$$

The wavefunction for the first excited state is given by [17]

$$\begin{aligned}\Psi_1(r) &= A^\dagger(r)\Psi_0 \\ &= \left[-\frac{\mathrm{d}}{\mathrm{d}r} + W(r)\right]\Psi_0.\end{aligned} \tag{19}$$

So we end up with algebraic expressions for the ground state as well as for the first excited state, with two constraints—one for each step. A simultaneous solution of two constraints (equations (9) and (18)) yields

$$b^2 - 4ac - 24c\sqrt{c} = 0. \tag{20}$$

Thus if only constraint (9) is satisfied, the energy of the ground state is given by equation (8); if only condition (18) is satisfied, the excitation energy of the first excited state is given by equation (17). On the other hand, if condition (20) together with equation (9) are satisfied, both the ground and first excited states are given algebraically. However, this corresponds to $l = \frac{1}{2}$, which is not a physical orbital angular momentum. That is, for a particular angular momentum l, only the parameters (a, b, c) can be adjusted to satisfy one of the two constraints.

Next, we apply the SUSY formalism to get the ground and excited states of SAHO and compare with the numerical solution of the Schrödinger equation. We choose three sets of parameters. In the first case, $a = 1$, $c = \frac{1}{7200}$; then the value of $b = 0.0243$, which is the solution of equation (20). In the second case, $a = 1$, $c = \frac{1}{6728}$ and the solution of equation (20) gives $b = 0.0252$. Finally, in the last case, we choose $a = 1$, $c = \frac{1}{6272}$, which gives $b = 0.0261$. In all the three cases the values of a and c are the same as chosen in [9], when b is calculated from equation (20). l is determined as 0.5 as required by equation (9) (in ground state) and equation (18) (in excited state). Although it seems unphysical, it corresponds to $l = 0$ in $N = 4$ dimensional space (obtained by equation (29)). In all the three cases, we calculate the ground-state energy E_0 from equation (8) analytically and present them in table 1. In the same table we also present the exact numerical solution of the Schrödinger equation, the ground-state energy is exactly reproduced in the SUSY formalism by analytical expression. The results for the first excited state are presented in table 2. Here we solve for the ground-state energy of V_2 with a translational set of parameters, which gives the first excited state of the original potential. The newly defined parameters (equation (12)) are $a' = a + 6\sqrt{c} = 1.0707$ (first set), 1.0731 (second set) and 1.0757 (third set); the value of l' becomes 0.75 (equation (12)) and the values of b and c remain unchanged. The ground-state energy of V_2 is in excellent agreement with the numerical results for the first excited state of V_1 in all sets. These results not only reproduce the first excited state, but at the same time they verify the existence of conditional shape-invariance symmetry with translational sets of parameters.

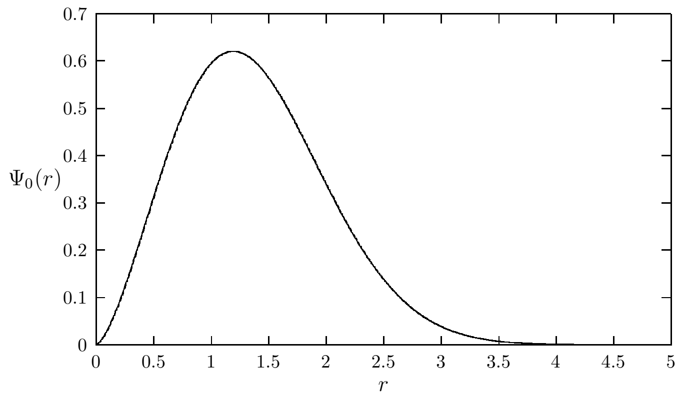

Figure 1. Ground-state wavefunction of sextic potential with $a = 1, b = 0.0243$ and $c = \frac{1}{7200}$ (arbitrary normalization).

Table 1. Ground-state energies of $V(r) = \frac{l(l+1)}{r^2} + ar^2 + br^4 + cr^6$ with $a = 1$ and different sets of parameters b and c. Numerical results are also presented.

b	c	E_{susy}	$E_{\text{numerical}}$
0.0243	$\frac{1}{7200}$	4.1390	4.1390
0.0252	$\frac{1}{6728}$	4.1437	4.1437
0.0261	$\frac{1}{6272}$	4.1487	4.1487

Table 2. First excited-state energy for the above combinations of table 1, with $a = 1$. Explanations are given in the text.

b	c	E_0 (for V_2)	E_1 (for V_1)
0.0243	$\frac{1}{7200}$	8.5356	8.5357
0.0252	$\frac{1}{6728}$	8.5531	8.5532
0.0261	$\frac{1}{6272}$	8.5718	8.5719

Table 3. The ground-state energy (E_0) and first excited-state energy (E_1) of sextic anharmonic potential with different combinations of a, b and c.

a	b	c	E_0^{susy}	E_0^{exact}	E_1^{susy}	E_1^{exact}
1.0	0.3845	0.02	5.4384	5.4384	12.7622	12.7625
5.0	0.6840	0.02	9.6734	9.6736	20.5948	20.5957
1.0	5.2915	1.0	10.5830	10.5833	27.1458	27.1484

The ground-state wavefunction is calculated from equation (10) and we plot it in figure 1 (with arbitrary normalization) for the parameters $a = 1.0$, $b = 0.0243$ and $c = \frac{1}{7200}$. For the same set of parameters, we calculate the first excited-state wavefunction using equation (19) and plot it in figure 2. Note that both the ground- and excited-state wavefunctions are calculated analytically. The results with higher anharmonicities are presented in table 3 together with the numerical solution of the Schrödinger equation. The SUSY results are in good agreement

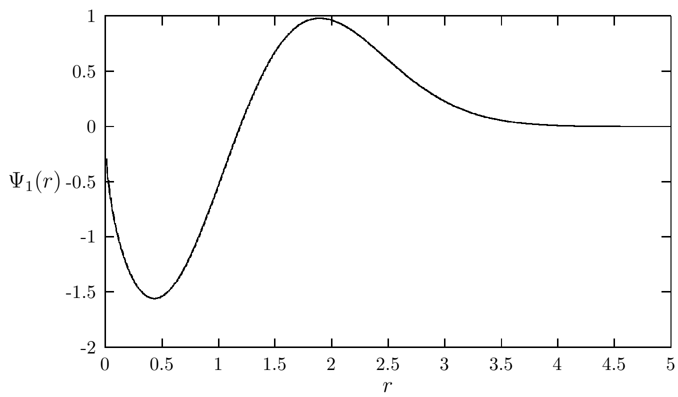

Figure 2. First excited state of sextic potential with $a = 1$, $b = 0.0243$ and $c = \frac{1}{7200}$ (arbitrary normalization).

with the exact numerical solution. The inclusion of higher anharmonicity is clear. In tables 1 and 2, anharmonicity was of small range, the ground and first excited states are almost equispaced, whereas higher anharmonic terms destroy the picture as shown in table 3.

It is clear that we can repeat our procedure to construct higher partner potentials in the hierarchy to get higher excited states. For the second excited state, we just repeat the procedure and set up the translational shape invariance as

$$\begin{aligned} l''(l''+1) &= l'(l'+1) + 2D' \\ a'' &= a' + 6\sqrt{c} \\ R'' &= -2A'D' + A', \end{aligned} \tag{21}$$

where A' and D' are given in equation (16). It yields the ground-state energy of the partner potential in the present hirarchy as

$$E_0'' = -\frac{b}{2\sqrt{c}}\left[10 + \frac{a}{\sqrt{c}} - \frac{b^2}{4c\sqrt{c}}\right] \tag{22}$$

subject to the constraint condition (as before)

$$\left(\frac{b^2}{8c\sqrt{c}} - \frac{a}{2\sqrt{c}} - \frac{15}{2}\right)^2 - \left(\frac{b^2}{8c\sqrt{c}} - \frac{a}{2\sqrt{c}} - \frac{15}{2}\right) = l''(l''+1). \tag{23}$$

It should produce the second excited state of the original potential according to the SUSY algebra, but as SAHO is basically a conditionally exactly solvable, simultaneous satisfaction of all three conditions (equations (9), (18) and (23)) this is impossible. However, a simultaneous solution of equations (18) and (23) is possible which will yield the first and second excited states at a time and the condition for that becomes

$$b^2 - 4ac - 48c\sqrt{c} = 0. \tag{24}$$

Similar arguments result in the ground state of the potential in the next hierarchy as

$$E_0''' = -\frac{b}{2\sqrt{c}}\left[14 + \frac{a}{\sqrt{c}} - \frac{b^2}{4c\sqrt{c}}\right] \tag{25}$$

with constraint condition

$$\left(\frac{b^2}{8c\sqrt{c}} - \frac{a}{2\sqrt{c}} - 11\right)^2 - \frac{1}{4} = l'''(l'''+1), \tag{26}$$

where l''' is related to l'' as $l'''(l'''+1) = l''(l''+1) + 2D''$, where $D'' = \frac{b^2}{8c\sqrt{c}} - \frac{15}{2} - \frac{a}{2\sqrt{c}}$. A simultaneous solution of equations (26) and (23) yields

$$b^2 - 4ac - 72c\sqrt{c} = 0. \tag{27}$$

So, we note that in each step condition for translational shape invariance is established and the corresponding ground-state energy is obtained analytically but in each step one additional constraint condition is satisfied. However, the number of states to be determined analytically is restricted as it depends on a simultaneous solution of constraint conditions.

Next, we want to mention another important point regarding the other solutions of the Riccati equation. It is well known that equation (3) is a special form of the solution of equation (2). However, the most general superpotential has the form $\mathcal{W}(r) = W(r) + \phi(r)$, which satisfies equations (5) and (11) [17]. $\mathcal{W}$ has the form $W(r) + \frac{d}{dr} ln[I(r) + \lambda]$, where $I(r) \equiv \int \psi_0^2(r')\,dr'$. It gives a family of potentials $\mathcal{V}_1(r) = V_1(r) - 2\frac{d^2}{dr^2} ln[I(r) + \lambda]$ having the same SUSY partner $V_2(r)$. For a normalized ground-state wavefunction, λ excludes the interval $-1 \leqslant \lambda \leqslant 0$. For $\lambda \to \pm\infty$, $\mathcal{V}_1 \to V_1$. $\mathcal{V}_1$ is isospectral to V_1 [17]. As we decrease λ from ∞ to zero, the shape changes drastically. The wavefunction also changes, however the energy eigenvalues will remain unchanged. So, the other possible solutions of Riccati equations will lead to the same eigenspectrum.

The concept of conditional shape invariance can easily be generalized to N dimensions. The radial Schrödinger equation for a spherically symmetric potential in an N-dimensional space is given by

$$-\left[\frac{d^2R}{dr^2} + \frac{N-1}{r}\frac{dR}{dr}\right] + \frac{l(l+N-2)}{r^2}R = [E - V(r)]. \tag{28}$$

Now taking $\psi(r) = r^{(N-1)/2}R(r)$, equation (28) is transformed to

$$-\frac{d^2\psi}{dr^2} + \left[\frac{\Lambda(\Lambda+1)}{r^2} + V(r)\right]\psi = E\psi, \tag{29}$$

where $\Lambda = l + \frac{N-3}{2}$.

So, the radial Schrödinger equation in N dimensions for a spherically symmetric potential has the same form as that in three dimensions, only angular momentum l has to be replaced by Λ. Next, to prove conditional shape invariance in CES models in an N-dimensional space, one can proceed in the same way as for three dimensions.

We conclude that the potential given by equation (1) is conditionally shape invariant in one or at most two steps, for a restricted set of parameters satisfying one or at most two conditions of constraints, respectively. Our 'superpotential ansatz' technique is a powerful tool, no initial input is necessary for our technique. From the structure of the potential we guess the form of the superpotential, and by using simple SUSY algebra we can obtain unknown parameters of the superpotential in terms of known parameters of the potential. This technique is applicable to get any excited state of the potential. Our approach also highlights the underlying conditional shape-invariance symmetry which is responsible for conditional exactness. To the best of our knowledge, this has not been pointed out earlier.

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References

[1] Reid C 1970 *J. Mol. Spectrosc.* **36** 183
[2] Wall F T and Glockler G 1937 *J. Chem. Phys.* **5** 314
[3] Kittle C 1986 *Introduction to Solid State Physics* (New York: Wiley)
[4] Bender C M and Wu T T 1968 *Phys. Rev. Lett.* **21** 406
[5] Jung P and Risken H 1985 *Z. Phys.* B **61** 367
[6] Chaudhuri R N and Mondal M 1989 *Phys. Rev.* A **40** 6080
[7] Tater M 1987 *J. Phys. A: Math. Gen.* **20** 2483
[8] Chaudhuri R N and Mukheree B 1984 *J. Phys. A: Math. Gen.* **17** 3327
[9] Chaudhuri R N and Mondal M 1995 *Phys. Rev.* A **52** 1850
[10] Killingbeck J 1981 *J. Phys. A: Math. Gen.* **14** 1005
Killingbeck J 1987 *J. Phys. A: Math. Gen.* **20** 601
[11] Bansal M, Srivastava S and Vishwamittar 1991 *Phys. Rev.* A **44** 8012
[12] Bender C and Wu T T 1969 *Phys. Rev.* **184** 1231
[13] Simon B 1970 *Ann. Phys., NY* **58** 76
[14] Keung W Y, Kovacs E and Sukhatme U P 1988 *Phys. Rev. Lett.* **60** 41
[15] Fernandez F M, Ma Q, Semat D J and Tipping R H 1989 *Can. J. Phys.* **67** 931
[16] Boya L, Kmiecik M and Bohm A 1987 *Phys. Rev.* D **35** 1255
[17] Cooper F, Khare A and Sukhatme U 1995 *Phys. Rep.* **251** 267 and references therein
[18] Gendenshtein L E 1983 *JETP Lett.* **38** 356
[19] de Souza Dutra A, de Castro A S and Boschi-Filho H 1995 *Phys. Rev.* A **51** 3480