Supersymmetric variational energies for the confined Coulomb system

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Abstract

The methodology based on the association of the Variational Method with - Supersymmetric Quantum Mechanics is used to evaluate the energy states of the confined hydrogen atom.

Introduction

Confined systems have motivated many studies in different areas of physics. Nowadays it culminates with low dimensional systems of technological applications like quantum dots in semiconductors, [1]. Several authors have worked in a variety of methods aiming the energy eigenvalues of such systems, [2]-[8]. Particularly, the conventional variational method has also been used, [9]-[10] and references therein.

In this context the association of the variational method applied within the formalism of Supersymmetric Quantum Mechanics, SQM, seems to be another appropriate alternative to tackle such problem.

SQM has provided good results concerning different nonrelativistic quantum mechanical systems, such as the exactly solvable, [11]-[12], the partially solvable, [13]-[14], the isospectral, [15] and the periodic potentials, [16]. In particular, it gave good results for the energy states of systems well fit by the Hulthén, the Morse and the screened Coulomb potentials, [17]-[19], which are all non-exactly solvable potentials in 3-dimensions. The latter were studied using a methodology based on the association of the variational method with SQM. Its starting point is the association of an Ansatz for the superpotential. Through the superalgebra the wave function is evaluated,
the so-called trial wave function containing the variational parameters, which will be varied until the energy expectation value reaches its minimum.

In this letter this approach is applied to the 3-dimensional confined hydrogen atom in order to get its the energy states. This system is analogous to the hydrogenic donor located at the centre of a spherical $GaAs - (Ga, Al)As$ quantum dot. The results obtained here for the $1s$, $2p$ and $3d$ states are very good when compared to recent results obtained from other approximative methods as well as numerical exact results, [10].

**The variational method associated to SQM**

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, [20]- [23].

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

(1)

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 $W_1(r)$,

$$A_1^\pm = \left( \pm \frac{d}{dr} + W_1(r) \right).$$

(2)

As a consequence of the factorization of the Hamiltonian $H_1$, the Riccati equation must be satisfied,

$$W_1^2 - W_1' = V_1(r) - E_0^{(1)}.$$  

(3)

Through the superalgebra, the eigenfunction for the lowest state is related to the superpotential $W_1$ by

$$\Psi_0^{(1)}(r) = N \exp(- \int_0^r W_1(\bar{r}) d\bar{r}).$$

(4)

It should be stressed that if the potential is non-exactly solvable, the Hamiltonian is not exactly factorizable which means that there is no superpotential that satisfies the Riccati equation. However, the Hamiltonian can be factorized in terms of a superpotential giving rise to an effective potential that best mimics the true potential. Thus, using the superalgebra we evaluate the wave function which will depend on free parameters, the variational parameters.

The variational method is an approximative technique 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 $\Psi(r)$ depending on a set of parameters, $\{\mu\}$. This is called the trial wave-function. The approach consists in varying these parameters in the expression for the expectation value of the energy

$$E = \frac{\int \Psi_\mu^* H \Psi_\mu dr}{\int |\Psi_\mu |^2 dr}$$

(5)
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, the aim of the variational method is the acquisition of this optimum wave-function. Conventionally one proposes a variational wavefunction depending on a set of parameters. At this crucial point, however, our strategy is to use SQM to obtain this function. Based on physical arguments, an Ansatz for the superpotential is proposed and, through the superalgebra, the trial wave function is evaluated, (equation (4)). By minimizing the energy expectation value with respect to the free parameters introduced by the Ansatz the minimum energy is found.

We stress that, in fact, by making an Ansatz in the superpotential corresponds to be dealing with an effective potential \( V_{\text{eff}} \) that satisfies the Riccati equation, i.e.,

\[
V_{\text{eff}}(r) = \bar{W}_1^2 - \bar{W}_1' + E(\bar{\mu})
\]

(6)

where \( \bar{W}_1 = W_1(\bar{\mu}) \) is the superpotential that satisfies (4) for \( \mu = \bar{\mu} \), the parameter that minimises the energy of eq.(5).

The Confined Coulomb Potential

The radial Hamiltonian equation for the Coulomb Potential, written in atomic units, is given by

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

(7)

We use the variational method associated to SQM in order to get the energy states of the confined Coulomb Potential. As the Coulomb 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

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

(8)

which depends on \( R \), the radius of confinement, and three variational parameters, \( \mu_1 \), \( \mu_2 \) and \( \mu_3 \). The first and the last terms are already known from the non-confined case, [23]. The second term deals with the confinement, as shown below in the effective potential.

Substituting this superpotential in the associated Riccati equation we arrive at a confining effective potential \( V_{\text{eff}} \), i.e., a potential which is infinite at \( r = R \). It is given by

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

\[
= \frac{\mu_1(\mu_1 - 1)}{r^2} + \frac{\mu_2(\mu_2 - 1)}{(R-r)^2} - \frac{2\mu_1\mu_3}{r} - \frac{2\mu_1\mu_2}{r(R-r)} + \frac{2\mu_2\mu_3}{R-r} + \mu_3^2 + E(\bar{\mu})
\]

(9)

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.
As mentioned before, 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 (8). It is given by

\[ \Psi(\mu_1, \mu_2, \mu_3, r) \propto r^{\mu_1} (R - r)^{\mu_2} e^{-\mu_3 r}. \]  

(10)

It depends on three free parameters, \(\mu_1, \mu_2\) and \(\mu_3\) and vanishes at \(r = R\).

The energy is obtained by minimisation of the energy expectation value with respect to the three parameters. The equation to be minimised is given by

\[ E(\mu_1, \mu_2, \mu_3) = \frac{\int_0^R \Psi(\mu_1, \mu_2, \mu_3, r)[-\frac{d^2}{dr^2} - \frac{2}{r} + \frac{l(l+1)}{r^2}]\Psi(\mu_1, \mu_2, \mu_3, r)dr}{\int_0^R \Psi(\mu_1, \mu_2, \mu_3, r)dr}. \]  

(11)

After the minimisation of (11) with respect to the parameters \(\mu_1, \mu_2\) and \(\mu_3\) we get \(E(\bar{\mu})\) which, from now on, will be referred as \(E_{VSQM}\).

The tables 1, 2 and 3 below show the results for different values of \(R\) and \(l\) and the comparison with the exact numerical, \(E_{EXACT}\), and conventional variational results, \(E_V\), contained in [10]. The comparison is made through the percentage errors,

\[ \delta_{VSQM} = \frac{|E_{EXACT} - E_{VSQM}|}{E_{EXACT}} \% \]  

(12)

and

\[ \delta_V = \frac{|E_{EXACT} - E_V|}{E_{EXACT}} \%. \]  

(13)
Table 1. Energy eigenvalues (in Rydbergs) and percentage errors for different values of $R$ for the $1s$ state, ($l = 0$). Comparison is made with results from [10].

| R  | $E_{EXACT}$ Ref. [10] | $E_V$ Ref. [10] | $\delta V$ | $E_{VSQM}$ | $\delta_{VSQM}$ |
|----|----------------------|----------------|------------|------------|----------------|
| 0.1 |      937.986         |      937.999   | 0.00       |      940.688 | 29.02         |
| 0.2 |      222.140         |      222.143   | 0.00       |      222.757 | 28.02         |
| 0.3 |       93.185         |      93.187    | 0.00       |      93.434  | 27.02         |
| 0.4 |       49.268         |      49.269    | 0.00       |      49.397  | 26.02         |
| 0.5 |       29.496         |      29.497    | 0.00       |      29.571  | 25.02         |
| 0.6 |      19.055          |      19.056    | 0.00       |      19.100  | 23.02         |
| 0.7 |      12.940          |      12.941    | 0.00       |      12.968  | 22.02         |
| 0.8 |      9.0868          |      9.0874    | 0.00       |      9.1055  | 21.02         |
| 0.9 |      6.5244          |      6.5249    | 0.00       |      6.5370  | 19.02         |
| 1.0 |      4.7480          |      4.7484    | 0.00       |      4.7565  | 18.02         |
| 1.2 |      2.5386          |      2.5388    | 0.00       |      2.5425  | 15.02         |
| 1.4 |      1.2942          |      1.2943    | 0.00       |      1.2958  | 13.02         |
| 1.6 |      0.54262         |      0.54263   | 0.00       |      0.54318 | 10.02         |
| 1.8 |      0.06511         |      0.06512   | 0.00       |      0.06522 | 17.02         |
| 2.0 |    -0.25000          |    -0.24990    | 0.00       |    -0.25000 | 0.00          |
| 2.2 |    -0.46407          |    -0.46376    | 0.00       |    -0.46391 | 0.03          |
| 2.4 |    -0.61280          |    -0.61216    | 0.00       |    -0.61227 | 0.09          |
| 2.6 |    -0.7196           |    -0.71682    | 0.00       |    -0.71697 | 0.14          |
| 2.8 |    -0.79333          |    -0.79152    | 0.00       |    -0.79186 | 0.19          |
| 3.0 |    -0.84793          |    -0.84523    | 0.00       |    -0.84706 | 10.00         |
| 3.2 |    -0.88781          |    -0.88396    | 0.00       |    -0.88545 | 27.00         |
| 3.4 |    -0.91710          |    -0.91184    | 0.00       |    -0.91440 | 30.00         |
| 3.6 |    -0.93870          |    -0.93174    | 0.00       |    -0.93575 | 32.00         |
| 3.8 |    -0.95469          |    -0.94571    | 0.00       |    -0.95156 | 32.00         |
| 4.0 |    -0.96653          |    -0.95518    | 0.00       |    -0.96509 | 15.00         |
Table 2. Energy eigenvalues (in Rydbergs) and percentage errors for different values of \( R \) for the \( 2p \) state, \( (l = 1) \). Comparison is made with results from [10].

| \( R \) | \( E_{EXACT} \) Ref. [10] | \( E_V \) Ref. [10] | \( \delta_V \) | \( E_{VSQM} \) | \( \delta_{VSQM} \) |
|---|---|---|---|---|---|
| 0.4 | 116.896 | 116.925 | 0.02 | 117.038 | 0.12 |
| 0.5 | 73.318 | 73.336 | 0.02 | 73.406 | 0.12 |
| 0.6 | 49.874 | 49.887 | 0.03 | 49.934 | 0.12 |
| 0.8 | 26.879 | 26.886 | 0.03 | 26.911 | 0.12 |
| 1.0 | 16.446 | 16.451 | 0.03 | 16.466 | 0.12 |
| 1.2 | 10.893 | 10.897 | 0.03 | 10.906 | 0.12 |
| 1.4 | 7.6138 | 7.6160 | 0.03 | 7.6225 | 0.12 |
| 1.6 | 5.5295 | 5.5311 | 0.03 | 5.5358 | 0.11 |
| 1.8 | 4.1308 | 4.1321 | 0.03 | 4.1355 | 0.11 |
| 2.0 | 3.1520 | 3.1530 | 0.03 | 3.1555 | 0.11 |
| 2.2 | 2.4438 | 2.4445 | 0.03 | 2.4465 | 0.11 |
| 2.4 | 1.9173 | 1.9178 | 0.03 | 1.9193 | 0.11 |
| 2.6 | 1.5170 | 1.5173 | 0.03 | 1.5185 | 0.10 |
| 2.8 | 1.2068 | 1.2070 | 0.02 | 1.2080 | 0.10 |
| 3.0 | 0.96250 | 0.96269 | 0.03 | 0.96346 | 0.10 |
| 3.5 | 0.54239 | 0.54245 | 0.01 | 0.54239 | 0.10 |
| 4.0 | 0.28705 | 0.28706 | 0.00 | 0.28732 | 0.09 |
| 4.5 | 0.12373 | 0.12375 | 0.01 | 0.12385 | 0.10 |
| 5.0 | 0.01519 | 0.01528 | 0.59 | 0.01523 | 0.29 |
| 5.5 | -0.05910 | -0.05887 | 0.38 | -0.05909 | 0.02 |
| 6.0 | -0.11111 | -0.11069 | 0.38 | -0.11111 | 0.00 |
| 6.5 | -0.14818 | -0.14748 | 0.47 | -0.14816 | 0.01 |
| 7.0 | -0.17496 | -0.17392 | 0.59 | -0.17490 | 0.03 |
| 7.5 | -0.19451 | -0.19304 | 0.75 | -0.19440 | 0.05 |
| 8.0 | -0.20890 | -0.20691 | 0.95 | -0.20882 | 0.04 |
Table 3. Energy eigenvalues (in Rydbergs) and percentage errors for different values of $R$ for the $3d$ state, $(l = 2)$. Comparison is made with results from [10].

| $R$ | $E_{EXACT}$ Ref. [10] | $E_V$ Ref. [10] | $\delta_V$ | $E_{VSQM}$ | $\delta_{VSQM}$ |
|-----|------------------------|------------------|-------------|-------------|-----------------|
| 0.4 | 116.896                | 116.925          | 0.02        | 117.038     | 0.12            |
| 0.5 | 126.320                | 126.396          | 0.06        | 126.417     | 0.08            |
| 1.0 | 29.935                 | 29.950           | 0.05        | 29.958      | 0.08            |
| 1.5 | 12.570                 | 12.576           | 0.05        | 12.579      | 0.07            |
| 2.0 | 6.6550                 | 6.6583           | 0.05        | 6.6601      | 0.08            |
| 2.5 | 3.9920                 | 3.9938           | 0.05        | 3.9950      | 0.08            |
| 3.0 | 2.5856                 | 2.5867           | 0.04        | 2.5876      | 0.08            |
| 3.5 | 1.7618                 | 1.7624           | 0.04        | 1.7631      | 0.07            |
| 4.0 | 1.2427                 | 1.2431           | 0.03        | 1.2437      | 0.08            |
| 4.5 | 0.89752                | 0.89776          | 0.03        | 0.89820     | 0.08            |
| 5.0 | 0.65823                | 0.65836          | 0.02        | 0.65873     | 0.08            |
| 5.5 | 0.48681                | 0.48686          | 0.01        | 0.48717     | 0.07            |
| 6.0 | 0.36068                | 0.36074          | 0.02        | 0.36095     | 0.08            |
| 6.5 | 0.26583                | 0.26583          | 0.00        | 0.26603     | 0.08            |
| 7.0 | 0.19318                | 0.19318          | 0.00        | 0.19333     | 0.08            |
| 7.5 | 0.13666                | 0.13668          | 0.02        | 0.13677     | 0.08            |
| 8.0 | 0.09212                | 0.09216          | 0.05        | 0.09220     | 0.08            |
| 9.0 | 0.02801                | 0.02815          | 0.50        | 0.02805     | 0.14            |
| 10.0| -0.01419               | -0.01390         | 1.98        | -0.01417    | 0.13            |
| 11.0| -0.04275               | -0.04229         | 1.09        | -0.04275    | 0.01            |
| 12.0| -0.06250               | -0.06181         | 1.11        | -0.06250    | 0.00            |
| 13.0| -0.07637               | -0.07540         | 1.27        | -0.07637    | 0.00            |
| 14.0| -0.08623               | -0.08479         | 1.66        | -0.08622    | 0.01            |
| 15.0| -0.09328               | -0.09160         | 1.81        | -0.09327    | 0.01            |

At this point we stress that for $R \to \infty$ the SQM results also agree with the exact non-confined problem, which corresponds to the removal of the infinite barrier. In this case the energy is exact and corresponds to

$$E = -\frac{1}{N^2}, \quad N = n + l + 1$$

(14)

The table 4 below shows the energy eigenvalues, $E_{VSQM}$, for the $1s$, $2p$ and $3d$ states, $(n = 0$ and $l = 0, 1, 2)$ for increasing values of $R$. Notice the convergency towards the energy of the exact non-confined case, given by equation (14).
Table 4. Energy eigenvalues, $E_{VSQM}$, (in Rydbergs) for different values of $R$ for the 1s, 2p and 3d states, ($n = 0$ and $l = 0, 1, 2$). It is also shown the exact result from (14).

| R  | $l = 0$  | $E_{R \to \infty} = -1.00000$ | $l = 1$  | $E_{R \to \infty} = -0.25000$ | $l = 2$  | $E_{R \to \infty} = -0.11111$ |
|----|---------|--------------------------------|---------|--------------------------------|---------|--------------------------------|
| 10 | -0.99985| -0.23754                       | -0.01417|                               |         |                               |
| 15 | -0.99998| -0.24941                       | -0.09327|                               |         |                               |
| 20 | -1.00000| 0.24990                        | -0.10788|                               |         |                               |
| 30 | -1.00000| -0.24999                       | -0.11103|                               |         |                               |
| 50 | -1.00000| -0.25000                       | -0.11111|                               |         |                               |

Comments and conclusions

When dealing with the variational method associated with SQM to get the energy states of a quantum dot we have used a confining effective potential depending on three variational parameters ($\mu_1$, $\mu_2$ and $\mu_3$). This was achieved through an Ansatz for the superpotential. Using the superalgebra the trial wave function was evaluated which depends on these three parameters.

Varying the trial wave function with respect to these parameters we found good results for increasing values of the radius $R$, for which the energy is negative, when compared to results obtained from other approximative variational method and exact numerical results, [10]. From the point of view of the number of variational parameters involved in the evaluation this improvement was indeed expected, since in ref. [10] there are two of such parameters present in the calculation. Nonetheless we stress that the great advantage of our method is the achievement of the trial wave function through the Ansatz for the superpotential, equation (8). This allowed us a previous comparative analysis between the original potential, contained in equation (7), and the effective potential, equation (9), which approaches the infinite at the neighbourhood of the barrier. Following this line of reasoning, the wave function, evaluated through the superalgebra, equation (4), vanishes at the border because it finds a potential barrier that increases until becoming impenetrable at $r = R$. These border effects become more perceptive for smaller values of $R$. For increasing values of $R$, smaller will be the border effects so that the variational results get better. In other words, for large values of $R$ the variational SQM Ansatz provides fast converging results as displayed in Table 4. In this way we recover the results for the non-confined system, when $R \to \infty$.

In conclusion, we remark that the results presented here suggest that the association of the superalgebra of SQM with the variational method provides an appropriate approach to analyse confined systems.
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