Supersymmetric Quantum Mechanics, the Variational Method and a New Shape Invariant Potential

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Born 2 decades ago in the study of the SUSY breaking mechanism of higher dimensional quantum field theories, Supersymmetric Quantum Mechanics (SQM) has so far been considered as a new field of research, providing not only a supersymmetric interpretation of the Schrödinger equation, but interesting answers in all sorts of non-relativistic quantum mechanical systems. Particular points to be mentioned include the better understanding it brought of the exactly solvable,\cite{2}-\cite{3}, the partially solvable,\cite{4},\cite{5}, the isospectral,\cite{6} and the periodic potentials,\cite{7}. Recently the association of the variational method with SQM formalism has been introduced to obtain the approximate energy spectra of non-exactly solvable potentials,\cite{8}-\cite{10}.

Works of reference\cite{8} introduce a scheme based in the hierarchy of Hamiltonians; it permits the evaluation of excited states for one-dimensional systems. In reference\cite{10} a new methodology based in an ansatz for the superpotential which is related to the trial wave function is proposed. This new methodology has been successfully applied to get the spectra of 3-dimensional atomic systems and it is illustrated here through systems well fit by the Hulthén, the Morse and the screened Coulomb potentials,\cite{11},\cite{12},\cite{13}. As a byproduct of this investigation a new exactly solvable potential has been found, a generalization of the Hulthén potential, which presents, in 1-dimension, the property of shape invariance.

Here, these results in a concise form and a sketch of the new potential are presented.

As we learn from the basis of quantum mechanics, (see for instance\cite{13}), the variational method was conceived to be an approximative method to evaluate the energy spectra of a Hamiltonian $H$ and, in particular, its ground state. Its central point is the search for an optimum wave-function $\Psi(r)$ that depends of a number of parameters. This is called the trial wave-function. The approach consists in varying these parameters in the expression for the expectation value of the energy

$$E = \frac{\int \Psi^* H \Psi dr}{\int |\Psi|^2 dr}$$ (1)

until this expectation value reaches its minimum value. This value is an upper limit of the energy level. Even though this method is usually applied to get the ground state energy only, it can also be applied to get the energy of the excited states.

Thus most important for the variational method to work is the acquisition of this optimum wave function. At this crucial point SQM is used to obtain this function. Based in

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physical arguments, an *ansatz* for the superpotential is proposed and, through the super-

algebra, the trial wave function is evaluated. By minimizing the energy expectation value

with respect to a free parameter introduced by the *ansatz* the minimum energy is found.

Consider a system described by a given potential \( V_1 \). The associated Hamiltonian \( H_1 \)

can be factorized in terms of bosonic operators, in \( \hbar = c = 1 \) units, [14]- [17].

\[
H_1 = -\frac{1}{2} \frac{d^2}{dr^2} + V_1(r) = A_1^+ A_1^- + E_0^{(1)}
\]  

(2)

where \( E_0^{(1)} \) is the lowest eigenvalue. Notice that the function \( V_1(r) \) includes the barrier

potential term. The bosonic operators are defined in terms of the so called superpotential \( W_1(r) \),

\[
A_1^\pm = \frac{1}{\sqrt{2}} \left( \mp \frac{d}{dr} + W_1(r) \right).
\]  

(3)

As a consequence of the factorization of the Hamiltonian \( H_1 \), the Riccati equation must

be satisfied,

\[
W_1^2 - W_1' = 2V_1(r) - 2E_0^{(1)}. 
\]  

(4)

Through the superalgebra, the eigenfunction for the lowest state is related to the super-
potential \( W_1 \) by

\[
\Psi_0^{(1)}(r) = N exp \left( - \int_0^r W_1(\bar{r}) d\bar{r} \right).
\]  

(5)

What is clear is that if the potential is non-exactly solvable, the Hamiltonian is not exactly factorizable, in other words, there is no superpotential that satisfies the Riccati equation. The Hamiltonian can however be factorized by an effective potential. In this case, the Riccati equation is exact. What we do is to make an *ansatz* for the superpotential using physical arguments that approximate the effective potential to the true potential. Having a superpotential we use the superalgebra to evaluate the wave function which will definitely depend on a free parameter, the variational parameter.

We stress that in fact we are dealing with an effective potential \( V_{eff} \) that satisfies Riccati equation, i.e.,

\[
V_{eff}(\mu) = \frac{W_1^2 - W_1'}{2} + E(\mu) 
\]  

(6)

where \( W_1 = W_1(\mu) \) is the superpotential that satisfies the Riccati equation, i.e.,

for \( \mu = \bar{\mu} \), the parameter that minimises the energy of eq.(1).

The Hulthén Potential

The Hulthén Potential, in atomic units, is given by

\[
V_H(r) = -\frac{\delta e^{-\delta r}}{1 - e^{-\delta r}},
\]  

(7)

where \( \delta \) is the screening parameter. This potential has been used in several branches of

Physics, (see [18] and references therein). Its Hamiltonian is written as

\[
H = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)}{2r^2}.
\]  

(8)
The associated Schrödinger equation is only solved in closed form for the case $l = 0$, (s waves), [19]. Other than this case, the potential barrier term prevent us to solve the Schrödinger equation and, in SQM superalgebra language, to build the superfamily as can be done when $l = 0$. This case however serves as a basis to construct a superpotential for the $l \neq 0$ case, [10],

$$W_1(r) = B_1 \frac{e^{-\delta r}}{1 - e^{-\delta r}} + C_1$$

(9)

where

$$B_1 = -\frac{\delta}{2} (1 + \sqrt{1 + 4l(l+1)}), \quad C_1 = -\frac{\delta B_1 + 2}{2B_1}.$$  

(10)

This in fact defines, through the Riccati equation, an effective potential whose functional form is

$$V_{\text{eff}}(r) = -\frac{\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)}{2} \frac{\delta^2 e^{-2\delta r}}{(1 - e^{-\delta r})^2} + C_1^2.$$  

(11)

We note that, for small values of $\delta$, the second term of (11) gives us a potential barrier term of (8) in first approximation.

For the state $2p$ we use equation (9) with $l = 1$ and evaluate the wave function, changing $\delta$ by the variational parameter $\mu$, i.e.,

$$\Psi_\mu = \Psi_0^{(1)}(r, \mu) = (1 - e^{-\mu r})^{-\frac{B_1}{\mu}} e^{-C_1 r}.$$  

(12)

The energy is obtained by minimisation with respect to $\mu$. Thus, the equation to be minimised is

$$E_\mu = \int_0^\infty \Psi_\mu(r)[\frac{1}{2} \frac{d^2}{dr^2} - \frac{\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)}{2r^2}]\Psi_\mu(r)dr.$$  

(13)

and the integration is carried out numerically. Our explicit values for the $2p$, ($l = 1$) energy states for some values of the parameter $\delta$ are listed below in Table 1. They are shown together with direct numerical integration data.

| State | Delta | Variational result | Numerical Integration |
|-------|-------|--------------------|-----------------------|
| 2p    | 0.025 | -0.112760          | -0.1127605            |
|       | 0.050 | -0.101042          | -0.1010425            |
|       | 0.075 | -0.089845          | -0.0898478            |
|       | 0.100 | -0.079170          | -0.0791794            |
|       | 0.150 | -0.059495          | -0.0594415            |
|       | 0.200 | -0.041792          | -0.0418860            |

Table 1. Energy eigenvalues as a function of the screening parameter for the states $2p$, [eq.(12)]. Comparison is made with numerical data of Ref.[18].

The Morse Potential

The three dimensional Morse oscillator, suitable to describe a diatomic system, can be written as,

$$V_M = D(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)})$$

(14)
where $D$ is the dissociation energy, $r_e$ is the equilibrium internuclear distance and $a$ is the range parameter. We rewrite the original Schrödinger equation $H\Psi = E\Psi$ in terms of a new variable $y$,

$$\left(-\frac{d^2}{dy^2} + \frac{l(l+1)}{y^2} + \lambda^2(e^{-2(y-y_e)} - 2e^{-(y-y_e)})\right)\Psi(y) = \epsilon\Psi(y)$$  \hspace{1cm} (15)

where $y = ar$ and the constants are set like

$$y_e = ar_e, \quad \lambda^2 = \frac{2mD}{\hbar^2}, \quad E = \epsilon\frac{\hbar^2a^2}{2m}$$  \hspace{1cm} (16)

and the parameter $m$ is the reduced mass of the molecule.

For the case $l = 0$ the system is again exactly solvable and it is used to provide information to the ansatz to be made to the superpotential for the $l \neq 0$ case, for which an analytical exact solution cannot be determined. The superpotential takes the form

$$W_1(y) = -\lambda e^{-(y-y_e)} - \frac{(l+1)}{y} + C.$$  \hspace{1cm} (17)

The argument is that the first term is taken from the one-dimensional results, [21], the case of $l = 0$. The knowledge of the second term comes from the study of three-dimensional potentials, [22]. The related effective potential is given by

$$V_{eff} = -\lambda e^{-(y-y_e)} + \left(-\lambda e^{-(y-y_e)} + \mu - \frac{l+1}{y}\right)^2 - \frac{l+1}{y} + E(\mu)$$  \hspace{1cm} (18)

The eigenfunction obtained from eq. (17) is then

$$\Psi(y) \propto e^{-\lambda e^{-(y-y_e)}} y^{l+1} e^{-Cy}.$$  \hspace{1cm} (19)

Using this expression as a trial wavefunction in the variational method we change the parameter $C$ by the variational parameter $\mu$, i.e.,

$$\Psi_\mu = \Psi(y, C = \mu) \propto e^{-\lambda e^{-(y-y_e)}} y^{l+1} e^{-\mu y}.$$  \hspace{1cm} (20)

The energy is then obtained by minimisation of the energy expectation value with respect to $\mu$. Thus, the equation to be minimised is

$$E_\mu = \frac{\int_0^\infty \Psi_\mu(y)\left[-\frac{d^2}{dy^2} + \lambda^2(e^{-2(y-y_e)} - 2e^{-(y-y_e)}) + \frac{l(l+1)}{y^2}\right]\Psi_\mu(y)dy}{\int_0^\infty \Psi_\mu(y)^2dy}.$$  \hspace{1cm} (21)

We have used this expression to minimize the energy expectation value of various molecules: $H_2$, $HCl$, $CO$ and $LiH$, [11]. The explicit values of the energy for $n = 0$ and different values of $l$ are shown below for the $H_2$ molecule, for known values of their respective potential parameters, [23]: $D, a, r_e$ and $m$. 


Table 2. Energy eigenvalues (in eV) for different values of \( l \) for \( H_2 \) molecule, with \( D = 4.7446 \text{eV}, a = 1.9426\AA^{-1}, r_e = 0.7416\AA \) and \( m = 0.50391\text{amu} \). Comparison is made with results from ref. [20].

The Screened Coulomb Potential

The screened Coulomb potential is given, in atomic units, by

\[
V_{SC} = -e^{-\delta r} \tag{22}
\]

where \( \delta \) is the screened length. The associated radial Schrödinger equation includes the potential barrier term and it is given by

\[
\left( -\frac{1}{2} \frac{d^2}{dr^2} - \frac{e^{-\delta r}}{r} + \frac{l(l+1)}{2r^2} \right) \Psi = E \Psi \tag{23}
\]

where the unit length is \( \hbar^2/m \) and the energy unit is \( \epsilon_0 = -me^4/\hbar^2 \).

In order to determine an effective potential similar to the potential in the Hamiltonian (23), that is the screened Coulomb potential plus the potential barrier term, the following ansatz to the superpotential is suggested

\[
W(r) = -(l+1)\delta e^{-\delta r} + \frac{1}{l+1} - \frac{\delta}{2} \tag{24}
\]

Substituting it into (23), one gets

\[
\Psi_0(r) = (1 - e^{-\delta r})^{l+1} e^{-\left(\frac{1}{(l+1) - \frac{\delta}{2}}\right)r}. \tag{25}
\]

Assuming that the radial trial wave function is given by (25), replacing \( \delta \) by the variational parameter \( \mu \), i.e.,

\[
\Psi_\mu(r) = (1 - e^{-\mu r})^{l+1} e^{-\left(\frac{1}{(l+1) - \frac{\mu}{2}}\right)r}, \tag{26}
\]

the variational energy is given by

\[
E_\mu = \frac{\int_0^\infty \Psi_\mu(r) \left[ -\frac{1}{2} \frac{d^2}{dr^2} - \frac{e^{-\mu r}}{r} + \frac{l(l+1)}{2r^2} \right] \Psi_\mu(r) dr}{\int_0^\infty \Psi_\mu(r)^2 dr}. \tag{27}
\]

Thus, minimizing this energy with respect to the variational parameter \( \mu \) one obtains the best estimate for the energy of the screened Coulomb potential, [12].
As our potential is not exactly solvable, the superpotential given by eq.(24) does not satisfy the Riccati equation (4) but it does satisfy it for an effective potential instead, \( V_{\text{eff}} \)

\[
V_{\text{eff}}(r) = \frac{W_1^2 - W_1'}{2} + E(\bar{\mu})
\]  

(28)

where \( W_1 = W_1(\delta = \bar{\mu}) \) is given by eq.(24) and \( \bar{\mu} \) is the parameter that minimises the energy expectation value, \( (27) \). It is given by

\[
V_{\text{eff}}(r) = -\frac{\delta e^{-\delta r}}{1 - e^{-\delta r}} + \frac{l(l+1)}{2} \frac{\delta^2 e^{-2\delta r}}{(1 - e^{-\delta r})^2} + \frac{1}{2} \left( \frac{1}{l+1} - \frac{\delta^2}{2} \right) + E(\delta),
\]

(29)

where \( \delta = \bar{\mu} \) that minimises energy expectation value. One observes that for small values of \( \delta \) the first term is similar to the potential (22) and the last is approximately the potential barrier term. This observation allows us to conclude that the superpotential (24) can be used to analyse the three dimensional screened Coulomb potential variationally through the trial wavefunction (25).

| \( \delta \) | Variational | Numerical | Variational | Numerical | Variational | Numerical |
|---|---|---|---|---|---|---|
| 0.001 | -0.2480 | -0.2480 | -0.10910 | -0.10910 | -0.06051 | -0.06052 |
| 0.005 | - | - | - | - | -0.52930 | -0.05294 |
| 0.010 | -0.2305 | -0.2305 | -0.09212 | -0.09212 | -0.04419 | -0.04420 |
| 0.020 | -0.2119 | -0.2119 | -0.07503 | -0.07503 | -0.02897 | -0.02898 |
| 0.025 | -0.2030 | -0.2030 | -0.06714 | -0.06715 | - | - |
| 0.050 | -0.1615 | -0.1615 | -0.03374 | -0.03383 | - | - |
| 0.100 | -0.09289 | -0.09307 | - | - | - | - |

Table 3. Energy eigenvalues as function of the screening parameters \( \delta \) for \( 2p \) \((l = 1) \), \( 3d \) \((l = 2) \) and \( 4f \) \((l = 3) \) states, in rydberg units of energy. Comparison is made with results from references [24]-[29].

Comments
We have proposed trial wavefunctions to be used in the variational calculation in order to determine the energy eigenvalues of some atomic systems described by the Hulthén, the Morse and the screened Coulomb potentials. These functions were induced from the formalism of SQM. Using physical arguments it is possible to make an \textit{ansatz} in the superpotential which satisfies the Riccati equation by an effective potential. The superalgebra enables us to take this superpotential and to evaluate the trial wavefunctions that contains the variational parameter, the parameter that minimises the energy expectation value of the energy. The results are in very good agreement with the ones available in the literature.

Thus this new methodology that associates the variational method with SQM is a simple and good alternative procedure that enables the evaluation of the energy spectra with reasonable accuracy. In particular, when applying the approach to the Hulthén potential it was found that its effective potential was linked to a new exactly solvable potential, that presents, in one-dimension the property of shape invariance. At that time the focus
of our attention was not on the properties of this new potential, whose main results are presented below.

**A new shape-invariant potential**

As mentioned above, in [10] when dealing with the evaluation of the trial wave function, the following one-dimensional potential, a generalization of the Hulthén potential, was found,

\[
V(x) = A \frac{e^{-2\delta x}}{(1 - e^{-\delta x})^2} - B \frac{\delta e^{-\delta x}}{1 - e^{-\delta x}}.
\]  

(30)

Notice that when setting \( A = 0 \) and \( B = 1 \) the original Hulthén potential is recovered, eq. (7). For convenience we redefine the constants \( A \) and \( B \) such that \( V(x) \) becomes

\[
V_1(x) = a_1(a_1 - \delta) \frac{e^{-2\delta x}}{2(1 - e^{-\delta x})^2} - a_1(2b_1 + \delta) \frac{e^{-\delta x}}{2(1 - e^{-\delta x})}.
\]  

(31)

From the basis of SQM the following superpotential

\[
W_1 = -a_1 \frac{e^{-\delta x}}{1 - e^{-\delta x}} + b_1
\]  

(32)

factorizes the related Hamiltonian

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

(33)

and satisfies the Riccati equation associated

\[
W_1^2(r) - W_1'(x) = 2V_1 - 2E_0^{(1)}
\]

\[
= a_1(a_1 - \delta) \frac{e^{-2\delta x}}{(1 - e^{-\delta x})^2} - a_1(2b_1 + \delta) \frac{e^{-\delta x}}{(1 - e^{-\delta x})} + b_1^2
\]

where the lowest energy-eigenvalue is given by

\[
E_0^{(1)} = -\frac{b_1^2}{2}
\]  

(34)

From the superalgebra, the associated eigenfunction, is given by

\[
\Psi_0^{(1)} = (1 - e^{-\delta x})^{\frac{a_1}{\delta}} e^{-b_1 x}.
\]  

(35)

The condition we must impose on the above wave-functions is to vanish at infinity and at the origin, i.e.,

\[
a_1 \delta > 0, \quad b_1 > 0 \quad \Rightarrow \quad a_1, b_1, \delta > 0
\]  

(36)

This process of factorization can be repeated and the whole hierarchy of this potential can be evaluated. The general form for the superpotential is written as

\[
W_{n+1} = -a_{n+1} \frac{e^{-\delta x}}{1 - e^{-\delta x}} + b_{n+1}
\]  

(37)
which are related to the potentials
\[
V_{n+1} = a_{n+1}(a_{n+1} - \delta) \frac{e^{-2\delta x}}{2(1 - e^{-\delta x})^2} - a_{n+1}(2b_{n+1} + \delta) \frac{e^{-\delta x}}{2(1 - e^{-\delta x})}
\] (38)
with lowest levels given by
\[
E^{(n+1)}_0 = -\frac{b^2_{n+1}}{2}
\] (39)
and with the constants being given by
\[
a_{n+1} = a_1 + n\delta 
\] (40)
and
\[
b_{n+1} = \frac{1}{2a_{n+1}}(a_1(2b_1 + \delta) - 2\delta(na_1 + \frac{n(n - 1)\delta}{2}) - \frac{\delta}{2}.
\] (41)
For the particular case where \(n = 0\) and fixing the constants to
\[
a_1 = \delta , \quad 2b_1 + \delta = 2
\] (42)
the original Hulthén potential is recovered,
\[
V_1(x) = -\delta \frac{e^{-\delta x}}{1 - e^{-\delta x}}
\] (43)
which can also be factorized, as already known, \([10]\). Its whole hierarchy of potentials is given by
\[
V_n = \frac{n(n - 1)\delta^2 e^{-2\delta x}}{2(1 - e^{-\delta x})^2} - \frac{\delta(2 + n(1 - n)\delta)e^{-\delta x}}{2(1 - e^{-\delta x})}
\] (44)
with lowest energy levels
\[
E^{(n)}_0 = -\frac{1}{2} \left( \frac{1}{n} - \frac{n\delta}{2} \right)^2
\] (45)
and related superpotentials
\[
W_n(x) = -a_n \frac{e^{-\delta x}}{1 - e^{-\delta x}} + b_n
\] (46)
where the lowest states are
\[
\Psi^{(n)}_0 = (1 - e^{-\delta x})^{a_n/\delta} e^{-b_n x}
\] (47)
with constants given by
\[
a_n/\delta = n , \quad b_n = \frac{1}{n} - \frac{n\delta}{2}.
\] (48)
At this point we remark that the Hulthén potential is non-shape-invariant, \([2]\). This is clear by observing the \(n = 1\) and \(n = 2\) cases of equation (44), whereas the new potential clearly is shape invariant, since all the potentials preserve the shape in the hierarchy eq. (38). More details shall soon be found in \([31]\).
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