Supersymmetric variational energies of 3d confined potentials\textsuperscript{1}

Elso Drigo Filho\textsuperscript{2,3}  
Instituto de Biociências, Letras e Ciências Exatas, IBILCE-UNESP  
Rua Cristovão Colombo, 2265 - 15054-000 São José do Rio Preto - SP

Regina Maria Ricotta\textsuperscript{4}  
Faculdade de Tecnologia de São Paulo, FATEC/SP-CEETPS-UNESP  
Praça Fernando Prestes, 30 - 01124-060 São Paulo-SP  
Brazil

Abstract

Within the approach of Supersymmetric Quantum Mechanics associated with the variational method a recipe to construct the superpotential of three dimensional confined potentials in general is proposed. To illustrate the construction, the energies of the Harmonic Oscillator and the Hulthén potential, both confined in three dimensions are evaluated. Comparison with the corresponding results of other approximative and exact numerical results is presented.
1. Introduction

Supersymmetric Quantum Mechanics, (SQM), was conceived in 1981 as the simplest field theory that would provide understanding of the supersymmetry breaking mechanism of higher dimensional field theories, [1]. Since then this formalism has become a new field of research and a great deal of work, both analytical and numerical, has been done to get better knowledge of the exactly solvable, the partially solvable, the isospectral, the periodic and the non-exactly solvable potential problems, (see [2] for the latest review). In particular, few of these latter have been investigated through a novel methodology based on the association of the variational method with SQM formalism. The conjunction of this well known quantum mechanism with SQM has given a simple framework to investigate spectral problems of Hamiltonian systems associated to the three dimensional Hulthén, Morse and Screened Coulomb potentials,[3]-[5]. The main basis of the method consists in setting an Ansatz for the superpotential. Based on the superalgebra intrinsic of SQM we are able to evaluate the wavefunction which naturally contains free parameters introduced by the Ansatz. Having in hands our ideal wavefunction, the calculations to be done are the usual variational calculations in which the parameters are varied until the energy expectation value reaches its minimum.

More recently the application of this methodology to exploit the energy spectra of a confined quantum mechanical system gave encouraging results: the confined 3-dimensional hydrogen atom showed results compatible with those obtained from other approximative methods and numerical calculation, [6].

Motivated by these results and considering the widespread interest in quantum confined systems, particularly in the studies of semiconductor heterostructures (nanostuctures like quantum dots, quantum wires, quantum wells), [7]-[9], as well as in field theory, [10], in this work we propose a systematic construction of the superpotential for 3d confined systems, that yields, through SQM, to the trial wavefunction pursued.

To illustrate the construction, the technique is applied here to get the 1s and 2p energy states for the confined Harmonic Oscillator and for the 1s, 2p and 3d energy states of the confined Hulthén, both in three dimensions. They are very good when compared to recent results obtained from other approximative methods as well as exact numerical results, [11]-[15].

In what follows, in order to be self consistent and to set up the notation, we present a brief description of SQM and its association with the variational method. At this point we introduce our recipe for the superpotential in the general case. Then we show the results of the application of this formalism to the confined Harmonic Oscillator and Hulthén potential. Comparison with the corresponding results of other approximative and exact numerical results is presented in the tables, followed by a discussion and our conclusions.

2. Supersymmetric Quantum Mechanics and the Variational Method

The starting point is the factorization of a Hamiltonian $H$ associated to a given
potential \( V(r) \), in terms of bosonic operators \( A^\pm \) and the lowest energy eigenvalue \( E_0 \). In \( \hbar = c = 1 \) units, this is written as

\[
H = -\frac{1}{2} \frac{d^2}{dr^2} + V(r) = A^+ A^- + E_0.
\]  

(1)

We recall that for the cases we are considering the potential is symmetric so that equation (1) is the radial equation and \( V(r) \) includes the barrier potential term. The bosonic operators are defined in terms of the so called superpotential \( W(r) \),

\[
A^\pm_1 = \frac{1}{\sqrt{2}} \left( \mp \frac{d}{dr} + W(r) \right).
\]  

(2)

Thus, substituting the bosonic operators into equation (1) we conclude that, as a consequence of the factorization of the Hamiltonian \( H \), the Riccati equation must be satisfied,

\[
W^2 - W' = 2 \left( V(r) - E_0 \right),
\]  

(3)

where \( W' = \frac{dW}{dr} \). Also through the superalgebra, the eigenfunction for the lowest state is related to the superpotential \( W \) by

\[
\Psi_0(r) = N \exp(-\int_0^r W(\bar{r}) d\bar{r}).
\]  

(4)

The above scheme works perfectly well if the potential is exactly solvable. However, if the potential is non-exactly solvable, the Hamiltonian is not exactly factorizable, i.e., there is no superpotential that satisfies equation (3). On the other hand, the Hamiltonian can be factorized in terms of an approximated superpotential giving rise to an effective potential. This is achieved by making an Ansatz for the superpotential, which naturally introduces free parameters in the problem, denoted by the set \( \{ \mu \} \).

Thus, through the superalgebra, the wavefunction, (equation (4)), is evaluated. It is the trial wavefunction of the usual variational method, denoted by \( \Psi_\mu \) and depending on \( \{ \mu \} \). Therefore, having in hands the main ingredient of the variational method, namely the trial wavefunction, the energy expectation value given by

\[
E_\mu = \frac{\int \Psi_\mu^* H \Psi_\mu dr}{\int |\Psi_\mu|^2 dr}
\]  

(5)

can be evaluated and the parameters can be varied until it reaches its minimum value, \( E(\bar{\mu}) \), which is an upper limit of the sought energy level. Indeed, the Ansatz in the superpotential drives us to an effective potential \( V_{eff} \) that has a similar form as the original potential, i.e.,

\[
V_{eff}(r) = \frac{1}{2} \left( \tilde{W}^2 - \tilde{W}' \right) + E(\bar{\mu})
\]  

(6)

where \( \tilde{W} = W(\bar{\mu}) \) is the superpotential for \( \{ \mu = \bar{\mu} \} \), the set of parameters that minimises (5). The above methodology was applied in the search of approximate
energy levels of 3-dimensional systems, like the Hulthén, Morse and Screened Coulomb potentials, [3]-[5].

Concerning the confinement, it is remarkable that for the confined cases we have treated so far, the confined Coulomb, [6], and the present cases of the confined Oscillator and Hulthén potentials, the Ansatz set in the superpotential is restricted to an extra confining term added to the superpotential used in the non-confined case, i.e.,

\[ W_{\text{confined}} = W_{\text{non-confined}} + \frac{\text{constant}}{R - r} \]  \hspace{1cm} (7)

where \( R \) is the radius of confinement. The advantage of this choice is that it allows us a previous comparative analysis between the original potential (non-confined) and the effective potential, containing the infinite (confining) barrier. This is corroborated by the fact that in the \( R \to \infty \) limit the non-confined superpotential is recovered. Moreover, the trial wavefunction will naturally vanish at the barrier \( R = r \) and not as an input, as it is usual in the variational calculation.

3. The Confined Harmonic Oscillator

The radial Hamiltonian equation for the Harmonic Oscillator potential, written in atomic units is given by

\[ H = -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l + 1)}{2r^2} + \frac{r^2}{2}. \]  \hspace{1cm} (8)

As the Harmonic Oscillator potential is symmetric, the confinement is introduced by an infinite potential barrier at radius \( r = R \). Thus we make the following Ansatz for the superpotential

\[ W(r) = -\frac{\mu_1}{r} + \frac{\mu_2}{R - r} + \mu_3 r \]  \hspace{1cm} (9)

which depends of \( R \), the radius of confinement, and of three variational parameters, \( \mu_1, \mu_2 \) and \( \mu_3 \). As stated in expression (7), the first and the last terms are already known from the non-confined case, [2]. The second term deals with the confinement. This is explicitly shown through the effective potential. From equation (6), it has the following form

\[ V_{\text{eff}}(r) = \frac{\bar{\mu}_3}{2} r^2 + \frac{\bar{\mu}_1(\bar{\mu}_1 - 1)}{2r^2} - \bar{\mu}_1 \bar{\mu}_3 - \frac{\bar{\mu}_3}{2} + \frac{\bar{\mu}_2(\bar{\mu}_2 - 1)}{2(R - r)^2} - \frac{\bar{\mu}_1 \bar{\mu}_2}{r(R - r)} + \frac{\bar{\mu}_2 \bar{\mu}_3 r}{(R - r)} + E(\bar{\mu}) \]  \hspace{1cm} (10)

which is clearly infinite at \( r = R \), as expected for a confining system. Notice that the effective potential is evaluated for the values of the set of parameters \( \{\bar{\mu}\} \) that minimise the energy. Our trial wavefunction for the variational method is obtained from the superalgebra through equation (4), using the superpotential given by the Ansatz made in equation (9). It is given by

\[ \Psi_\mu(r) = \Psi(\mu_1, \mu_2, \mu_3, r) \propto r^{\mu_1} (R - r)^{\mu_2} e^{-\mu_3 r^2/2}. \]  \hspace{1cm} (11)
It depends on three free parameters, $\mu_1$, $\mu_2$ and $\mu_3$ and vanishes at $r = R$. We use this trial wavefunction to calculate the energy expectation value, given by the equation (5), evaluated with the Hamiltonian (8). Its minimisation with respect to the three parameters gives $E(\bar{\mu})$, which, from now on, we call $E_{\text{vsqm}}$. The results are given in the tables below for different values of the confining radius $R$ and states 1s and 2p, corresponding to the values of $l = 1$ and 2 of the angular momentum, respectively. Comparison is made with exact numerical, $E_{\text{exact}}$, perturbative, $E_{\text{pert}}$, [11], other variational, $E_{\text{var}}$, [12], WKB, $E_{\text{wkb}}$, [13] and modified WKB results, $E_{\text{centri}}$, [15], through the percentage errors,

$$\delta_{\text{vsqm}} = \frac{|E_{\text{exact}} - E_{\text{vsqm}}|}{E_{\text{exact}}} \%$$

and

$$\delta_{\text{pert}} = \frac{|E_{\text{exact}} - E_{\text{pert}}|}{E_{\text{exact}}} \%.$$  

The same percentage errors are applied to the other results. We must note that the perturbative results lost their accuracy for large values of the radius of confinement, for which they are outside the convergence region. For the results of Table 1, $R < 1.72$ and of the Table 2, $R < 1.84$.

It should be stressed that in the limit of no-confinement, i.e. $R \to \infty$, the variational SQM results also agree with the exact non-confined problem, corresponding to the removal of the infinite barrier. In this case the energy is exact and is given by

$$E = 2n + L + 3/2.$$  

Thus for $n = 0$ and $l = 0$, state 1s, the exact result is $E_{R \to \infty} = 1.5000$, (Table 1), and for $n = 0$ and $l = 1$, state 2p, the exact result is $E_{R \to \infty} = 2.5000$, (Table 2).

Table 1. Energy eigenvalues (in Rydbergs) and percentage errors for different values of $R$ for the 1s state, ($l = 0$).

| R     | $E_{\text{exact}}$ | $E_{\text{vsqm}}$ | $\delta_{\text{vsqm}}$ | $E_{\text{pert}}$ | $\delta_{\text{pert}}$ | $E_{\text{wkb}}$ | $\delta_{\text{wkb}}$ | $E_{\text{var}}$ | $\delta_{\text{var}}$ |
|-------|--------------------|-------------------|------------------------|-------------------|------------------------|----------------|------------------------|----------------|------------------------|
| 1.0   | 5.0755             | 5.0865            | 0.22                   | -                 | -                      | 5.0627        | 0.25                   | 5.1313        | 1.10                   |
| 1.5   | 2.5050             | 2.5104            | 0.22                   | 2.5046            | 0.02                   | 2.5082        | 0.13                   | 2.5265        | 0.86                   |
| 2.0   | 1.7648             | 1.7664            | 0.09                   | 1.7588            | 0.34                   | 1.9882        | 12.7                   | 1.7739        | 0.52                   |
| 2.5   | 1.5514             | 1.5529            | 0.10                   | -                 | -                      | 1.5564        | 0.32                   | 1.5567        | 0.34                   |
| 3.0   | 1.5061             | 1.5069            | 0.05                   | 1.1532            | 23.4                   | 1.5061        | 0.00                   | 1.5105        | 0.29                   |
| 4.0   | 1.5000             | 1.5002            | 0.01                   | -                 | 4.341728              | 1.5000        | 0.00                   | 1.5033        | 0.22                   |
| 5.0   | 1.5000             | 1.5000            | 0.00                   | -                 | -8.076319             | 1.5000        | 0.00                   | 1.5025        | 0.17                   |
| 10.0  | 1.5000             | 1.5000            | 0.00                   | -                 | -                      | 1.5000        | 0.00                   | -             | -                      |
### Table 2. Energy eigenvalues (in Rydbergs) and percentage errors for different values of $R$ for the $2p$ state, ($l = 1$).

| $R$ | $E_{exact}$ | $E_{vsqm}$ | $\delta_{vsqm}$ | $E_{pert}$ | $\delta_{pert}$ | $E_{wkb}$ | $\delta_{wkb}$ | $E_{var}$ | $\delta_{var}$ | $E_{centri}$ | $\delta_{centri}$ |
|-----|-------------|------------|----------------|-----------|----------------|---------|--------------|---------|--------------|-------------|----------------|
| 0.3 | 112.188     | 112.231    | 0.04           | 112.188   | 0.00           | -       | -            | -       | -            | -           | -              |
| 1.0 | 10.2822     | 10.2847    | 0.02           | -         | -              | 10.2643 | 0.17         | 10.3188 | 0.36         | 10.2876     | 0.05           |
| 1.5 | 4.9036      | 4.9046     | 0.02           | 4.9034    | 0.00           | 4.9084  | 0.01         | 4.9169  | 0.27         | 4.9068      | 0.07           |
| 2.0 | 3.2469      | 3.2471     | 0.01           | 3.2434    | 0.11           | 3.2490  | 0.07         | 3.2514  | 0.14         | 3.3081      | 1.88           |
| 2.5 | 2.6881      | 2.6891     | 0.04           | -         | -              | 2.7079  | 0.74         | 2.6901  | 0.07         | 2.6835      | 0.17           |
| 3.0 | 2.5313      | 2.5322     | 0.04           | 2.3104    | 0.73           | 2.5310  | 0.01         | 2.5337  | 0.10         | 2.5313      | 0.00           |
| 4.0 | 2.5001      | 2.5003     | 0.01           | -1.5656   | 163            | 2.5001  | 0.00         | 2.5015  | 0.06         | 2.5001      | 0.00           |
| 5.0 | 2.5000      | 2.5000     | 0.00           | -34.0358  | -              | 2.5000  | 0.00         | 2.5012  | 0.05         | 2.5000      | 0.00           |
| 10.0| 2.5000      | 2.5000     | 0.00           | -         | -              | 2.5000  | 0.00         | -       | -            | -           | -              |

### 4. The Confined Hulthén Potential

The radial Hamiltonian equation for the Hulthén potential, written in atomic units is given by

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

(15)

Once again, as the potential is symmetric, the confinement is introduced by the infinite potential barrier at radius $r = R$. The associated Ansatz for the superpotential follows the equation (7) and the expression for the superpotential given for the unconfined case, as in [3],

$$W(r) = B_1 \frac{e^{-\mu_1 r}}{(1 - e^{-\mu_1 r})} + C_1 + \frac{\mu_2}{R - r}$$

(16)

where

$$B_1 = -\mu_1 (l + 1), \quad C_1 = -\frac{1}{2} \mu_1 + \frac{1}{l + 1}.$$  

(17)

This superpotential gives rise through the superalgebra, (4), to the following trial wavefunction

$$\Psi_\mu = \Psi(\mu_1, \mu_2, r) \propto (1 - e^{-\mu_1 r})^{-\frac{\mu_1}{\mu_1}} e^{-C_1 r} (R - r)^{\mu_2}.$$  

(18)

It depends of two free parameters, $\mu_1$ and $\mu_2$ and vanishes at $r = R$, as expected, since the effective potential, evaluated by using equations (6), (16) and (17), is infinite at this point. Its general form is

$$V_{eff}(r) = -\frac{\mu_1 e^{-\mu_1 r}}{1 - e^{-\mu_1 r}} + \frac{l(l+1)}{2} \frac{\mu_1^2 e^{-2\mu_1 r}}{(1 - e^{-\mu_1 r})^2} + \frac{\mu_2 (\mu_2 - 1)}{(R - r)^2} - \frac{(l+1)\mu_1 \mu_2 e^{-\mu_1 r}}{(R - r)(1 - e^{-\mu_1 r})} - \frac{\mu_1 \mu_2}{2(R - r)} + \frac{\mu_2}{(l+1)(R - r)} + \frac{1}{2} (-\frac{\mu_1}{2} + \frac{1}{l+1})^2 + E(\bar{\mu}).$$

(19)
As in the previous case, \( \{ \bar{\mu} \} \) is the set of parameters that minimise the energy, given by \( E(\bar{\mu}) \), which we also call, from now on, \( E_{\text{vsqm}} \). The results are in the tables below, for different values of the parameter \( \delta \) and the confining radius \( R \), for the states 1s, 2p and 3d, corresponding to the values of \( l = 1, 2 \) and 3 of the angular momentum, respectively. Comparison is made with exact numerical, \( E_{\text{exact}} \), from the 1/N approximation, \( E_{1/N} \), [14] and modified WKB results, \( E_{\text{centri}} \), [15].

For \( R \to \infty \) exact values of the energy are only for the \( l = 0 \) case, and are given by

\[
E = -\frac{1}{2} \left( \frac{1}{n} - \frac{n\delta}{2} \right)^2
\]

(20)

Thus for \( \delta = 0.1 \) and \( n = 1 \) the exact result is \( E_{R \to \infty} = -0.45125 \), (Table 3).

**Table 3.** Energy eigenvalues (in Rydbergs) for different values of \( R \), \( n = 1 \) and \( l = 0, 1, 2 \), (states 1s, 2p and 3d) and \( \delta = 0.1 \).

| R  | 1  | \( E_{\text{exact}} \) | \( E_{\text{vsqm}} \) | \( \delta_{\text{vsqm}} \) | \( E_{1/N} \) | \( \delta_{1/N} \) | \( E_{\text{centri}} \) | \( \delta_{\text{centri}} \) |
|----|----|----------------|----------------|---------------|-------------|--------------|----------------|----------------|
| 6.0| 0  | -0.45053       | -0.44945       | 0.24          | -0.45109    | 0.12         | -0.00782       | 9.60           |
|    | 1  | -0.00865       | -0.00808       | 6.59          | -0.00294    | 66.0         | -0.00782       | 9.60           |
| 7.0| 0  | -0.45111       | -0.45043       | 0.15          | -0.45181    | 0.16         | -0.00782       | 9.60           |
|    | 1  | -0.04069       | -0.04037       | 0.79          | -0.03324    | 18.3         | -0.03976       | 2.29           |
| 8.0| 0  | -0.45122       | -0.45076       | 0.10          | -0.45193    | 0.16         | -0.00782       | 9.60           |
|    | 1  | -0.05783       | -0.05762       | 0.36          | -0.05293    | 8.47         | -0.05510       | 4.72           |
| 9.0| 0  | -0.45125       | -0.45090       | 0.08          | -0.45188    | 0.14         | -0.00782       | 9.60           |
|    | 1  | -0.06728       | -0.06712       | 0.24          | -0.06389    | 5.04         | -0.06612       | 1.72           |
| 10.0| 0   | -0.45125     | -0.45098      | 0.06          | -0.45179    | 0.12         | -0.00782       | 9.60           |
|    | 1  | -0.07257       | -0.07243       | 0.19          | -0.07008    | 3.43         | -0.07196       | 0.84           |
| 25.0| 0  | -0.45125       | -0.45125       | 0.00          | -0.45131    | 0.01         | -0.00782       | 9.60           |
|    | 1  | -0.07918       | -0.07915       | 0.04          | -0.07920    | 0.03         | -0.07921       | 0.04           |
|    | 2  | -0.01390       | -0.01380       | 0.72          | -0.01332    | 4.17         | -0.01381       | 0.65           |
| 50.0| 0  | -0.45125       | -0.45125       | 0.00          | -0.45126    | 0.00         | -0.00782       | 9.60           |
|    | 1  | -0.07918       | -0.07918       | 0.00          | -0.07920    | 0.03         | -0.07920       | 0.03           |
|    | 2  | -0.01448       | -0.01448       | 0.00          | -0.01450    | 0.14         | -0.01450       | 0.14           |

**Table 4.** Energy eigenvalues (in Rydbergs) and percentage errors for different values of \( R \) for the 2p state, \( l = 1 \) and \( \delta = 0.2 \).

| R  | \( E_{\text{exact}} \) | \( E_{\text{vsqm}} \) | \( \delta_{\text{vsqm}} \) | \( \tilde{E}_{1/N} \) | \( \delta_{1/N} \) | \( E_{\text{centri}} \) | \( \delta_{\text{centri}} \) |
|----|----------------|----------------|---------------|-------------|--------------|----------------|----------------|
| 8  | -0.01731       | -0.01708       | 1.33          | -0.01242    | 28.3         | -0.01607       | 7.16           |
| 9  | -0.02749       | -0.02731       | 0.65          | -0.02428    | 11.7         | -0.02612       | 4.98           |
| 10 | -0.03339       | -0.03323       | 0.48          | -0.03118    | 6.62         | -0.03389       | 1.50           |
| 25 | -0.04188       | -0.04178       | 0.24          | -0.04199    | 0.26         | -0.04192       | 0.10           |
| 50 | -0.04189       | -0.04189       | 0.00          | -0.04196    | 0.17         | -0.04191       | 0.05           |
5. Discussion and conclusions

The study of the two 3-dimensional confined quantum systems considered here was made through the mechanism based on the association of the variational method with SQM, using the recipe given to construct the superpotential, equation (7). For the two cases considered, namely, the Harmonic Oscillator and the Hulthén potential, the Ansatz, as given by equations (9) and (16), respectively, naturally introduced free parameters in the superpotential. Thus, using the superalgebra the wave functions were evaluated, showing, of course, explicit dependence on these parameters, equations (11) and (18), respectively. They were our optimal wave functions, used to calculate the energy expectation values, equation (5), as in the usual variational method. The parameters were varied until this expectation value reached its minimum, giving rise to the searched energy states.

The peculiar feature of the approach is that, when doing the Ansatz to the superpotential following the recipe of equation (7), we were able to evaluate the effective potential, equation (6), and also equations (10) and (19), which resemble the real, confining potential under consideration. In both cases, the effective potential is surely infinite at the border, \( r = R \), and as a result the wave function, evaluated through the superalgebra, equation (4), naturally vanishes at the border because it finds a potential barrier that increases until becoming impenetrable at \( r = R \). Furthermore, for increasing values of \( R \) the border effects vanish and our effective potential becomes the original non-confined potential. The results for the energies improved, when compared with the corresponding results of other approximative and exact numerical results, converging to the results of the non-confined system. On the other hand, for small values of \( R \), stronger are the border effects, but even so very small deviation from the exact numerical results were found.

We conclude that our main result is the recipe given for the superpotential when confinement takes place, equation (7). The inclusion of the confining term \( \frac{1}{r} \) in the superpotential was crucial to describe border effects. This prescription showed to be appropriate to get good results for the cases considered so far and can be a first trial to exploit other confined systems through this method. It is remarkable that the approach was applied to different systems. Contrary to the Coulomb potential, [6], and the Harmonic Oscillator, the Hulthén potential is not exactly solvable in three dimensions. This makes our recipe good enough to work in the general case and reinforces the fact that the association of the superalgebra of SQM with the variational method gives a simple and useful framework to investigate confined systems in general.
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