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General structures of Hamiltonian hierarchies

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Abstract. Three dimensional exactly solvable quantum potentials for which an extra term of form $\frac{1}{r^2}$ has been added are shown to maintain their functional form which allows the construction of the Hamiltonian hierarchy and the determination of the spectra of eigenvalues and eigenfunctions within the Supersymmetric Quantum Mechanics formalism. For the specific cases of the harmonic oscillator and the Coulomb potentials, known as pseudo-harmonic oscillator and pseudo-Coulomb potentials, it is shown here that the inclusion of the new term corresponds to rescaling the angular momentum and it is responsible for maintaining their exact solvability.

1. Introduction

In the context of supersymmetric quantum mechanics, [1], the Hamiltonian hierarchy, introduced by Sukumar, [2], is an important algebraic structure that introduces a formalism which allows us to solve the Schrödinger equation, not only for the exactly solvable potentials but for the partially solvable ones, [3]-[7].

Few potentials in three dimensions are known to permit the construction of their complete hierarchy. The harmonic oscillator and the Coulomb potentials are examples of this property. It has been observed that the inclusion of an extra term of form $\frac{1}{r^2}$ in these potentials is such that their exact solvability is preserved, [8]. They are so called pseudo-harmonic oscillator and pseudo-Coulomb potentials, respectively, [9]-[15]. Variations of the pseudo-Coulomb potentials are the Kratzer potential, [16], or Mie-type potential, [17]. The study of these potentials is motivated by the fact that the new term is followed by an extra parameter, useful for applications in quantum chemistry and atomic and molecular physics, [17] -[25]. The reason why the factorization is possible is because the term added to the potential acts as a rescaling of the angular momentum barrier term. In this way, the exact solvability and shape invariance of both potentials are preserved.

In this work the Hamiltonian hierarchy of the pseudo-harmonic and pseudo-Coulomb potentials in three dimensions are shown and their spectra of eigenvalues and eigenfunctions are indicated.

2. The Hamiltonian hierarchy

Through the super-algebra, for a given Hamiltonian H_1 , factorized in terms of the bosonic operators, it is possible to construct its hierarchy of Hamiltonians. For the general spontaneously

broken supersymmetric case we have

$$H_1 = -\frac{d^2}{dx^2} + V_1(x) = A_1^+ A_1^- + E_0^{(1)} \quad (1)$$

where $E_0^{(1)}$ is the lowest eigenvalue, written in $\frac{\hbar^2}{2m}$ units. The bosonic operators are defined by

$$A^\pm = \mp \frac{d}{dx} + W_1(x) \quad (2)$$

where the superpotential $W_1(r)$ satisfies the Riccati equation

$$W_1^2 - W_1' = V_1(x) - E_0^{(1)}. \quad (3)$$

The eigenfunction for the lowest state is related to the superpotential W_1 by

$$\Psi_0^{(1)}(x) = N \exp\left(-\int_0^x W_1(\bar{x}) d\bar{x}\right). \quad (4)$$

The supersymmetric partner Hamiltonian is given by

$$H_2 = A_1^- A_1^+ + E_0^{(1)} = -\frac{d^2}{dr^2} + (W_1^2 + W_1') + E_0^{(1)}. \quad (5)$$

Thus, factorizing H_2 in terms of a new pair of bosonic operators, A_2^\pm we get,

$$H_2 = A_2^+ A_2^- + E_0^{(2)} = -\frac{d^2}{dx^2} + (W_2^2 - W_2') + E_0^{(2)} \quad (6)$$

where $E_0^{(2)}$ is the lowest eigenvalue of H_2 and W_2 satisfy the Riccati equation,

$$W_2^2 - W_2' = V_2(x) - E_0^{(2)}. \quad (7)$$

Thus a whole hierarchy of Hamiltonians can be constructed, with simple relations connecting the eigenvalues and eigenfunctions of the n -members, [2],

$$H_n = A_n^+ A_n^- + E_0^{(n)} \quad (8)$$

$$A_n^\pm = \mp \frac{d}{dx} + W_n(x) \quad (9)$$

$$\Psi_n^{(1)} = A_1^+ A_2^+ \dots A_n^+ \psi_0^{(n+1)}, \quad E_n^{(1)} = E_0^{(n+1)} \quad (10)$$

where $\Psi_0^{(1)}(x)$ is given by (4).

3. The pseudo-harmonic oscillator

The potential for this case is given by

$$V_{PH} = \left(br + \frac{a}{r}\right)^2 = \frac{a^2}{r^2} + 2ab + b^2 r^2. \quad (11)$$

The factorized radial Hamiltonian H_1 , first member of the hierarchy, is given by

$$H_1 = A_1^+ A_1^- + E_0^{(1)} = -\frac{d^2}{dr^2} + V_1(r) \quad (12)$$

where $V_1(r)$ incorporates the potential barrier term, $V_1(r) = V_{PH} + l(l+1)/r^2$.

In order to simplify the calculation, we rescale the angular momentum l to a new constant γ ,

$$a^2 + l(l+1) = \gamma(\gamma+1) \quad (13)$$

whose solution for γ is

$$\gamma = -\frac{1}{2} + \frac{1}{2}\sqrt{1 + 4(a^2 + l(l+1))}. \quad (14)$$

Writing the superpotential as

$$W_1(r) = \beta r - \frac{\alpha}{r} \quad (15)$$

and substituting it into equation (3) we arrive at

$$\alpha = \gamma + 1, \quad \beta = b. \quad (16)$$

As a result, the groundstate energy is given by

$$E_0^{(1)} = 2ab + 2\gamma b + 3b. \quad (17)$$

In terms of the parameters, the superpotential (15) is rewritten as

$$W_1(r) = br - \frac{\gamma+1}{r}. \quad (18)$$

With the above superpotential through the equation (4), a convergent ground state wavefunction. It is given by

$$\Psi_0^{(1)}(r) = Ne^{-\frac{ab}{\gamma+1}r} r^{\gamma+1}. \quad (19)$$

Repeating the same procedure we can evaluate the $(n+1)$ -th member of the hierarchy. The results are the following, [8],

$$W_{n+1} = br - \frac{\gamma+n+1}{r}, \quad (20)$$

the ground state wavefunction is

$$\Psi_0^{(n+1)}(r) = Ne^{-\frac{b}{2}r^2} r^{\gamma+n+1}. \quad (21)$$

and the ground state energy is

$$E_0^{(n+1)} = 2ab + 2\gamma b + (4n+3)b, \quad (22)$$

where γ is defined by (14). Thus the potentials of the hierarchy are given by

$$V_{n+1} = b^2 r^2 + \frac{(\gamma+n)(\gamma+n+1)}{r^2} + 2nb + 2ab. \quad (23)$$

From the above results we notice that this is a shape invariant potential, as defined by [26].

4. Pseudo-Coulomb potential

The pseudo-Coulomb potential is given, in atomic units, as

$$V_{PC} = c - \frac{b}{r} + \frac{a^2}{r^2} \quad (24)$$

and the factorized Hamiltonian associated is given by

$$H_1 = A_1^+ A_1^- + E_0^{(1)} = -\frac{d^2}{dr^2} + V_1(r). \quad (25)$$

$V_1(r)$ is the potential of the first Hamiltonian of the hierarchy, $V_1(r) = V_{PC} + l(l+1)/r^2$. Similarly as in the previous case, we rescale the angular momentum l to a new constant γ , as in (13), whose solution for γ is exactly like (14). Writing the superpotential as

$$W_1(r) = \beta - \frac{\alpha}{r} \quad (26)$$

and substituting it into equation (3) we arrive at

$$\alpha = \gamma + 1, \quad \beta = \frac{b}{2(\gamma + 1)}. \quad (27)$$

As a result, the energy is given by

$$E_0^{(1)} = c - \beta^2 = c - \frac{b^2}{4(\gamma + 1)^2}. \quad (28)$$

In terms of the parameters, the superpotential (26) is rewritten as

$$W_1(r) = \frac{b}{2(\gamma + 1)} - \frac{\gamma + 1}{r} \quad (29)$$

The convergent ground state wavefunction is

$$\Psi_0^{(1)}(r) = N e^{-\frac{b}{2(\gamma+1)}r} r^{\gamma+1}. \quad (30)$$

Repeating the same procedure we can evaluate the $(n+1)$ -th member of the hierarchy. The results are the following, [8],

$$W_{n+1} = \frac{b}{2(\gamma + n + 1)} - \frac{\gamma + n + 1}{r} \quad (31)$$

or given in terms of the potentials

$$V_{n+1} = c - \frac{b}{r} + \frac{(\gamma + n)(\gamma + n + 1)}{r^2} \quad (32)$$

with groundstate wavefunctions

$$\Psi_0^{(n+1)}(r) = N e^{-\frac{b}{2(\gamma+n+1)}r} r^{\gamma+n+1}. \quad (33)$$

The corresponding ground state energy

$$E_0^{(n+1)} = c - \frac{b^2}{4(\gamma + n + 1)^2} \quad (34)$$

For the particular case where

$$c^2 \rightarrow b^2, \quad b \rightarrow 2ab \quad (35)$$

the pseudo-Coulomb potential takes the usual form as shown in the literature, [15], [24]. Once again we notice that this pseudo-Coulomb potential is shape invariant in the sense of [26].

5. Conclusions

The Hamiltonian hierarchy of pseudo-harmonic and pseudo-Coulomb potentials were evaluated. These potentials are constructed through the introduction of a term proportional to $\frac{1}{r^2}$ into the original harmonic oscillator and Coulomb potentials, respectively. However, the introduction of this additional term, important for studies of molecular systems, is such that it acts as a centrifugal term. This is the reason why the exact solvability and the shape invariance of both potentials are preserved. It is important to remark the fact that the method allows us to evaluate the spectra of energy and eigenfunctions of the original potential.

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6. References

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