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Solving Schrödinger equation for two dimensional potentials using supersymmetry*

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ABSTRACT: The formalism of supersymmetric Quantum Mechanics can be extended to arbitrary dimensions. We introduce this formalism and explore its utility to solve the Schrödinger equation for a bidimensinal potential. This potential can be applied in several systems in physical and chemistry context , for instance, it can be used to study benzene molecule.

KEYWORDS: Quantum Mechanics; supersymmetry, bidimensional systems, Schrödinger equation.

Introduction

Supersymmetric Quantum Mechanics (SQM) in one dimension has been used in several contexts to analyze the Schrödinger equation. For example, in analytical solutions for determination of shape invariant potentials,[6] in the study of partially solvable potentials,[9] to obtain isoespectral potentials[8] and used in WKB approximation[1] and in Variational Method.[5]

Recently, a formalism of SQM for two or more dimensions was introduced and this formalism can be used, for example, to solve the Scrodinger equation.[4]

In this work, the two dimensional realization for the superalgebra is presented and applies to obtain the solution (eigenvalues and eigenfunctions) for Schrödinger equation for the general potential:

$$V(\vec{r})=\frac{c}{2r^2}+\frac{b_1+b_2+(b_1-b_2)\cos\theta}{2r^2\sin^2\theta}+\frac{1}{2}(a_1+a_2)+\frac{1}{2}(a_1-a_2)\cos\theta \qquad (1)$$

where a_1, a_2, b_1, b_2 and c are parameters. With special values of these parameters one can obtain, for example, Hartmann potential or Coulomb plus an Akaranov-Bohm potential. A different approach, based in so (2,1) dynamic algebra, to study the solutions of this potential is presented in ref 2. In particular, the Hartmann potential has been applied to study the benzene molecule.[7]

SQM in two-dimensions

In SQM we have the nilpotent operators Q and Q^+ that satisfy the algebra

$$\{Q, Q^+\} = H; \; Q^+ = Q^{+2} = 0 \qquad (2)$$

The standard realization for the operators is a matrix of rank two.[1,5,6,8-10] However, the superalgebra (2) can also be realized by[4]

$$Q = dl^- x s_- \text{ and } Q^+ = dl^+ x s_+ \qquad (3)$$

where: $dl^- = \begin{bmatrix} a^- & 0 \\ 0 & b^- \end{bmatrix}$, $dl^+ = \begin{bmatrix} a^+ & 0 \\ 0 & b^+ \end{bmatrix}$; $\sigma_+ = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$ and $\sigma_- = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$;

$a^\pm$ and $b^\pm$ are bosonic operators which may be written as

$$dl^\pm = \begin{bmatrix} \pm \frac{d}{dx} + W(x) & 0 \\ 0 & \pm \frac{d}{dy} + Z(y) \end{bmatrix} \qquad (4)$$

W(x) and Z(y) are the superpotential for the coordinates x and y, respectively

In this two dimensional (2D) realization Q and Q^+ are 4 x 4 matrices; and the super Hamiltonian is

$$H_{SS} = \begin{bmatrix} a^+a^- & 0 & 0 & 0 \\ 0 & b^+b^- & 0 & 0 \\ 0 & 0 & a^-a^+ & 0 \\ 0 & 0 & 0 & b^-b^+ \end{bmatrix} = \begin{bmatrix} H_+^a & 0 & 0 & 0 \\ 0 & H_+^b & 0 & 0 \\ 0 & 0 & H_-^a & 0 \\ 0 & 0 & 0 & H_+^b \end{bmatrix} = \begin{bmatrix} H_+ & 0 \\ 0 & H_- \end{bmatrix} \qquad (5)$$

Restricting the approach to 2D systems which are separable into two 1D Hamiltonians, the original 2D Hamiltonian is written as

$$H_o = \mathrm{tr}\, H_+ = a^+a^- + b^+b^- \qquad (6)$$

This formalism allows the immediate extension of the results obtained for 1D systems into two dimensions. Specifically, it is possible to construct a family of Hamiltonians[10]

$$dl_n^+ dl_n^- = H_n - E_n^{(o)} \qquad (7)$$

and obtain the relation among their members:

$$E_n^{(1)} = E_o^{(n+1)} \text{ and } \psi_n^{(1)} = dl_1^+ dl_2^+ \cdots dl_n^+ \psi_o^{(n+1)} \qquad (8)$$

Thus, the n-th member of the super-family is related with the (n+1)-th state of the original Hamiltonian. The ground state of each member $y_o^{(n)}$ is given in terms of the superpotential:

$$dl_n^- \psi_o^n = 0 \Rightarrow \psi_o^b \alpha \begin{bmatrix} e^{-\int^x W_n(Z)dz} \\ e^{-\int^y Z_n(Z)dz} \end{bmatrix} \tag{9}$$

Then, if it is possible to construct the superfamily, one can obtain the spectrum and eigenfunctions from the original problem by the relations in (8). In the next section, the potential (1) is studied by this formalism.

Solving a 2D Schrödinger equation

In parabolic rotational coordinates (x , h , j) [x = x h cos j , y = x h sin j and Z = $(x^2 + h^2)/2$] we can write the Hamiltonian to potential (1) in two 1D equations:[2]

$$H_1^a \chi^a(\xi) = \left\{ -\frac{d^2}{d\xi^2} + \frac{2M}{\hbar^2}(a_1 - E)\xi^2 + \left[\frac{2M}{\hbar^2} b_1 - m^2 - \frac{1}{4}\right]\xi^{-2} \right\}\chi^a(\xi) =$$
$$= \frac{2M}{\hbar^2}\varepsilon_1 \chi^a(\xi) \tag{10}$$

$$H_1^b \chi^b(\eta) = \left\{ -\frac{d^2}{d\eta^2} + \frac{2M}{\hbar^2}(a_2 - E)\eta^2 + \left[\frac{2M}{\hbar 2} b_2 - m^2 - \frac{1}{4}\right]\eta^{-2} \right\}\xi^b(\eta) =$$
$$= \frac{2M}{\hbar^2}\varepsilon_2 \chi^b(\eta) \tag{11}$$

where

$$e_1 + e_2 + c = 0 \tag{12}$$

and the eigenfunctions in the new coordinates are

$$y(x , h , j) = (xh)^{1/2}\, c^a (x) c^b(h) e^{imj} \tag{13}$$

Proceeding as in the 1D case, the superfamily can be constructed and $dl_n^{\pm}$ determined:

$$dl_n^{\pm} = \begin{bmatrix} \pm\frac{d}{d\xi} + \left[\frac{2M}{\hbar^2}(a_1 - E\right]^{1/2}\xi - \left[\left(\frac{2Mb_1}{\hbar^2} - m^2\right)^{1/2} - \frac{1}{2} + \eta_1\right]\frac{1}{\xi} & 0 \\ 0 & \pm\frac{d}{d\eta} + \left[\frac{2M}{\hbar^2}(a_2 - E\right]^{1/2}\eta - \left[\frac{2Mb_2}{\hbar^2} - m^2\right]^{1/2} - \frac{1}{2} + \eta_2 \end{bmatrix} \tag{14}$$

where h_1, h_2 = 0, 1, 2... From eq. (6) and (7) we get

$$E_n^{(1)} = \begin{pmatrix} b_1 A_1 & 0 \\ 0 & b_2 A_2 \end{pmatrix} \tag{15}$$

where

$$_1=\left(\frac{2\hbar^2}{M}(a_1-E)\right)^{1/2},\ b_2=\left(\frac{2\hbar}{M}(a_2-E)\right)^{1/2},\ \nu_1=\left(\frac{2M}{\hbar^2}b_1-m^2\right)^{1/2},$$

$$_2=\left(\frac{2M}{\hbar^2}b_2-m^2\right)^{1/2},\ A_1=1+\nu_1+2\eta,\ \text{and}\ A_2=1+\nu_2+2\eta$$

Using the constraint (12) we get

$$E_{n_1,n_2,m}=\left\{\frac{\left(a_1A_1^2-a_2A_2^2\right)\left(A_1^2-A_2^2\right)+\frac{Mc^2}{2\hbar^2}\left(A_1^2+A_2^2\right)\pm\frac{2c}{M}A_1A_2\left[\left(\frac{Mc}{2\hbar}\right)^2+\frac{M}{2}\left(A_1^2-A_2^2\right)\left(a_2-a_1\right)\right]^{1/2}}{\left(A_1^2-A_2^2\right)^2}\right\}, \tag{16}$$

for $A_1 \# A_2$, and

$$E_{n_1,n_2,m}=\frac{A}{2c^2}\frac{\hbar^2}{M}\left(a_1-a_2\right)^2+\frac{1}{2}\left(a_1+a_2\right)+\frac{c^2M}{8\hbar^2A^2} \tag{17}$$

for $A_1 = A_2 = A$ ($n_1 = n_2 = 2n$, $n=0, \pm 1, \pm 2...$).

These results are in agreement with those in ref.[2] The eigenfunctions are obtained in the usual form from the relations (8) and (9):

$$\chi_n^{(1)}=d|_1^+\, d|_2 \cdots d|_n^+\ \chi_o^{(n+1)} \tag{18}$$

where $c_o^{(n)}$ are given by

$$d|_n^-\ \chi_o^{(n)}=0 \Rightarrow \chi_o^{(n)}=\begin{pmatrix} \xi^{\left(\frac{2Mb_1}{\hbar^2}-m^2\right)^{1/2}-\frac{1}{2}+n_1} & \exp\left\{\left[\frac{M}{2\hbar^2}(a_1-E)\right]^{1/2}\xi^2\right\} \\ \eta^{\left(\frac{2Mb_2}{\hbar^2}-m^2\right)^{1/2}-\frac{1}{2}+n_2} & \exp\left\{\left[\frac{M}{2\hbar^2}(a_2-E)\right]^{1/2}\eta^2\right\} \end{pmatrix} \tag{19}$$

Then, the eigenfunctions for the original problem are y (x , h , j) = (x h)$^{1/2}$ c^a (x) c^b (h) e^{imj} , where c^a(x) and c^b (h) are the components of $c_n^{(1)}$.

Conclusions

A non-usual formalism for SQM and a constructive method to solve Schrodinger equation for 2D potentials is presented. The solution for the potential given in (1) is explicitly determined and the results are the same as obtained from so(2,1) dynamic algebra.[2]

In principle, all results in SQM for 1D systems can be extended for 2D ones. Up to now the formalism presented here is used only to solve Schrodinger equation[4] and to determine isoespectral potentials.[3] However, in principle, all results in SQM for 1D systems (for instance, ref.1,5,6,8,9) can be extended for two dimensions.

Finally, we note that the approach presented can be directly extended to higher dimensional systems.

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RESUMO: O formalismo da mecânica quântica supersimétrica pode ser estendido para dimensões arbitrarias. Nós introduzimos este formalismo e exploramos sua utilidade na resolução da equação de Schrödinger para um potencial bidimensional. Este potencial possuí varias aplicações em física e química, por exemplo, no estudo da molécula de benzeno.

PALAVRAS-CHAVE: Mecânica quântica; supersimetria; sistemas bidimensionais; equação de Schrödinger.

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