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Supersymmetry and the Hartmann potential of theoretical chemistry

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Abstract. An exactly solvable ring-shaped potential in quantum chemistry given by

$$V = \eta\sigma^2\varepsilon_0\left(\frac{2a_0}{r} - \frac{\eta a_0^2}{r^2 \sin^2\theta}\right)$$

was introduced by Hartmann in 1972 to describe ring-shaped molecules like benzene. In this article, the supersymmetric features of the Hartmann potential are discussed. We first review the results of a previous paper in which we rederived the eigenvalues and radial eigenfunctions of the Hartmann potential using a formulation of one-dimensional supersymmetric quantum mechanics (SUSYQM) on the half-line $[0, \infty)$. A reformulation of SUSYQM in the full line $(-\infty, \infty)$ is subsequently developed. It is found that the second formulation makes a connection between states having the same quantum number L but different values of $\eta\sigma^2$ and quantum number N. This is in contrast to the first formulation, which relates states with identical values of the quantum number N and $\eta\sigma^2$ but different values of the quantum number L.

Key words: Supersymmetry – Hartmann potential – Supersymmetric quantum mechanics – Ring-shaped potential – Superpotential

1 Introduction

The unification of the four fundamental forces of nature (namely, the gravitational, electromagnetic, weak and strong interactions) has been a major goal in theoretical particle physics ever since Einstein started out with this idea during the early 1900s. Some degree of success has been achieved in partially unifying the electromagnetic and weak interactions. Viable theories which unify the electromagnetic, weak and strong interactions have also been put forth. A major stumbling block is putting gravity into the picture. Efforts to circumvent this problem led to the discovery of supersymmetry (SUSY) in 1971 by Gel'fand and Likhtman [1]. At present, many physicists believe that supersymmetry is a necessary ingredient in the theory which will eventually unify the four fundamental interactions.

Symmetry plays a crucial role in contemporary theoretical particle physics. The very successful Standard Model of particle physics is based on a "gauge" symmetry which relates fermions (half-integer spin particles) to fermions and also bosons (integer spin particles) to bosons. Supersymmetry is a symmetry which relates fermions to bosons and vice versa. In a more general sense, supersymmetry relates the "fermionic" and "bosonic" degrees of freedom of a quantum system.

One of the most important predictions of SUSY models is the existence of supersymmetric partners for each of the presently observed particles. For instance, an electron (spin $\frac{1}{2}$) has a SUSY partner called a "selectron" (spin 1) while a photon (spin 1) has a SUSY partner called a "photino" (spin $\frac{1}{2}$). An important property of SUSY partners is that they have the same mass as their corresponding ordinary particles.

The mass degeneracy of SUSY partners and ordinary particles is not observed at ordinary energies. Hence, supersymmetry is said to be "broken" at some energy scale. In an attempt to study SUSY breaking in quantum field theory, Witten [2] developed the simplest case of supersymmetric quantum mechanics (SUSYQM) in 1981. Consequently, early studies in SUSYQM were focused on the study of SUSY breaking. Soon, however, it was realized that SUSYQM can have interesting applications in atomic physics, statistical physics, nuclear physics, etc. [3] and most recently in quantum chemistry [4]. The present paper is meant to extend the application of SUSYQM techniques on the Hartmann potential which we started in Ref. [4].

In 1972, Hartmann [5] proposed a potential of the form

$$V = \eta\sigma^2\varepsilon_0\left(\frac{2a_0}{r} - \frac{\eta a_0^2}{r^2\sin^2\theta}\right), \tag{1}$$

with

$$a_0 = \frac{\hbar^2}{\mu e^2} \quad \text{and} \quad \varepsilon_0 = -\frac{1}{2}\frac{\mu e^4}{\hbar^2} \tag{2}$$

in which η and σ are positive real parameters ranging from 1 to 10 in theoretical chemistry applications [6], μ is the mass of the particle and r and θ are in spherical coordinates. The above potential has been very useful in describing ring-shaped molecules like benzene. In a previous paper [4], SUSYQM techniques were used to rederive the eigenvalues and radial eigenfunctions of the Hartmann potential. In this article, we further explore its supersymmetric quantum mechanical features by a second formulation of SUSYQM. This analysis is inspired by the analysis made for the hydrogen atom using supersymmetry in Ref. [7]. It is the author's hope to further contribute to the use of SUSYQM techniques in solving important problems in theoretical chemistry.

Section 2 gives a brief introduction to SUSYQM techniques. We explore the supersymmetric features of the Hartmann potential in Sect. 3 by looking at two different formulations. To facilitate the comparison of these two formulations, we briefly review the first formulation (see Ref. [4] for a very detailed discussion) in Sect. 3.1. Section 3.2 gives a detailed discussion of the second formulation and subsequently compares it to the first.

Some conclusions are given in Sect. 4.

2 Supersymmetry in quantum mechanics

As alluded to in Sect. 1, supersymmetry was first introduced in particle physics [8, 9]. The language of particle physics is quantum field theory (which is a theory describing systems with an infinite number of quantum mechanical variables). To describe a system, a Lagrangian density $\mathscr{L}(\varphi_i, \partial_\mu \varphi_i)$ where $[\partial_\mu \equiv ((1/c)\partial/\partial t, \nabla)]$, is specified. φ_i are quantum fields describing the dynamics of the particles in a system. Supersymmetry is introduced by imposing the invariance of $\mathscr{L}$ with respect to supersymmetric transformations given by a SUSY algebra. Invariance of $\mathscr{L}$ dictates a relationship between fields χ and ψ in which the spins of χ and ψ differ by $\frac{1}{2}\hbar$. In the present paper, we will use the word "supersymmetry" in a more general sense. Supersymmetric systems are systems which can be described by the SUSY algebra.

A quantum mechanical system is considered supersymmetric if it can be characterized by charge operators Q_i, $i = 1, 2, \ldots, N$. The SUSY algebra (denoted by sqm(N)) is then given by

$$\{Q_i, Q_j\} = \delta_{ij} H_{\mathrm{ss}}, \quad [Q_i, H_{\mathrm{ss}}] = 0, \tag{3}$$

where { } and [ ] are anticommutator and commutator, respectively, and H_{ss} is the supersymmetric Hamiltonian describing the system. For most applications of SUSYQM, like this article, only two charge operators Q_1 and Q_2 will be considered (i.e. sqm(2) algebra).

It is more useful to construct non-Hermitian charge operators from Q_1 and Q_2 given by

$$Q = \frac{1}{\sqrt{2}}(Q_1 + \mathrm{i}Q_2) \quad \text{and} \quad Q^\dagger = \frac{1}{\sqrt{2}}(Q_1 - \mathrm{i}Q_2). \tag{4}$$

The SUSY algebra of Eq. (3) becomes

$$\{Q, Q^\dagger\} = H_{\mathrm{ss}}, \quad Q^2 = 0, \quad (Q^\dagger)^2 = 0 \tag{5}$$

and

$$[Q, H_{\mathrm{ss}}] = 0 \quad \text{and} \quad [Q^\dagger, H_{\mathrm{ss}}] = 0. \tag{6}$$

A simple way of realizing Eqs. (5) and (6) is by letting

$$Q = \begin{bmatrix} 0 & 0 \\ A^- & 0 \end{bmatrix}, \quad Q^\dagger = \begin{bmatrix} 0 & A^+ \\ 0 & 0 \end{bmatrix} \tag{7}$$

in which

$$(A^-)^\dagger = A^+. \tag{8}$$

Equations (5) and (7) give

$$H_{\mathrm{ss}} = \begin{bmatrix} A^+A^- & 0 \\ 0 & A^-A^+ \end{bmatrix} \equiv \begin{bmatrix} H_1 & 0 \\ 0 & H_2 \end{bmatrix}. \tag{9}$$

H_1 and H_2 are said to be supersymmetric partner Hamiltonians. H_1 is often called the "Bose" sector while H_2 is referred to as the "Fermi" sector. Let us now discuss how we can relate the preceding formalism to quantum mechanics.

Given a Hamiltonian H_1 in quantum mechanics,

$$H_1 = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_1(x) \tag{10}$$

satisfying the Schrödinger equation

$$H_1\psi^n_{(1)} = \left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_1(x)\right]\psi^n_{(1)} = E^n_{(1)}\psi^n_{(1)}, \tag{11}$$

it is well known that it can be factorized [3] by defining the operators

$$A_1^- \equiv \frac{1}{\sqrt{2}}\left(\frac{\mathrm{d}}{\mathrm{d}x} + W_1\right) \quad \text{and} \quad A_1^+ \equiv \frac{1}{\sqrt{2}}\left(-\frac{\mathrm{d}}{\mathrm{d}x} + W_1\right), \tag{12}$$

where W_1 (called the "superpotential") satisfies the Ricatti equation

$$V_1(x) = \frac{1}{2}\left[W_1^2 - \frac{\mathrm{d}W_1}{\mathrm{d}x}\right]. \tag{13}$$

In Eq. (10) above, the potential $V_1(x)$ is chosen such that the ground-state energy E_1^0 is zero.

From Eq. (9) we get

$$H_1 = A_1^+ A_1^- \quad \text{and} \quad H_2 = A_1^- A_1^+, \tag{14}$$

and thus we can form H_{ss} as in Eq. (9). The preceding discussion essentially tells us that given a potential $V_1(x)$, any Hamiltonian H_1 in one-dimensional quantum mechanics has a SUSY partner H_2 and thus can be an element of an H_{ss}, as long as one can solve for the superpotential W_1 in Eq. (13).

Expanding H_2 in Eq. (14) using Eq. (12), we get

$$H_2 = A_1^- A_1^+ = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_2(x), \tag{15}$$

where

$$V_2(x) = \frac{1}{2}\left[W_1^2 + \frac{\mathrm{d}W_1}{\mathrm{d}x}\right]. \tag{16}$$

One notices that H_2 in Eq. (15) is altogether a new Hamiltonian with a new potential $V_2(x)$. We can then construct another set of operators similar to Eq. (12),

$$A_2^- \equiv \frac{1}{\sqrt{2}}\left(\frac{\mathrm{d}}{\mathrm{d}x} + W_2\right) \quad \text{and} \quad A_2^+ \equiv \frac{1}{\sqrt{2}}\left(-\frac{\mathrm{d}}{\mathrm{d}x} + W_2\right), \tag{17}$$

where this time the superpotential W_2 satisfies an equation similar to Eq. (13),

$$V_2(x) = \frac{1}{2}\left[W_2^2 - \frac{\mathrm{d}W_2}{\mathrm{d}x}\right]. \tag{18}$$

Solving Eq. (18) for W_2 enables us to construct the operators in Eq. (17) from which we can construct a new SUSY-partner Hamiltonian

$$H_3 = A_2^- A_2^+ = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_3(x) \tag{19}$$

with

$$V_3(x) = \frac{1}{2}\left[W_2^2 + \frac{\mathrm{d}W_2}{\mathrm{d}x}\right]. \tag{20}$$

It is apparent that we can generate a "hierarchy" of SUSY-partner Hamiltonians $H_1, H_2, H_3, \ldots$ with the above procedure.

The construction of the operators $A_1^{\pm}$ from H_1 is reminiscent of the raising and lowering operators of the simple harmonic oscillator in elementary quantum mechanics. These operators give a convenient way of solving the energy eigenvalues and eigenfunctions. Since $A_1^{\pm}$ determines H_1 and H_2, we expect the eigenvalues and eigenfunctions of H_1 and H_2 to be related. Let us illustrate how this happens.

Consider an eigenfunction of H_1, namely, $\psi^n_{(1)}$ such that

$$E^n_{(1)}\psi^n_{(1)} = H_1\psi^n_{(1)} = A_1^+ A_1^- \psi^n_{(1)}. \tag{21}$$

Multiplying Eq. (21) by A_1^-,

$$E^n_{(1)}(A_1^- \psi^n_{(1)}) = A_1^- A_1^+ (A_1^- \psi^n_{(1)}) = H_2(A_1^- \psi^n_{(1)}). \tag{22}$$

Equation (22) means that given an eigenfunction $\psi^n_{(1)}$ of H_1, one can form an eigenfunction $A_1^- \psi^n_{(1)}$ of H_2 with the same eigenvalue $E^n_{(1)}$. Similarly, one can start with H_2 and show that

$$E^n_{(2)}(A_1^+ \psi^n_{(2)}) = H_1(A_1^+ \psi^n_{(2)}). \tag{23}$$

Note that since we have chosen the eigenvalue of the ground state of H_1 to be zero, Eqs. (14) and (11) imply that

$$0 = (A_1^+ A_1^-)\psi^0_{(1)} \tag{24}$$

which leads to

$$A_1^- \psi^0_{(1)} = 0. \tag{25}$$

Equations (22), (23) and (25) imply that H_1 and H_2 have identical eigenvalues except for the ground state of H_1 (in which $A_1^- \psi^0_{(1)} = 0$, implying non-normalizability). In addition, these equations imply that we can get eigenfunctions of H_2 (H_1) by applying A_1^- (A_1^+) to eigenfunctions of $H_1(H_2)$. This analysis can clearly be extended to the hierarchy of Hamiltonians $H_1, H_2, H_3, \ldots$. We illustrate these ideas in Fig. 1.

An important consequence of SUSYQM is the intimate relationship of the eigenfunctions and eigenvalues of the SUSY-partner Hamiltonians. This can be very useful in solving the Schrödinger equation of a more complicated potential if the solution of its corresponding SUSY partner is known.

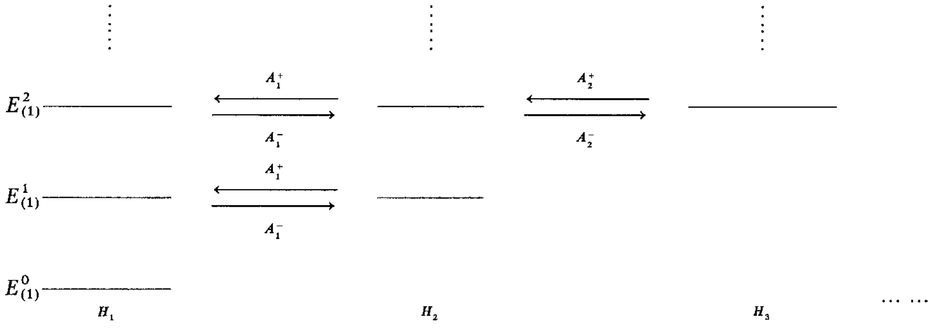

Fig. 1. The hierarchy of Hamiltonians and the action of the operators $A_n^{\pm}$ on the degenerate eigenstates.

3 SUSYQM of the Hartmann potential

The Schrödinger equation of a particle with mass μ subjected to the Hartmann potential is given in spherical coordinates by

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + \left[\frac{2\eta\sigma^2\varepsilon_0 a_0}{r} - \frac{\eta^2\sigma^2 a_0^2\varepsilon_0}{r^2\sin^2\theta}\right]\psi = E\psi. \tag{26}$$

The discussion of SUSYQM in the preceding section involves only one dimension. In order to be able to apply SUSYQM in one dimension to the three-dimensional Hartmann potential, we do a separation of variables to get three one-dimensional differential equations [5]. Assuming a solution

$$\psi = R(r)\Theta(\theta)\Phi(\phi), \tag{27}$$

we get from Eqs. (26) and (27)

$$\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} = -m^2, \tag{28}$$

$$\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) - \left(\frac{M^2}{\sin^2\theta} - L(L+1)\right)\Theta = 0, \tag{29}$$

$$\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R}{\mathrm{d}r}\right) - L(L+1)\frac{R}{r^2} + \frac{8\pi^2\mu}{h^2}\left(E + \frac{\eta\sigma^2 e^2}{r}\right)R = 0, \tag{30}$$

where

$$M^2 = m^2 + \eta^2\sigma^2. \tag{31}$$

For a one-dimensional differential equation to be solvable by SUSYQM [10], it must be of the form of Eq. (11) (no first derivative term) and must yield an infinite tower of states as in Fig. 1. As shown in Ref. [4], only the radial equation of Eq. (30) gives an interesting SUSY. Equations (28) and (29) can be solved by conventional methods [5]. Their solutions are given by

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}m\phi}, \quad m = 0, \pm 1, \pm 2, \dots, \tag{32}$$

$$\Theta(\theta) \sim \mathscr{P}_L^{|M|}(\cos\theta), \quad L = v' + |M|, \; v' = 0, 1, 2, \dots, \tag{33}$$

respectively. From hereon, we focus on Eq. (30).

Equation (30) can be shown to have the form of Eq. (11) by making the change of variables [4]

$$R = \frac{u}{r}. \tag{34}$$

Putting Eq. (34) into Eq. (30), yields

$$H_L u = \left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{L(L+1)}{2r^2} - \frac{\gamma}{r} \right] u = \frac{\mu E}{\hbar^2} u, \tag{35}$$

where

$$\gamma \equiv \frac{\mu\eta\sigma^2 e^2}{\hbar^2}. \tag{36}$$

Let us next review the results of Ref. [4].

3.1 *Calculation of the eigenvalues and radial eigenfunctions*

One useful thing to note about Eqs. (28)–(30) is that they resemble closely the separated equations of the hydrogen atom [11]. The eigenvalues and radial eigenfunctions of the hydrogen atom had been solved by SUSYQM methods [12]. Thus, we can just utilize some of the useful results from the hydrogen atom problem. In this subsection, we will simply quote the major results of our previous paper [4]. The reader can refer to Ref. [4] for more details.

In order to solve the eigenvalues and radial eigenfunctions of the Hartmann potential by SUSYQM, we construct a Hamiltonian similar to Eq. (35):

$$\mathscr{H}_L = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{L(L+1)}{2r^2} - \frac{\gamma}{r} + \frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2. \tag{37}$$

Note that the Hamiltonians in Eqs. (37) and (35) differ only by a constant. Hence, any eigenfunction of $\mathscr{H}_L$ will also be an eigenfunction of H_L. The eigenvalues of H_L can be obtained by simply letting H_L act on its eigenfunctions.

The resulting Ricatti equation of Eq. (37) is given by (from Eqs. (11), (37) and (13))

$$\frac{L(L+1)}{2r^2} - \frac{\gamma}{r} + \frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2 = \frac{1}{2}\left[W_L^2 - \frac{\mathrm{d}W_L}{\mathrm{d}r} \right] \tag{38}$$

which yields a superpotential

$$W_L = -\frac{L+1}{r} + \frac{\gamma}{L+1}. \tag{39}$$

From Eq. (39) we construct the operators (using Eq. (12))

$$A_L^{\pm} = \frac{1}{\sqrt{2}}\left(\mp\frac{\mathrm{d}}{\mathrm{d}r} - \frac{L+1}{r} + \frac{\gamma}{L+1}\right) \tag{40}$$

Using Eqs. (40) and (14) we construct a SUSY-partner Hamiltonian

$$\mathscr{H}_{L+1} = A_L^- A_L^+ = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{(L+1)(L+2)}{2r^2} - \frac{\gamma}{r} + \frac{1}{2}\left(\frac{\gamma}{L+1}\right)^2. \tag{41}$$

With $L = |M|, |M|+1, |M|+2, \ldots$ as in Eq. (33), a hierarchy of Hamiltonians similar to Fig. 1 will be formed but with $H_1, H_2, H_3, \ldots$ replaced by $\mathscr{H}_{|M|}$, $\mathscr{H}_{|M|+1}$, $\mathscr{H}_{|M|+2}, \ldots$. We then expect a similar set of states for $H_{|M|}$, $H_{|M|+1}, H_{|M|+2}, \ldots$. This is illustrated in Fig. 2. The states at the lowest rung of the infinite tower of states of each of the Hamilotonians are shown and labeled by the corresponding L quantum number.

From Eqs. (25) and (40), we get

$$\frac{1}{\sqrt{2}}\left(\frac{\mathrm{d}}{\mathrm{d}r} - \frac{L+1}{r} + \frac{\gamma}{L+1}\right)\psi^0_{(L)} = 0 \tag{42}$$

with the solution

$$\psi^0_{(L)} = \mathscr{N}_L r^{L+1}\exp(-\kappa_L r), \tag{43}$$

where

$$\kappa_L \equiv \frac{\gamma}{L+1} \tag{44}$$

and $\mathscr{N}_L$ is a normalization constant.

Since L is arbitrary, Eq. (43) is the expression for the radial eigenfunctions at the bottom rung of the ladder of states of the hierarchy of Hamiltonians in Fig. 2. Hence, we can write

$$u_L = \mathscr{N}_L r^{L+1}\exp(-\kappa_L r). \tag{45}$$

Letting H_L of Eq. (35) act on Eq. (45), we get

$$H_L u_L = \left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \left(\frac{L(L+1)}{2r^2} - \frac{\gamma}{r}\right)\right]u_L = \frac{\mu E_L}{\hbar^2}u_L. \tag{46}$$

Solving for the energy yields

$$E_L = -\frac{\Lambda}{(L+1)^2}, \quad \Lambda = \eta^2\sigma^4|\varepsilon_0|. \tag{47}$$

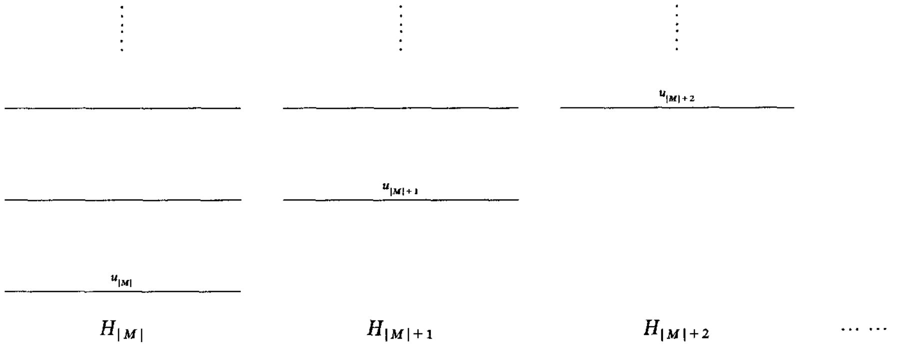

Fig. 2. The hierarchy of Hamiltonians of the Hartmann potential and their ground states. The H_L here are the actual radial Hamiltonian for a particular L value.

We illustrate these energy levels in Fig. 3. By carefully examining in Fig. 3, the labels of the states and their corresponding energies as given by Eq. (47), it can be shown [4] that the energy is actually labeled by the quantum number N and is given by the following expression:

$$E_N = -\frac{\Lambda}{N^2}; \quad \Lambda = \eta^2\sigma^4|\varepsilon_0|, \quad N = L + 1 + n', \quad n' = 0, 1, 2, \ldots \tag{48}$$

with $N \geqslant |M| + 1$ (from Eqs. (48) and (33)).

From Fig. 3, it is apparent that the states must be labeled by $u_{|M|+1,|M|}$; $u_{|M|+2,|M|}$; $u_{|M|+3,|M|}$; … for a given $L = |M|$ value for instance. These are shown in Fig. 4.

We can obtain the rest of the eigenfunctions by the action of A_L^+ on the u_L's of Eq. (45) for different values of L. Figure 4 illustrates this too.

With the above procedure, one can obtain the radial eigenfunctions R_{NL} (since we can get the $u(r)$'s and then use Eq. (34)) found in Ref. [6]. We have shown that SUSYQM can be used to obtain the energy and radial eigenfunctions of the Hartmann potential.

It is important to note that comparing Eqs. (37) and (41) (discounting the common constant $\frac{1}{2}(\gamma/(L+1))^2$ which just rescales the ground state such that its energy eigenvalue is zero) and with Fig. 4, we realize that states with quantum numbers (N, L) has for its SUSY partner, states with quantum numbers $(N, L + 1)$.

3.2 Relating eigenstates with different values of $\eta\sigma^2$ and quantum number N

One thing to note about the analysis of Sect. 3.1 is that the one-dimensional SUSYQM problem was formulated in the half-line $[0, \infty)$ (since $0 \leqslant r < \infty$). Let us now see the consequences of formulating the SUSYQM problem in the full line $(-\infty, \infty)$ [7].

As a first step, let us rewrite Eq. (35) by a change of variables given by

$$y \equiv \gamma r = \frac{(\eta\sigma^2)\mu e^2}{\hbar^2} r \tag{49}$$

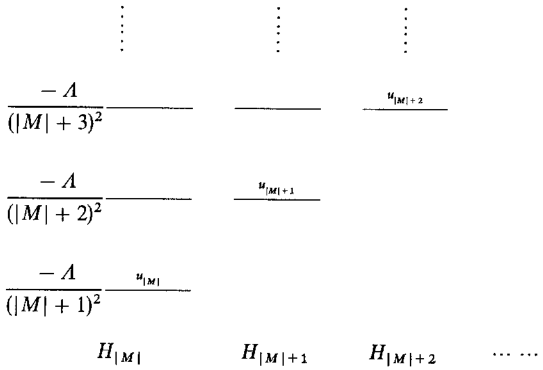

Fig. 3. Figure 2 with the energy levels labeled.

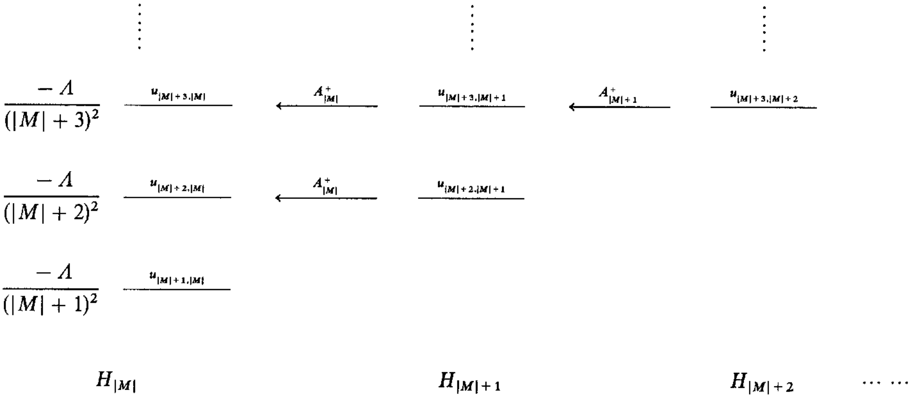

Fig. 4. The energy eigenstates of the Hartmann potential. The action of the A_L^+ operators are explicitly shown to indicate how the other states are obtained from the states at the lowest rung of the hierarchy of Hamiltonians.

with y given by Eq. (36). Using Eq. (49) and the equation for the energy given by Eq. (48), we can rewrite Eq. (46) as

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}y^2}+\frac{L(L+1)}{2y^2}-\frac{1}{y}\right]u_{NL}=-\frac{1}{2N^2}u_{NL}. \tag{50}$$

We now make a second change of variables from y to x such that

$$y=\mathrm{e}^x,\quad u_{NL}=\mathrm{e}^{x/2}\psi \tag{51}$$

to turn Eq. (50) into a differential equation in the full line $(-\infty,\infty)$ given by

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{\mathrm{e}^{2x}}{2N^2}-\mathrm{e}^x\right]\psi=-\tfrac{1}{2}(L+\tfrac{1}{2})^2\psi. \tag{52}$$

It is interesting to note that Eq. (52) describes a Morse potential $\mathrm{e}^{2x}/2N^2-\mathrm{e}^x$ with eigenvalues $-\frac{1}{2}(L+\frac{1}{2})^2$. We next find the SUSY-partner Hamiltonian of Eq. (52).

In order to be able to use the results of Sect. 2, we have to chose $V_1(x)$ of Eq. (52) such that its ground-state eigenvalue is zero. Given N, the L values are (from Eq. (48) and as can be deduced from Fig. 4) $N-1, N-2, N-3, \ldots, |M|$. Hence, the ground-state eigenvalue of Eq. (52) is $-\frac{1}{2}(N-1+1/2)^2 = -\frac{1}{2}(N-1/2)^2$. We rewrite Eq. (52) as

$$H_1\psi = \left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{e^{2x}}{2N^2} - e^x + \tfrac{1}{2}(N-\tfrac{1}{2})^2\right]\psi = [-\tfrac{1}{2}(L+\tfrac{1}{2})^2 + \tfrac{1}{2}(N-\tfrac{1}{2})^2]\psi \tag{53}$$

with

$$V_1(x) = \frac{e^{2x}}{2N^2} - e^x + \tfrac{1}{2}(N-\tfrac{1}{2})^2 \tag{54}$$

chosen such that the ground-state eigenvalue is zero. We are now ready to get the SUSY-partner Hamiltonian of Eq. (53). From Eqs. (54) and (13), we get the Ricatti equation

$$\frac{e^{2x}}{2N^2} - e^x + \tfrac{1}{2}(N-\tfrac{1}{2})^2 = \frac{1}{2}\left[W_1^2 - \frac{dW_1}{dx}\right] \tag{55}$$

whose solution is

$$W_1 = \frac{e^x}{N} + \frac{1}{2} - N. \tag{56}$$

From Eqs (56) and (12), we construct

$$A_1^- = \frac{1}{\sqrt{2}}\left(\frac{d}{dx} + \frac{e^x}{N} + \frac{1}{2} - N\right) \quad \text{and} \quad A_1^+ = \frac{1}{\sqrt{2}}\left(-\frac{d}{dx} + \frac{e^x}{N} + \frac{1}{2} - N\right). \tag{57}$$

The SUSY-partner Hamiltonian of H_1 in Eq. (53) is given by Eqs (57) and (15) yielding

$$H_2 = A_1^- A_1^+ = -\frac{1}{2}\frac{d^2}{dx^2} + \frac{e^{2x}}{2N^2} - \left(1 - \frac{1}{N}\right)e^x + \frac{1}{2}(N-\tfrac{1}{2})^2. \tag{58}$$

From the discussion in Sect. 2, we know that H_2 has the same eigenvalues as H_1 except for the ground state where $L = N-1$ and that the eigenstates $\tilde{\psi}$ of H_2 are related to that of the eigenstates of H_1 by $\tilde{\psi} \sim A_1^- \psi$. We then write the eigenvalue equation for Eq. (58) as

$$\begin{aligned} H_2\tilde{\psi} &= \left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{e^{2x}}{2N^2} - \left(1 - \frac{1}{N}\right)e^x + \frac{1}{2}(N-\tfrac{1}{2})^2\right]\tilde{\psi} \\ &= \left[-\frac{1}{2}(L+\tfrac{1}{2})^2 + \frac{1}{2}(N-\tfrac{1}{2})^2\right]\tilde{\psi}. \end{aligned} \tag{59}$$

Summarizing, we have the SUSY-partner eigenvalue equations given by Eqs. (53) and (59) (with the rescaling constant term $\frac{1}{2}(N-\frac{1}{2})^2$ cancelled out)

$$\left[-\frac{1}{2}\frac{d^2}{dx^2}+\frac{e^{2x}}{2N^2}-e^x\right]\psi=-\tfrac{1}{2}(L+\tfrac{1}{2})^2\psi$$

$$\left[-\frac{1}{2}\frac{d^2}{dx^2}+\frac{e^{2x}}{2N^2}-\left(1-\frac{1}{N}\right)e^x\right]\tilde{\psi}=-\tfrac{1}{2}(L+\tfrac{1}{2})^2\tilde{\psi}. \tag{60}$$

Transforming back to the variable r and the eigenstate u_{NL} using Eqs. (49) and (51), we get from Eq. (60)

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}-\delta\frac{\mu e^2}{\hbar^2}\frac{1}{r}+\frac{L(L+1)}{2r^2}\right]u_{NL}=-\frac{\delta^2}{N^2}\frac{\mu^2e^4}{2\hbar^4}u_{NL},$$

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}-\delta'\frac{\mu e^2}{\hbar^2}\frac{1}{r}+\frac{L(L+1)}{2r^2}\right]\tilde{u}_{N'L}=-\frac{\delta'^2}{N'^2}\frac{\mu^2e^4}{2\hbar^4}\tilde{u}_{N'L}, \tag{61}$$

where

$$\delta\equiv\eta\sigma^2,$$

$$\delta'=\left(1-\frac{1}{N}\right)\delta,$$

$$N'=N-1. \tag{62}$$

From Eqs. (61) and (62), it becomes apparent that if we formulate the SUSYQM problem in the full line by the change of variables given by Eq. (51), states with the quantum numbers (N, L) in a potential with parameter $\eta\sigma^2$ is the SUSY partner of states with quantum numbers $(N-1, L)$ but in a potential with parameter $(1-1/N)\eta\sigma^2$. This relationship is in sharp contrast to that of Sect. 3.1 in which states with quantum numbers (N, L) with a potential having parameter $\eta\sigma^2$ has as their SUSY partners, states with quantum numbers $(N, L+1)$ with the potential having the *same* parameter $\eta\sigma^2$. By SUSYQM, we have related states with different $\eta\sigma^2$ and N as SUSY partners in the Hartmann potential.

An illustration of the observations put forth in the preceding paragraph is illustrated in Fig. 5 for $N=|M|+3$ in which $L=|M|+2$, $|M|+1$, $|M|$. The SUSY-partner states will have $N'=|M|+2$ with $L=|M|+1$, $|M|$. If $\eta\sigma^2$ is the value for the first set of eigenstates, then its SUSY partners will have a value of $(1-1/N)\eta\sigma^2=((|M|+2)/(|M|+3))\eta\sigma^2$. Note that the actual SUSY eigenvalues are given by $-\frac{1}{2}(L+\frac{1}{2})^2$ as in Eq. (60). In addition, note carefully that in Eq. (61), the *energy* eigenvalues of the SUSY-partner eigenvalue equations are *identical* since from Eq. (62)

$$\frac{\delta'}{N'}=\frac{(1-1/N)\delta}{N-1}=\frac{(N-1)\delta/N}{N-1}=\frac{\delta}{N}. \tag{63}$$

Hence, in Fig. 5, the eigenstates have the same energy eigenvalue but different SUSY eigenvalues. We have here a case in which the SUSY partnership does not involve the actual energy eigenvalues.

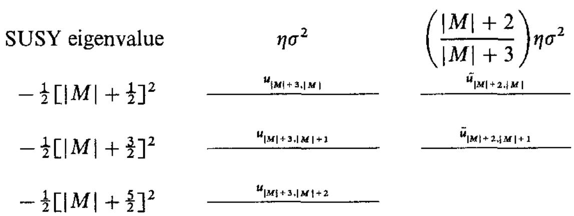

Fig. 5. An illustration of SUSY-partner eigenstates identified by $(N, L, \eta\sigma^2)$ and $(N-1, L, (1-1/N)\eta\sigma^2)$ given $N = |M| + 3$ for the SUSYQM formulation of the Hartmann potential in the full line $(-\infty, \infty)$. Of course, one can again relate the different eigenstates with the same SUSY eigenvalues by $A_1^{\pm}$ of Eq. (57).

Another thing to note from Fig. 5 is that indeed, the spectrum of states of the Fermi sector has all the corresponding states of the Bosonic sector except for its ground state, as expected.

4 Conclusion

In the preceding discussions, we have demonstrated how SUSYQM techniques can be used in the radial equation of the Hartmann potential in theoretical chemistry. By formulating SUSYQM in the half line $[0, \infty)$, we are able to establish a connection between the states with quantum numbers (N, L) and $(N, L+1)$ and the same parameter values $\eta\sigma^2$. This enabled us to derive the energy eigenvalues and radial eigenfunctions. On the other hand, formulating SUSYQM in the full line $(-\infty, \infty)$, established an interesting SUSY connection between states with quantum numbers (N, L) and the parameter value $\eta\sigma^2$ with that of states with quantum numbers $(N-1, L)$ and the parameter value $(1-1/N)\eta\sigma^2$.

The first formulation basically tells us that SUSYQM techniques can be used as an alternative method of solving the Schrödinger equation. The second formulation reveals the possibility of unraveling new and unexpected relationships between eigenstates with different parameters and quantum numbers.

A very important result in SUSYQM is the close relationship of the eigenvalues and the eigenfunctions of the SUSY-partner Hamiltonians. Knowing the eigenvalues and eigenfunctions of one of the Hamiltonians, can yield the eigenvalues and eigenfunctions of its SUSY-partner Hamiltonian. This can be useful in solving a complicated Hamiltonian if the solution of its SUSY partner is known.

Using SUSYQM simplifies the problem of solving the second-order Schrödinger differential equation to that of solving a first-order differential equation given by $A^-\psi^0 = 0$. This yields the eigenfunctions at the lowest rung of the tower of states. The rest of the eigenfunctions are obtained by letting A_L^+ act on the eigenfunctions obtained from $A^-\psi^0 = 0$.

As mentioned in Sect. 3.1, the separated differential equations of the Schrödinger equation of the Hartmann potential closely resembles that of the hydrogen atom. There had been work on the SUSY features of the hydrogen atom [10, 13, 14]. These works can possibly give further insights to the role of SUSYQM in the Hartmann potential due to the resemblance of the differential equations of the Hartmann potential to that of the hydrogen atom.

With the above comments, the author hopes to stimulate further examples of applications of SUSYQM to important problems in theoretical chemistry.

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