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Generalized Non-Relativistic Supersymmetric Quantum Mechanics

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1. Introduction

Symmetry has long been recognized as a powerful formal and computational tool in quantum mechanics, beginning with the seminal work of Wigner Wigner & Fano (1960) and Weyl Weyl (1950). Indeed, it is well understood that so-called "accidental degeneracies" were, in fact, not accidents at all but rather the result of "hidden symmetry" (*e.g.* the $2l$+1 degeneracy of the hydrogen atom energy states). Because of this fundamental role in quantum mechanics, the discovery of new symmetries (and their possible "breaking" by interactions) is of enormous interest Griffiths (1987). In the latter half of the 20^{th} century, a new hidden symmetry was discovered that led to much speculation in relativistic quantum field theory as applied to elementary particles. The essence of this so-called "supersymmetry" (SUSY) is that for every boson, there is also a fermion of the same mass (energy) and vice versa. Of course, this has not been observed in nature, leading to speculation that there exists some interaction in nature that "breaks" the symmetry. On the other hand, there is also substantial opinion held by many physicists that SUSY has no connection to physical reality.

This chapter is not aimed at addressing such issues. Rather, it was observed by many Junker (1996) that one did not have to deal with quantum field theory to encounter SUSY. Indeed, SUSY is also an intrinsic feature of ordinary, non-relativistic quantum mechanics (SUSY-QM). In this case, attention has not been focused on whether the symmetry exists in nature. Instead, it has been used primarily as a pedagogical tool. The reason for this lies in the intimate connection of SUSY-QM and the ladder operator approach to the harmonic oscillator, angular momentum, and the hydrogen atom Dirac (1958).

The essence of SUSY-QM is the factorization of the Hamiltonian for a one dimensional system in analogy with the harmonic oscillator. For most bound-state quantum systems, it is possible to define operators analogous to the lowering ($\hat{a}$) and raising ($\hat{a}^\dagger$) operators that factor the harmonic oscillator Hamiltonian. However, in the general case, these operators do not possess all the properties of the harmonic oscillator $\hat{a}$ and $\hat{a}^\dagger$, but rather they behave as so-called "charge operators". As such, the SUSY charge operators not only allow factorization of the one dimensional Hamiltonian, they form a Lie algebraic structure. This structure results in the generation of isospectral "sector Hamiltonians". Unfortunately, almost all previous research concentrated on exactly soluble, one dimensional model systems. We became interested in the possibility of taking computational advantage of SUSY. Our idea was that symmetry in QM has long been known to lead to significant computational simplifications and advantages. We

therefore asked whether this could be the case for SUSY. It turns out that SUSY does, in fact, lead to significant computational advantages Kouri et al. (2010a); Kouri, Markovich, Maxwell & Bittner (2009); Kouri, Markovich, Maxwell & Bodman (2009). In particular, the structure of the degeneracies between sector Hamiltonians makes it possible to achieve significant progress in more accurate calculations of excited state energies and wave functions. Below we outline how the theory can be used as a new computational tool, first for one dimension and later for higher dimensional systems. In addition, we also introduce an entirely new class of system dependent coherent states.

There have been a number of suggested generalizations of SUSY-QM to treat more than one dimensional systems Andrianov et al. (1985); Andrianov, Borisov & Ioffe (1984a;b;c); Andrianov et al. (1986); Andrianov, Borisov, Ioffe & Eides (1984); Andrianov & Ioffe (1988); Andrianov et al. (2002); Cannata et al. (2002); Das & Pernice (1996). For the most part, these have involved the introduction of new "spin-like" variables. One early study instead introduced tensorial operators Stedman (1985), but at the cost of seriously affecting the nature of the energy level degeneracies. In addition, in the tensorial operator approach, he did not consider the application to any system in detail other than writing down the equations for the hydrogen atom without exploring their solutions. In the following sections, we present our generalization of SUSY-QM to allow the treatment of multi-particle, multi-dimensional systems. These include clusters of distinguishable particles and the electronic structure of atoms.

2. Introduction to supersymmetric quantum mechanics in one dimension

The general starting point is to define the so-called "superpotential", usually denoted as W. In the theory, W is related to the ground state wave function through the well-known Riccati substitution Jafarpour & Afshar (2002):

$$\psi_0^1(x) \;=\; Ne^{-\int_0^x W(x')\,dx'}\,. \tag{2.1}$$

The relationship between the superpotential W and the physical interaction $V(x)$ results from assuming that Equation (2.1) solves the standard Schrödinger equation with energy zero. This does not impose any restriction since the energy can be changed by adding any constant to the Hamiltonian. Thus,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_0^1}{dx^2} + V_1\psi_0^1 \;=\; 0 \tag{2.2}$$

If we solve for W_1 in Equation (2.1), we find that

$$W_1 \;=\; -\frac{\frac{d\psi_0^1}{dx}}{\psi_0^1} \;=\; -\frac{d}{dx}\ln\psi_0^1 \tag{2.3}$$

and, if W_1 is known, V_1 is given by

$$V_1(x) \;=\; \frac{\hbar^2}{2m}\left(W_1^2(x) - \frac{dW_1}{dx}\right) \tag{2.4}$$

It is then evident that

$$-\frac{d^2\psi_0^1}{dx^2} + \left(W_1^2(x) - \frac{dW_1}{dx}\right)\psi_0^1 \;=\; 0 \tag{2.5}$$

The Hamiltonian operator now can be factored in the form

$$-\frac{d^2}{dx^2} + W_1^2(x) - \frac{dW_1}{dx} \;=\; \left[-\frac{d}{dx} \;+\; W_1(x) \right] \left[\frac{d}{dx} \;+\; W_1(x) \right] \tag{2.6}$$

We define the "charge" operator and its adjoint by (assuming W_1 is hermitian; *i.e.*, ψ_0^1 is real)

$$Q_1 \;=\; \frac{d}{dx} + W_1, \; Q_1^\dagger \;=\; -\frac{d}{dx} + W_1 \tag{2.7}$$

Then the "first sector" Hamiltonian is defined as

$$\mathcal{H}_1 \;=\; Q_1^\dagger Q_1 \tag{2.8}$$

Then it follows that for $n > 0$, (since for $n \;=\; 0$, $E_0 \;=\; 0$),

$$Q_1^\dagger Q_1 \psi_n^1 \;=\; E_n^1 \psi_n^1 \tag{2.9}$$

We then apply Q_1 to the equation, to obtain

$$Q_1 Q_1^\dagger (Q_1 \psi_n^1) \;=\; E_n^1 Q_1 \psi_n^1 \tag{2.10}$$

Thus, $Q_1 \psi_n^1$ is an eigenstate of $\mathcal{H}_2$ with the same energy, E_n^1, as the state ψ_n^1. Similarly, consider the eigenstates of $\mathcal{H}_2$:

$$\mathcal{H}_2 \psi_n^2 \;=\; Q_1 Q_1^\dagger \psi_n^2 \;=\; E_n^2 \psi_n^2. \tag{2.11}$$

Application of $Q^\dagger$, then implies that $Q_1^\dagger \psi_n^2$ is an eigenstate of $\mathcal{H}_1$:

$$(Q_1^\dagger Q_1)(Q_1^\dagger \psi_n^2) \;=\; E_n^2 Q_1^\dagger \psi_n^2 \tag{2.12}$$

It follows that the Hamiltonians $\mathcal{H}_1$ and $\mathcal{H}_2$ have identical spectra with the exception of the ground state, since the $E_0^1 \;=\; 0$ wave function is unique. In the case of the ground state ψ_0^1, we recall that

$$Q_1 \psi_0^1 \;=\; 0 \tag{2.13}$$

which shows that the quantity $Q_1 \psi_0^1$ cannot be used to generate the ground state of the second sector. Indeed, Equation (2.13) indicates that such a ψ_0^2 would vanish identically.
Because of the uniqueness of the $E_0^1 = 0$ state, the indexing of the first and second sector levels must be modified. Consider

$$Q_1 Q_1^\dagger \psi_n^2 \;=\; E_n^2 \psi_n^2 \tag{2.14}$$

Then

$$Q_1^\dagger Q_1 (Q_1^\dagger \psi_{n+1}^1) \;=\; E_{n+1}^1 (Q_1^\dagger \psi_{n+1}^1) \tag{2.15}$$

since $Q \psi_0^1 \equiv 0$. So

$$E_n^2 \;=\; E_{n+1}^1 \tag{2.16}$$

and we conclude that

$$\psi_n^2 = \frac{Q_1\psi_{n+1}^1}{\sqrt{E_{n+1}^1}} \text{ and } \psi_{n+1}^1 = \frac{Q_1^\dagger\psi_n^2}{\sqrt{E_n^2}} \tag{2.17}$$

The next step in building a hierarchy of isospectral Hamiltonians is to define a second superpotential, W_2, according to

$$W_2 = -\frac{d}{dx}\ln\psi_0^2 \tag{2.18}$$

in much the same way as we did before. It is then clear that we can define an alternate form for $\mathcal{H}_2$, given by

$$\mathcal{H}_2 = Q_2^\dagger Q_2 + E_0^2, \tag{2.19}$$

where

$$Q_2 = \frac{d}{dx} + W_2 \tag{2.20}$$

We observe that ψ_0^2 is automatically an eigenstate of this form for $\mathcal{H}_2$

$$\mathcal{H}_2\psi_0^2 = E_0^2\psi_0^2 \tag{2.21}$$

Next consider the first excited state eigenvalue equation for the second sector:

$$\mathcal{H}_2\psi_1^2 = E_1^2\psi_1^2 \tag{2.22}$$

We apply Q_2 to Equation (2.22) to find

$$\left(Q_2Q_2^\dagger + E_0^2\right)Q_2\psi_1^2 = E_n^2Q_2\psi_1^2 \tag{2.23}$$

Then, by similar reasoning, we deduce that

$$Q_2\psi_1^2 = \sqrt{E_1^2 - E_0^2}\psi_0^3. \tag{2.24}$$

Using the new charge operators Q_2 and $Q_2^\dagger$, we then define the third sector Hamiltonian,

$$\mathcal{H}_3 = Q_2Q_2^\dagger + E_0^2, \tag{2.25}$$

with ground state equation

$$\mathcal{H}_3\psi_0^3 = E_0^3\psi_0^3 \tag{2.26}$$

It follows that

$$Q_2^\dagger\psi_0^3 = \sqrt{E_1^2 - E_0^2}\psi_1^2 \tag{2.27}$$

and,

$$Q_2Q_2^\dagger\psi_0^3 = \left(E_1^2 - E_0^2\right)\psi_0^3 = E_0^3\psi_0^3 \tag{2.28}$$

Thus, we conclude that

$$E_0^3 = E_1^2 - E_0^2 \tag{2.29}$$

It is clear that this procedure can be continued until one exhausts the number of bound excited states supported by $\mathcal{H}_1$. We also see that determining the excited state energies and wave

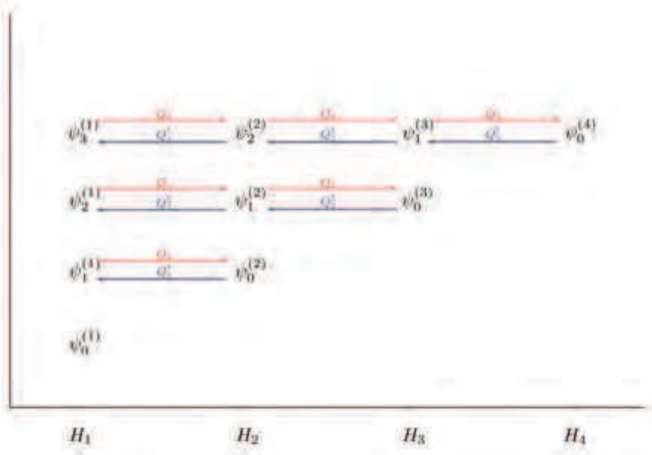


Fig. 1. Above, we display graphically how this hierarchical degenarcy is realized.

functions for $\mathcal{H}_1$ involves solving for the ground state energies and wave functions for each sector Hamiltonian, $\mathcal{H}_j$, $j > 1$.
For a more concrete example, we present a general family of anharmonic oscillator. The ubiquity of this example in chemistry and physics is best exemplified by the fact that all nuclear vibrations in molecules are anharmonic, with the effect increasing as the vibrational energy gets closer to the dissociation limit Wilson et al. (1955). Additionally, anharmonicity is also present when studying the effects of rotation, through the centrifugal potential. For the one dimensional case, we consider an oscillator on the domain $-\infty < x < \infty$. In order to have potentials that are guaranteed to possess bound states, we shall postulate a superpotential

$$W(x) \;=\; \sum_{j=0}^{J} d_j x^{2j+1} \tag{2.30}$$

Then the corresponding sector one potential, $V_1(x)$, is

$$V_1(x) \;=\; \sum_{j=0}^{J}\sum_{j'=0}^{J} d_j d_{j'} x^{2(j+j'+1)} - \sum_{j\,=\,0}^{J} d_J(2j+1)x^{2j} \tag{2.31}$$

The "charge" operators are given by

$$Q_1 \;=\; \frac{d}{dx} + W_1 \;\text{ and }\; Q_1^{\dagger} \;=\; -\frac{d}{dx} + W_1. \tag{2.32}$$

Then the first sector ground state for a general member of this family is

$$\psi_0^{+}(x) \;=\; Ne^{-\sum_{j=0}^{J} \frac{d_j x^{2j+2}}{(2j+2)}} \tag{2.33}$$

We stress that contrary to the periodic case Kouri, Markovich, Maxwell & Bodmann (2009), the solution of the sector two equation,

$$Q^{\dagger}\psi_0^2(x) \;=\; 0 \tag{2.34}$$

is not allowed because it is not normalizable. Thus, the ground state for the second sector satisfies

$$Q_1 Q_1^\dagger \psi_0^2(x) \;=\; E_0^2 \psi_0^2(x) \;=\; E_1^1 \psi_0^2(x) \tag{2.35}$$

where

$$E_1^1 \neq 0 \tag{2.36}$$

However, once $\psi_0^2(x)$ is known, one can generate the first excited state $\psi_1^1(x)$ according to

$$Q_1^\dagger \psi_0^2(x) \;=\; \sqrt{E_0^2}\psi_0^1(x) \tag{2.37}$$

The energy, E_1^1, of $\psi_1^1(x)$ is, of course, equal to E_0^2.
We remark that the ground state, $\psi_0^1(x)$ is equal to the product of the ground states for each separate term in W. This is to say that,

$$\psi_0^1(x) \;=\; N \prod_{j=0}^{J} e^{\frac{d_j x^{2j+2}}{(2j+2)}}, \tag{2.38}$$

where N is the normalization constant. This is true even though $V_1(x)$ contains cross terms of the form

$$d_j d_{j'} x^{2(j+j'+1)}, \;\; j \neq j' \tag{2.39}$$

In fact, even more general anharmonic oscillators can be dealt with. Thus, any function, $g(x)$ can be added to $W(x)$ in Equation (2.30), provided only that $e^{-\int_0^x g(x')\,dx'}$ is $\mathcal{L}_2$. Thus, not only polynomic anharmonic potentials can be treated but many others.

3. Computational examples

In the following section we will explore the computational aspects of our SUSY-QM approach using two example anharmonic oscillator systems. To illustrate this approach to polynomic anharmonic oscillation we define $W(x)$ to be

$$W_1(x) \;=\; x^3 + 2x, \tag{3.1}$$

which obviously yields a potential for the first sector of

$$V_1(x) = x^6 + 4x^4 + x^2 - 2. \tag{3.2}$$

Where x is defined on the domain $-\infty < x < \infty$. We can thus define $\mathcal{H}_1$ as:

$$\mathcal{H}_1 \;=\; \left[-\frac{d}{dx} \;+\; W_1(x) \right] \left[\frac{d}{dx} \;+\; W_1(x) \right] \tag{3.3}$$

which satisfies the equation

$$\mathcal{H}_1 \psi(x)_0^{(1)} \;=\; 0, \tag{3.4}$$

and possesses an analytic ground state wave function of

$$\psi_0^{(1)} \;=\; N e^{-\left(\frac{x^4}{4} + x^2\right)}. \tag{3.5}$$

To get the second Hamiltonian in the hierarchy we next define $\mathcal{H}_2$ as

$$\mathcal{H}_2 \;=\; \left[\frac{d}{dx} \;+\; W_1(x) \right] \left[-\frac{d}{dx} \;+\; W_1(x) \right] \tag{3.6}$$

so

$$V_2 \;=\; x^6 + 4x^4 + 7x^2 + 2 \tag{3.7}$$

and we must solve the equation

$$\mathcal{H}_2\psi_0^{(2)} \;=\; E_0^{(2)}\psi_0^{(2)}. \tag{3.8}$$

Possessing $\psi_0^{(2)}$, we may develop the next Hamiltonian in the hierarchy. To do so, we begin by expressing $\mathcal{H}_2$ in the following form

$$\mathcal{H}_2 \;=\; \left[\, -\frac{d}{dx} \;+\; W_2(x) \,\right]\left[\, \frac{d}{dx} \;+\; W_2(x) \,\right] + E_0^{(2)} \tag{3.9}$$

where

$$W_2(x) \;=\; -\frac{d}{dx}\ln\psi_0^{(2)}. \tag{3.10}$$

with

$$\psi_0^{(3)} \;=\; \frac{Q_2\psi_1^{(2)}}{\sqrt{E_1^{(2)} - E_0^{(2)}}}. \tag{3.11}$$

From this point, one can obviously generate as many Hamiltonians as needed. It should also be noted that the excited state wave functions can be obtained by using the charge operators we have previously defined. We now turn to the proof of principle for this approach as a computational scheme to obtain improved excited state energies and wave functions in the Rayleigh-Ritz variational method. We should note that these results can be generalized to any system where a hierarchy of hamiltonians can be generated because of the nature of the Rayleigh-Ritz scheme. In the standard approach one calculates the energies and wave functions variationally, relying on the Hylleraas-Undheim theorem for convergence Hylleraas & Undheim (1930). This, however, is unattractive for higher energy states because they require a much larger basis to converge to the same error. We stress that this is true regardless of the specific basis set used. Of course, some bases will be more efficient than others but it is generally true that for a given basis, the Rayleigh-Ritz result is less accurate for excited states. We address this situation by always solving for ground states in the variational part of the problem.

To demonstrate our computational scheme, we investigate the first example system from the previous section. For this potential Equation (3.2), exact solutions are known for all states of $\mathcal{H}_1$. We use the exact results to assess the accuracy of the variational calculations. For our first variational calculations, we use the harmonic oscillator basis functions where:

$$\phi_n(x) = \frac{1}{\sqrt{2^n n!\sqrt{\pi}}}\mathcal{H}_n(x)e^{-\frac{x^2}{2}}, \tag{3.12}$$

with each matrix element determined using

$$\langle\phi_{n'}|\mathcal{H}_i|\phi_n\rangle \tag{3.13}$$

Using the hierarchy of hamiltonians, we present the converged eigenvalues in Table 1. In Table 1, all energies were obtained for each of the Hamiltonians, $\mathcal{H}_1$ and $\mathcal{H}_2$, by standard variational calculations using basis set sizes to achieve an accuracy of 10^{-6}. It is easily seen that the ground state of $\mathcal{H}_2$ is degenerate with the first excited state of $\mathcal{H}_1$. More interesting is the behavior of the excited state wave functions. Using the Cauchy criterion to measure

convergence, we show the basis set size (N) needed in a standard variational approach to obtain various eigenstates to the accuracy shown in Table 2. Clearly, excited state wave functions require substantially larger basis sets to achieve a high degree of accuracy. In Table 3 we show the results obtained for the same excited state wave functions obtained by applying the charge operator to the ground state wave function for $\mathcal{H}_2$. Again, N denotes the basis set required, and ΔN is the reduction of basis set achieved by use of the charge operators.

n	${}_N\psi_0^n$	$\mathcal{H}_1$	${}_N\psi_1^n$	$\mathcal{H}_2$	Δ N
0	${}_{44}\psi_0^1$	6.9441187e-07	${}_{34}\psi_0^1$	5.024450	18
1	${}_{52}\psi_1^1$	5.024449	${}_{42}\psi_0^1$	11.696825	20
2	${}_{62}\psi_2^1$	11.696820	${}_{50}\psi_0^1$	19.497666	-

Table 1. Energies for the Anharmonic Polynomic Oscillator using Hierarchy of Hamiltonians.

n	${}_N\psi_0^n$	$\mathcal{L}_2$	$\mathcal{L}_\infty$
0	${}_{56}\psi_0^1$	5.835283e-07	1.110223-16
1	${}_{78}\psi_1^1$	1.975656e-07	4.019723e-16
0	${}_{68}\psi_0^2$	2.303928e-07	2.220446e-16

Table 2. Wave function errors for the Anharmonic Polynomic Oscillator using the standard variational method for each hierarchy Hamiltonian. Each value has six significant figures.

n	ΔN	${}_N\psi_0^n$	$\mathcal{L}_2$	$\mathcal{L}_\infty$
1	4	${}_{74}\psi_1^1$	4.083823e-07	2.086041e-16

Table 3. Wave function errors for the Anharmonic Polynomic Oscillator using Charge Operators to find excited states. Each value has six significant figures.

To find the solutions we used LAPACK routines to find these eigenvalues and vectors and GSL routines for numerical integration. Clearly, the use of the hierarchy of hamiltonians and charge operators provides more rapid convergence, which provides us with better methods to calculate the excited states.
The second example results from taking

$$W_1(x) = x^3 + x + e^x. \tag{3.14}$$

In this case,

$$\begin{aligned} V_1(x) &= x^6 + 2x^4 + 2x^3e^x + \\ & 2xe^x + x^2 + e^{2x} - 3x^2 - e^x - 1 \end{aligned} \tag{3.15}$$

Then

$$\mathcal{H}_1 = \left[-\frac{d}{dx} + x^3 + x + e^x \right] \left[\frac{d}{dx} + x^3 + x + e^x \right] \tag{3.16}$$

with

$$\mathcal{H}_1 \psi_0^1 \;=\; 0 \tag{3.17}$$

and the analytical ground state is

$$\psi_0^{(1)} \;=\; N e^{-(\frac{x^4}{4}+\frac{x^2}{2}+e^x)}. \tag{3.18}$$

Then the second sector Hamiltonian is

$$\mathcal{H}_2 \;=\; \left[\, \frac{d}{dx} \;+\; x^3 + x + e^x \,\right] \left[\, -\frac{d}{dx} \;+\; x^3 + x + e^x \,\right] \tag{3.19}$$

The ground state satisfies

$$\mathcal{H}_2 \psi_0^2 \;=\; E_0^2 \psi_0^2 \tag{3.20}$$

which must be solved numerically.
We performed the Rayleigh-Ritz calculations and found similar results for the second system described by $W \;=\; x^3 + x + e^x$. Because the excited states of this oscillator are not known analytically, we use the Cauchy convergence criterion

$$\int_{-\infty}^{\infty} |{}_N\psi_n - {}_{N-1}\psi_n|^2 \, dx, \tag{3.21}$$

where N is the basis size. In Table 4, we give the converged energy levels (to 5 significant figures) obtained by standard variational calculations applied to $\mathcal{H}_1$ and $\mathcal{H}_2$. In Table 5, we show the basis set sizes needed in standard variational calculations to converge the wave functions for $\mathcal{H}_1$ and $\mathcal{H}_2$ (again, the Cauchy criterion of convergence was used.) Finally, in Table 6, we show the results for excited states obtained using the charge operators applied to the ground state wave functions of $\mathcal{H}_2$. Again, ΔN shows the reduction in the basis size gained by the charge operator approach.
Finally, we compared the numerical accuracy of the first excitation energy of the anharmonic oscillator described by Equation (3.2), but now using a n-point discrete variable representation (DVR) based upon the Tchebychev polynomials to compute the eigenspectra of the first and second sectors. In Figure 2 we show the numerical error in the first excitation energy by comparing $E_1^1(n)$ (the first excited state energy from the standard variational calculation with n-DVR basis functions) and $E_0^2(n)$ (the ground state of the sector two Hamiltonian computed with n-DVR basis functions) from an n point DVR to the numerically "exact" value corresponding to a 100 DVR points,

$$\epsilon_1^1(n) = \log_{10} |E_1^1(n) - E_1^1(exact)|.$$

Likewise,

$$\epsilon_0^2(n) = \log_{10} |E_0^2(n) - E_1^1(exact)|.$$

For any given basis size, $\epsilon_0^2 < \epsilon_1^1$. Moreover, over a range of $15 < n < 40$ points, the excitation energy computed using the second sector's ground state is between 10 and 100 times more accurate than $E_1^1(n)$. This effectively reiterates our point that by using the SUSY hierarchy, one can systematically improve upon the accuracy of a given variational calculation. It also illustrates that our conclusion does not depend on the basis set used.

n	${}_N\psi_0^n$	$\mathcal{H}_1$	${}_N\psi_1^n$	$\mathcal{H}_2$
0	${}_{50}\psi_0^1$	2.703955e-06	${}_{44}\psi_0^1$	5.263075
1	${}_{60}\psi_1^1$	5.263075	${}_{56}\psi_0^1$	12.109712
2	${}_{64}\psi_2^1$	12.109717	${}_{66}\psi_0^1$	20.186019

Table 4. Energies for the Anharmonic Non-Polynomic Oscillator using Hierarchy of Hamiltonians, determined variationally.

n	${}_N\psi_0^n$	$\mathcal{L}_2$	$\mathcal{L}_\infty$
0	${}_{70}\psi_0^1$	3.7158761e-07	2.220446e-16
1	${}_{88}\psi_1^1$	6.477328e-08	1.221245e-15
0	${}_{76}\psi_0^2$	5.659010e-07	2.109424e-15

Table 5. Errors for the Anharmonic Non-Polynomic Oscillator wave functions using Hierarchy of Hamiltonians all determined variationally.

n	ΔN	${}_N\psi_0^n$	$\mathcal{L}_2$	$\mathcal{L}_\infty$
1	14	${}_{74}\psi_1^1$	9.750546e-07	3.181791e-16

Table 6. Errors for the Anharmonic Non-Polynomic Oscillator using wave functions Charge Operators to find excited states by applying the correct charge operator to the appropriate ground state

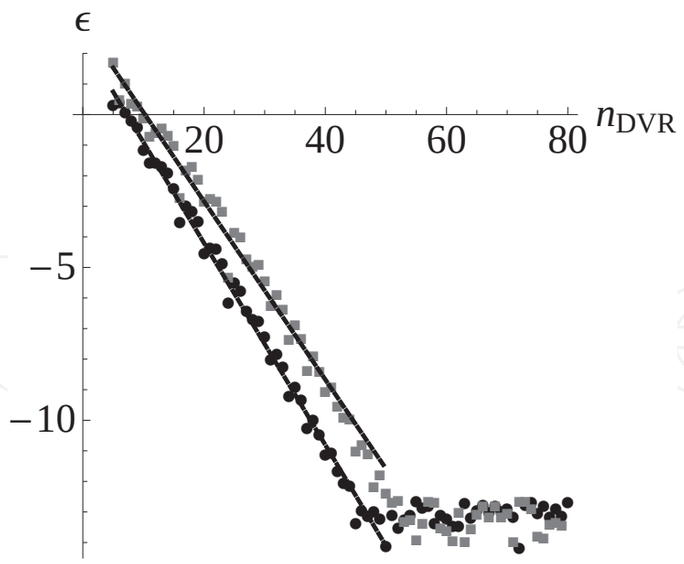


Fig. 2. Convergence of first excitation energy E_1^1 for model potential $V_1 = x^6 + 4x^4 + x^2 - 2$ using a n-point discrete variable representation (DVR). Gray squares: $\epsilon = \log_{10} |E_1^1(n) - E_1^1(exact)|$, Black squares: $\epsilon = \log_{10} |E_0^2(n) - E_1^1(exact)|$. Dashed lines are linear fits.

Another way to approximate excited state energies and wave functions of bound quantum systems is to take advantage of the Ricatti substitution for the purpose of constructing dynamically-adapted, system-specific coherent states. Perhaps the simplest procedure for creating an overcomplete set of such coherent states is to follow the work of Kouri, et al. Klauder & Skagerstam (1985); Kouri et al. (2003). In their approach, it was observed that the "fiducial" function, $\langle x|\psi(0)\rangle = \psi_0^1(x)$, could be translated an amount x_0 by application of the shift operator $e^{-x_0\frac{d}{dx}}$

$$\begin{aligned}\psi(\alpha|x) &= Ne^{ik_0(x-x_0)}e^{-x_0\frac{d}{dx}}\psi(0|x) \\ &= Ne^{ik_0(x-x_0)}e^{-\int_0^{x-x_0}W(x')\,dx'},\end{aligned} \tag{3.22}$$

where $\alpha = x_0 + ik_0$ is a point in the phase space Klauder & Skagerstam (1985) which completely describes the coherent state and the de Broglie relation tells us that $\langle \hat{p}_x \rangle = k_0$. Using the set of coherent states defined above, we can select a finite subset which remains overcomplete by discretizing the otherwise continuous label $\alpha = q + ik$ and setting up a von Neumann lattice in phase space with an appropriate density, D. We define an overcomplete basis of coherent states

$$\{\phi(\alpha_i|x) = Ne^{ik_i(x-q_i)}e^{-\int_0^{x-q_i}W(x')\,dx'} : 1 \leq i \leq M,\ M \in \mathbb{N}\}, \tag{3.23}$$

where M is the number of basis functions and the phase space grid points are given by

$$\{(q_i, k_i)\} = \left\{\left(m\Delta x\sqrt{\frac{2\pi}{D}}, \frac{n}{\Delta x}\sqrt{\frac{2\pi}{D}}\right)\right\}, m, n \in \mathbb{Z}, \tag{3.24}$$

and i being a joint index consisting of m and n Andersson (2001).
Due to the fact that the ground state of the system of interest solves the time-independent Schrödinger equation for the corresponding Hamiltonian, the coherent states defined above build in the dynamics of the system under investigation. This property leads to the expectation that these system-specific coherent states will prove more rapidly convergent in the approximation of excited state energies of bound quantum systems using variational methods.
For $W(x) = x^3$, and thus $V(x) = x^6 - 3x^2$, we carried out a variational calculation using the system-specific coherent states defined above and compared the accuracy in the approximation of the first three excited state energy eigenvalues with that achieved using the standard harmonic oscillator basis and the harmonic oscillator coherent states. To evaluate the accuracy of each method, we compare the results with a Chebyshev polynomial DVR (Discrete Variable Representation) calcuation using 1000 points Littlejohn (2002). The number of decimal places reported in Tables 7-10 correspond to the number of decimal places of agreement with the DVR plus an additional significant figure which is either rounded up or down.

E_0	E_1	E_2	E_3
0.000000000	1.935482104	6.298495901	11.680970886

Table 7. DVR Comparison.

M	E_0	E_1	E_2	E_3
9	0.000000000	1.9355	6.3	11.69
15	0.000000000	1.93548218	6.2985	11.681

Table 8. System-Specific Coherent States.

M	E_0	E_1	E_2	E_3
9	0.2	2.0	15.0	43.0
15	0.2	2.0	9.0	43.0

Table 9. Harmonic Oscillator Coherent States.

M	E_0	E_1	E_2	E_3
9	0.07	2.0	6.9	23.0
15	0.01	1.99	6.5	12.0

Table 10. Harmonic Oscillator Basis.

The results indicate that, in fact, the system-specific coherent states provide more accurate approximations of the excited state energies for the anharmonic oscillator given by $V(x) = x^6 - 3x^2$ when compared with other bases. Namely, they give seven decimal places of agreement with the DVR when 15 basis functions are used. The same number of harmonic oscillator basis functions only provides one decimal point of agreement, and 15 harmonic oscillator coherent states fails to give agreement in the ones place with the DVR. Despite the accuracy achieved using a small number of system-specific coherent states, the non-orthogonality and complex-valued nature of the basis necessitates the calculation of a complex overlap matrix, whose elements must be computed by numerical integration, which is computationally demanding. In order to eliminate numerical integration from the calculation, one can expand the ground state wave function used in the construction of the coherent states into an incomplete set of scaled Gaussians centered about the $\{q_i : 1 \leq i \leq M\}$. This expansion would allow us to compute the overlap matrix elements analytically, replacing numerical integration with function evaluation. In particular, we propose to use the Levenberg-Marquardt least-squares curve-fitting algorithm to build an arbitrarily-accurate approximation of each system-specific coherent state in the following manner:

$$\phi(\alpha_i|x) \approx Ne^{ik_i(x-q_i)} \sum_{j=1}^{\tilde{M}} c_j e^{-(x-q_i)^2/\sigma_j} . \tag{3.25}$$

4. Generalization to multi-dimensions

In our generalization, we make use of a vectorial approach that simultaneously treats more than one dimension and any number of distinguishable particles. We consider, therefore, a system of n-particles in three-dimensional space. We denote the coordinates of particle i by (x_i, y_i, z_i). We then define an orthogonal hyperspace of dimension $3n$. We take the Hamiltonian for this system to be given by

$$\mathcal{H}_1 = -\nabla^2 + V_1 \tag{4.1}$$

where

$$\vec{\nabla} = \sum_j \vec{\epsilon}_j \frac{\partial}{\partial u_j} \tag{4.2}$$

and $\vec{\epsilon}_j \cdot \vec{\epsilon}_k = \delta_{jk}$. The subscript "1" indicates this is the "sector one" Hamiltonian. For simplicity we take the masses of the particles to be equal and use units such that $\hbar^2/2m = 1$. For the development here we assume a Cartesian coordinate space, but have provided an extension to more general curvilinear coordinates in a previous publication Kouri et al. (2010b).

As per usual in quantum mechanics, the ground-state wave function is a solution of the Schrödinger equation,

$$\mathcal{H}_1 \psi_0^{(1)} = E_0^{(1)} \psi_0^{(1)}. \tag{4.3}$$

We also emphasize that the lowest energy state, $\psi_0^{(1)}$, is nodeless.

We now define a vector superpotential, $\vec{W}$, as

$$\vec{W} = -\vec{\nabla} \ln \psi_0^{(1)}, \tag{4.4}$$

which is to say

$$\vec{W} = \sum_{j=1}^{3n} \vec{\epsilon}_j W_j = -\sum_{j=1}^{3n} \vec{\epsilon}_j \frac{\partial}{\partial u_j} \ln \psi_0^{(1)}. \tag{4.5}$$

It is straightforward to see that one can write $\mathcal{H}_1$ in terms of $\vec{W}$ as

$$\begin{aligned} (\mathcal{H}_1 - E_0^{(1)}) &= (-\vec{\nabla} + \vec{W}) \cdot (+\vec{\nabla} + \vec{W}) \\ &= (-\partial_i + W_i)(\partial_i + W_i) \\ &= Q_i^\dagger \cdot Q_i, \end{aligned} \tag{4.6}$$

where, according to the Einstein convention, we sum over repeated indices. Since $(\vec{\nabla} + \vec{W})\psi_0^{(1)} \equiv \vec{Q}\psi_0^{(1)} \equiv \vec{0}$, it is clear that $(\mathcal{H}_1 - E_0^{(1)})\psi_0^{(1)} = 0$ as required. We can now define the sector two Hamiltonian such that, above the ground-state $(E_0^{(1)})$, it is isospectral with $\mathcal{H}_1$. We do this as follows: for the first excited state in sector one we can write

$$Q_i^\dagger \cdot Q_i \psi_1^{(1)} = (E_1^{(1)} - E_0^{(1)})\psi_1^{(1)}. \tag{4.7}$$

We then form the tensor product by operating on the left with $\vec{Q}$ so that

$$(\vec{Q}\vec{Q}^\dagger) \cdot \vec{Q}\psi_1^{(1)} = (E_1^{(1)} - E_0^{(1)})\vec{Q}\psi_1^{(1)}. \tag{4.8}$$

That is to say, using Einstein notation,

$$(Q_i Q_j^\dagger) Q_j \psi_1^{(1)} = (E_1^{(1)} - E_0^{(1)}) Q_i \psi_1^{(1)}. \tag{4.9}$$

It then follows that $\vec{Q}\psi_1^{(1)}$ is an eigenstate of the tensor Hamiltonian $\overleftrightarrow{\mathcal{H}}_2 = (\vec{Q}\vec{Q}^\dagger)$ with energy $E_0^{(2)} = E_1^{(1)} - E_0^{(1)}$. Since we are free to set the energy origin, taking $E_0^{(1)} = 0$ gives $E_0^{(2)} = E_1^{(1)}$. It is also clear that $\vec{Q}\psi_0^{(1)}$ cannot generate a lower energy eigenstate of $\overleftrightarrow{\mathcal{H}}_2$ since $\vec{Q}\psi_0^{(1)} = \vec{0}$, so

that $\vec{Q}\psi_1^{(1)}$ is indeed proportional to the ground state of $\overleftrightarrow{\mathcal{H}}_2$. The precise relation for obtaining the sector one state from a sector two state is given by

$$\psi_{n+1}^{(1)} = \frac{1}{\sqrt{E_{n+1}^{(1)} - E_0^{(1)}}} \vec{Q}^\dagger \cdot \vec{\psi}_n^{(2)}. \tag{4.10}$$

It is very instructive to illustrate this by considering a simple two dimensional separable harmonic oscillator model problem. This is because we can learn something of how our SUSY formalism works with an exactly soluble problem. We therefore consider a system described by the Hamiltonian

$$\mathcal{H} = -\frac{\partial^2}{\partial u_1^2} - \frac{\partial^2}{\partial u_2^2} + u_1^2 + u_1^2 \tag{4.11}$$

where again, we set $\hbar^2/2m_1 = \hbar^2/2m_2 = 1$. The solution of the Schrödinger equation is well known to be the product of one dimensional harmonic oscillator states,

$$\psi_{(n_1,n_2)}^{(1)} = N_{n_1,n_2} \mathcal{H}_{n_1}(u_1) \mathcal{H}_{n_2}(u_2) e^{-(u_1^2+u_2^2)/2} \tag{4.12}$$

where N_{n_1,n_2} is the normalization constant and $\mathcal{H}_n$ denotes the n^{th} Hermite polynomial. The ground state is

$$\psi_{(0,0)}^{(1)} = N_{0,0} e^{-(u_1^2+u_2^2)/2} \tag{4.13}$$

with the zero point energy in this case equals to 2. We next generate the vector superpotential, $\vec{W}_1$, as

$$\vec{W}_1 = -\vec{\nabla} \ln \psi_{(0,0)}^{(1)} = u_1 \hat{\epsilon}_1 + u_2 \hat{\epsilon}_2 \tag{4.14}$$

where

$$\vec{\nabla} = \hat{\epsilon}_1 \frac{\partial}{\partial u_1} + \hat{\epsilon}_2 \frac{\partial}{\partial u_2}. \tag{4.15}$$

We consider

$$(-\vec{\nabla} + \vec{W}_1) \cdot (\vec{\nabla} + \vec{W}_1) = -\nabla^2 + \vec{W}_1 \cdot \vec{W}_1 - \vec{\nabla} \cdot \vec{W}_1 \tag{4.16}$$

we see that $\vec{W}_1 \cdot \vec{W}_1 - \vec{\nabla} \cdot \vec{W}_1 = u_1^2 + u_2^2 - 2 = V - 2$, so that

$$\mathcal{H}_1 = \vec{Q}_1^\dagger \cdot \vec{Q}_1 + 2 \tag{4.17}$$

It is easily verified that

$$\mathcal{H}_1 \psi_{(0,0)}^{(1)} = 2\psi_{(0,0)}^{(1)}, \tag{4.18}$$

as required. The first excited states of $\mathcal{H}_1$ are doubly degenerate with energy $E_{(1,0)}^{(1)} = E_{(0,1)}^{(1)} = 3$ and denoted by $\psi_{(1,0)}^{(1)}$ and $\psi_{(0,1)}^{(1)}$. The next excited state, $\psi_{(1,1)}^{(1)}$ is degenerate with $\psi_{(0,2)}^{(1)}$ and $\psi_{(2,0)}^{(1)}$ with energy $E_{(1,1)}^{(1)} = E_{(2,0)}^{(1)} = E_{(0,2)}^{(1)} = 4$.

We construct the rigorous sector two Hamiltonian as

$$\overleftrightarrow{\mathcal{H}}_2 = \vec{Q}_1\vec{Q}_1^{\dagger} + 2\overleftrightarrow{1}\ , \quad \overleftrightarrow{1} = \hat{\epsilon}_1\hat{\epsilon}_1 + \hat{\epsilon}_2\hat{\epsilon}_2, \tag{4.19}$$

which is a second rank tensor in this case. The Hamiltonian $\overleftrightarrow{H}_2$ is then given by

$$\begin{aligned}\overleftrightarrow{\mathcal{H}}_2 = \hat{\epsilon}_1\hat{\epsilon}_1[-\frac{\partial^2}{\partial u_1^2} + u_1^2 + 3] + \hat{\epsilon}_1\hat{\epsilon}_2[-\frac{\partial^2}{\partial u_1 \partial u_2} + u_1u_2 - u_1\frac{\partial}{\partial u_2} + u_2\frac{\partial}{\partial u_1}] \\ + \hat{\epsilon}_2\hat{\epsilon}_1[-\frac{\partial^2}{\partial u_1 \partial u_2} + u_1u_2 - u_2\frac{\partial}{\partial u_1} + u_1\frac{\partial}{\partial u_2}] + \hat{\epsilon}_2\hat{\epsilon}_2[-\frac{\partial^2}{\partial u_2^2} + u_2^2 + 3].\end{aligned} \tag{4.20}$$

The eigenvalue equation is

$$\overleftrightarrow{\mathcal{H}}_2 \cdot \vec{\psi}^{(2)}_{(n)} = E^{(2)}_{(n)}\vec{\psi}^{(2)}_{(n)} \tag{4.21}$$

with eigenstates

$$\vec{\psi}^{(2)}_{(n)} = \hat{\epsilon}_1\psi^{(2)}_{(n)1} + \hat{\epsilon}_2\psi^{(2)}_{(n)2}. \tag{4.22}$$

It is not difficult to show that there are two degenerate ground state solutions given by

$$\vec{\psi}^{(2)}_{(0)1} = \hat{\epsilon}_1 e^{-(u_1^2+u_2^2)/2} \tag{4.23}$$

and

$$\vec{\psi}^{(2)}_{(0)2} = \hat{\epsilon}_2 e^{-(u_1^2+u_2^2)/2}, \tag{4.24}$$

respectively. This is extremely interesting and in contrast to the usual situation in quantum mechanics. For most systems (excluding spin effects) the ground state is unique, i.e., non-degenerate.
We shall see that the degenerate states, Equation (4.23)-(4.24), are exactly what is required for the charge operator, $\vec{Q}_1^{\dagger}$ to produce the doubly degenerate states $\psi^{(1)}_{(1,0)}$ and $\psi^{(1)}_{(0,1)}$. Thus, recall that

$$\vec{Q}_1^{\dagger} = \hat{\epsilon}_1(-\frac{\partial}{\partial u_1} + u_1) + \hat{\epsilon}_2(-\frac{\partial}{\partial u_2} + u_2) \tag{4.25}$$

Then

$$\vec{Q}_1^{\dagger} \cdot \vec{\psi}^{(2)}_{0(1)} = 2u_1 e^{-(u_1^2+u_2^2)/2} \propto \psi^{(1)}_{(1,0)} \ \text{ and } \ \vec{Q}_1^{\dagger} \cdot \vec{\psi}^{(2)}_{0(2)} = 2u_2 e^{-(u_1^2+u_2^2)/2} \propto \psi^{(1)}_{(0,1)} \tag{4.26}$$

Our results Equation (4.23)-(4.24) possess a remarkable property. Only one component is nonzero! We shall see that this is indicative of an extremely interesting property that we observe in the non-separable examples that we consider next. Indeed, we recall that in relativistic quantum mechanics, one obtains a tensor Hamiltonian and the solutions are characterized by large and small components. In the present case, the small component is exactly zero. In the degenerate pair of solutions, which component is zero changes. We stress, however, that any linear combination of the two degenerate solutions is also a solution of the same energy.

With a view toward the next section, where we consider a two dimensional, nonseparable anharmonic oscillator(or equivalently a pair of one dimensional coupled oscillators), we form the equivalent degenerate solutions

$$\vec{\phi}^{(2)}_{(0)1} = Ne^{-(u_1^2+u_2^2)/2}[\hat{\epsilon}_1 + \hat{\epsilon}_2] \text{ and } e^{-(u_1^2+u_2^2)/2}[\hat{\epsilon}_1 - \hat{\epsilon}_2] \tag{4.27}$$

In this case, both components of the 2-degenerate solutions are non-zero, of the same magnitude and of definite sign. In dealing with the two dimensional separable harmonic oscillator, the most convenient form is given by Equation (4.26).
A major concern is whether our approach satisfies the supersymmetric algebra which we will consider here. It is clear that we can define our Hamiltonian operator by

$$\mathcal{H} = \begin{pmatrix} \vec{Q}^\dagger \cdot \vec{Q} & 0 \\ 0 & \vec{Q}\vec{Q}^\dagger \cdot \end{pmatrix} = \begin{pmatrix} \mathcal{H}_1 & 0 \\ 0 & \overleftrightarrow{\mathcal{H}}_2 \end{pmatrix} \tag{4.28}$$

where the zero in the upper right is a row vector and the zero in the lower left is a column vector. This Hamiltonian will act on the state

$$\vec{\psi} = \begin{pmatrix} \psi_n^{(1)} \\ \vec{\psi}^{(2)}_{n-1} \end{pmatrix}. \tag{4.29}$$

Then, we can define a "super-charge" operator as

$$\mathcal{Q} = \begin{pmatrix} 0 & 0 \\ \vec{Q} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ Q_1 & 0 & 0 \\ Q_2 & 0 & 0 \end{pmatrix} \tag{4.30}$$

with the adjoint being

$$\mathcal{Q}^\dagger = \begin{pmatrix} 0 & \vec{Q}^\dagger \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & Q_1^\dagger & Q_2^\dagger \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{4.31}$$

If we take the product of $\mathcal{Q}^\dagger$ and $\mathcal{Q}$, we find that

$$\overleftrightarrow{\mathcal{H}}_1 = \begin{pmatrix} \vec{Q}^\dagger \cdot \vec{Q} & 0 \\ 0 & 0 \end{pmatrix} \tag{4.32}$$

and similarly, if we take the product of $\mathcal{Q}$ and $\mathcal{Q}^\dagger$, we find that

$$\overleftrightarrow{\mathcal{H}}_2 = \begin{pmatrix} 0 & 0 \\ 0 & \vec{Q}\vec{Q}^\dagger \cdot \end{pmatrix}. \tag{4.33}$$

It's straightforward to show that

$$[\mathcal{Q}, \mathcal{H}] = 0, \tag{4.34}$$

$$[\mathcal{Q}^\dagger\mathcal{Q}, \mathcal{Q}\mathcal{Q}^\dagger] = 0, \tag{4.35}$$

$$\mathcal{Q}\mathcal{Q} = \mathcal{Q}^\dagger\mathcal{Q}^\dagger = 0, \tag{4.36}$$

and

$$\overleftrightarrow{\mathcal{H}} = \{\mathcal{Q}, \mathcal{Q}^\dagger\} \tag{4.37}$$

where the braces indicate the anticommutator bracket. According to Wess and Bagger's text on supersymmetry, these are the necessary conditions for a superalgebra Wess & Bagger (1992).
We now consider in more detail the degeneracy between the two sectors, $\vec{Q}_1$ and $\vec{Q}_1^\dagger$ and the sector Hamiltonians $\mathcal{H}_1$ and $\overleftrightarrow{\mathcal{H}}_2$. An important consequence of the algebra is the existence of "inter-twining" relations. These are of fundamental importance because they underlie the isospectral property and in addition, they can be used to establish the unique correspondence between the eigenstates of sectors 1 and 2. Indeed, they are responsible for establishing the completeness of the eigenvectors $\{\vec{\psi}_n^{(2)}\}$ of $\overleftrightarrow{\mathcal{H}}_2$. It is of interest to note that inter-twining relations are essential to the fact that in ordinary quantum scattering, the continua of the full Hamiltonian, $\mathcal{H}$, and the unperturbed Hamiltonian $\mathcal{H}_0$ (where $\mathcal{H} = \mathcal{H}_0 + V$, with V the perturbation responsible for scattering) coincide. In that case, the inter-twining relation is

$$\Omega^+ e^{i\mathcal{H}_0 t/\hbar} = e^{i\mathcal{H}t/\hbar}\Omega^+. \tag{4.38}$$

It is useful to derive the SUSY inter-twining relations explicitly. We have

$$\mathcal{H}_1\psi_n^{(1)} = E_n^{(1)}\psi_n^{(1)}, \tag{4.39}$$

where $\mathcal{H}_1$ is a standard Schrödinger operator (comprised of a Laplacian for the kinetic energy and a Hermitian potential V_1). One result of this fact is that the ground state of $\mathcal{H}_1$ is nodeless. In addition, $\mathcal{H}_1$ is Hermitian and a well known postulate of quantum mechanics asserts that its eigenstates are complete. Essentially from a physical standpoint (as opposed to pure mathematics) $\mathcal{H}_1$ is required to be Hermitian because (a) it represents an observable, implying only real eigenvalues (b) quantum mechanics further asserts that these eigenvalues are the only values that can be obtained when measuring the energy for the physical system represented by $\mathcal{H}_1$. This implies that any physically realizable state, ψ, of the system must be a superposition (in general) of these and only these eigenvectors. This then implies that the set $\{\psi_n^{(1)}\}$ is complete on the physically allowed space of state vectors.
To derive the inter-twining relation, we again recall that the charge operator (which exactly factors $\mathcal{H}_1$) is such that

$$\mathcal{H}_1 = \vec{Q}_1^\dagger \cdot \vec{Q}_1 + E_0^{(1)} \tag{4.40}$$

where

$$\vec{Q}_1\psi_0^{(1)} \equiv \vec{0} \tag{4.41}$$

The general sector 1 Schrödinger equation is

$$(\vec{Q}_1^\dagger \cdot \vec{Q}_1 + E_0^{(1)})\psi_n^{(1)} = E_n^{(1)}\psi_n^{(1)} \tag{4.42}$$

where we now assume that $n > 0$; i.e., $\psi_n^{(1)}$ is an excited state of $\mathcal{H}_1$. We apply $\vec{Q}_1$ to Equation (4.42) to find

$$(\vec{Q}_1\vec{Q}_1^\dagger \cdot \vec{Q}_1 + E_0^{(1)})\psi_n^{(1)} = E_n^{(1)}\vec{Q}_1\psi_n^{(1)} \tag{4.43}$$

We define $\overleftrightarrow{\mathcal{H}}_2$ as

$$\overleftrightarrow{\mathcal{H}}_2 \equiv \vec{Q}_1 \vec{Q}_1^\dagger + E_0^{(1)} \tag{4.44}$$

so that Equation (4.43) yields

$$\vec{Q}_1 \mathcal{H}_1 = \overleftrightarrow{\mathcal{H}}_2 \cdot \vec{Q}_1. \tag{4.45}$$

This is the inter-twining relation. Let us explore inter-twining consequences further. Suppose we consider an eigenstate , $\psi_n^{(1)}$ of $\mathcal{H}_1$. It follows from Equation (4.45) that there is also a unique eigenstate of $\overleftrightarrow{\mathcal{H}}_2$, $\vec{Q}_1 \psi_n^{(1)}$ with the same energy. Next, assume that $\overleftrightarrow{\mathcal{H}}_2$ possesses an eigenvalue $E_\lambda^{(2)}$ that differs from all of the $E_n^{(1)}$. Then we have

$$\overleftrightarrow{\mathcal{H}}_2 \cdot \vec{\psi}_\lambda^{(2)} = E_\lambda^{(2)} \vec{\psi}_\lambda^{(2)} \tag{4.46}$$

Now $\overleftrightarrow{\mathcal{H}}_2$ and $\mathcal{H}_1$ are manifestly Hermitian. Taking the adjoint of Equation (4.45) yields

$$\mathcal{H}_1 \vec{Q}_1^\dagger = \vec{Q}_1^\dagger \cdot \overleftrightarrow{\mathcal{H}}_2 \tag{4.47}$$

which is again an inter-twining relation. We then take the scalar product of Equation (4.46) with $\vec{Q}_1^\dagger$

$$\vec{Q}_1^\dagger \cdot \overleftrightarrow{\mathcal{H}}_2 \cdot \vec{\psi}_\lambda^{(2)} = E_\lambda^{(2)} \vec{Q}_1^\dagger \cdot \vec{\psi}_\lambda^{(2)} \tag{4.48}$$

But by the adjoint inter-twining relation, we have

$$\mathcal{H}_1 \vec{Q}_1^\dagger \cdot \vec{\psi}_\lambda^{(2)} = E_\lambda^{(2)} \vec{Q}_1^\dagger \cdot \vec{\psi}_\lambda^{(2)} \tag{4.49}$$

Thus, we find that $\mathcal{H}_1$ also has the scalar eigenvector

$$\psi_\lambda^{(1)} \propto \vec{Q}_1^\dagger \cdot \vec{\psi}_\lambda^{(2)} \tag{4.50}$$

and its eigenvalue is equal to $E_\lambda^{(2)}$. This violates our initial assertion that $\mathcal{H}_1$ did not have the eigenvalue $E_\lambda^{(2)}$. We conclude that for eigenvectors $\vec{\psi}_n^{(2)}$, there corresponds a unique eigenvector $\psi_{n'}^{(1)}$, where $n' \equiv n+1$. That is, $\vec{\psi}_0{}^{(2)}$ must have the same energy as the first excited state $\psi_1^{(1)}$. It can not be lower than $E_1^{(1)}$ because it is the lowest eigenvalue of $\overleftrightarrow{\mathcal{H}}_2$ and it cannot equal $E_0^{(1)}$. In fact, the inter-twining relation is sufficient to establish that $\overleftrightarrow{\mathcal{H}}_2$ is a Schrödinger operator and as such, its eigenvectors must be complete on the space $\vec{\psi}$. Note that we are not saying that the $\vec{\psi}_n^{(2)}$ span the the space generated by $\mathcal{H}_1$. They are completely separate vector spaces arising from two distinct Hermitian Hamiltonians. All of the above can be made mathematically rigorous but our purpose here is to supply a physically reasonable argument for the properties of the tensor sector. Finally, at no point in this discussion have we imposed a condition that the spectra of $\mathcal{H}_1$ (and $\overleftrightarrow{\mathcal{H}}_2$) are strictly discrete. The inter-twining relations hold for systems with a mixed discrete and continuous spectra and even for systems with a purely continuous spectrum.

5. Clusters of distinguishable particles

5.1 Degenerate case

We next consider a model non-separable two dimensional anharmonic oscillator system for sector one for which the ground state energy is zero and the ground state wave function is exactly given by

$$\psi^{(1)}_{(0)}(u_1,u_2) = N\exp(-u_1^2u_2^2 - u_1^2 - u_2^2) \tag{5.1}$$

We can generate the superpotential corresponding to this ground state as

$$\vec{W}_1 = -\vec{\nabla}\ln\psi^{(1)}_{(0)}(u_1,u_2) \tag{5.2}$$

having the components $W_{11} = (2u_1u_2^2 + 2u_1)$ and $W_{12} = (2u_1^2u_2 + 2u_2)$, respectively. Now using these components we can generate the model potential for sector one. Thus we get the Hamiltonian for sector one of the following form

$$\begin{aligned}\mathcal{H}_1 = -\nabla^2 + V_1(u_1,u_2) = &-\frac{\partial^2}{\partial u_1^2} - \frac{\partial^2}{\partial u_2^2} + (2u_1u_2^2 + 2u_1)^2 + (2u_1^2u_2 + 2u_2)^2 \\ &- 2(u_1^2+1) - 2(u_2^2+1)\end{aligned} \tag{5.3}$$

In this case, the exact ground state energy is $E_0^{(1)} = 0$. The sector two tensor Hamiltonian can be generated with $\vec{\nabla}$ and $\vec{W}_1$. The calculation for sector one and sector two eigenvalues and eigenfunctions is done variationally by diagonalizing each sector Hamiltonian in an approximate truncated basis. We choose to employ a basis of the direct product of the eigenstates of a harmonic oscillator in each dimension, each with frequency $\omega = 2\sqrt{2}$. The trial wave function for sector one is

$$\psi^{(1)}_{(trial)}(u_1,u_2) = \sum_{m,n} C^{(1)}_{m,n}\phi_m(\alpha,u_1)\phi_n(\alpha,u_2) \tag{5.4}$$

where $\alpha = \sqrt{m\omega/\hbar}$. Similarly for the sector two the trial wave functions for each component are

$$\begin{aligned}\psi^{(2)}_{(trial)1}(u_1,u_2) &= \sum_{m,n} C^{(2)}_{1_{m,n}}\phi_m(\alpha,u_1)\phi_n(\alpha,u_2) \\ \psi^{(2)}_{(trial)2}(u_1,u_2) &= \sum_{m,n} C^{(2)}_{2_{m,n}}\phi_m(\alpha,u_1)\phi_n(\alpha,u_2)\end{aligned} \tag{5.5}$$

Using these trial wave functions and treating the $C_{m,n}$ as a variational parameters, we arrive at the Hermitian eigenvalue equation for both sectors. For sector one the form is

$$\mathcal{H}_1C^{(1)} = EC^{(1)} \tag{5.6}$$

and that for sector two is

$$\begin{pmatrix}\mathcal{H}^{(2)}_{11} & \mathcal{H}^{(2)}_{12}\\ \mathcal{H}^{(2)}_{21} & \mathcal{H}^{(2)}_{22}\end{pmatrix}\begin{pmatrix}C^{(2)}_1\\ C^{(2)}_2\end{pmatrix} = E\begin{pmatrix}C^{(2)}_1\\ C^{(2)}_2\end{pmatrix} \tag{5.7}$$

Each term of the Hamiltonian matrix can be calculated analytically in the harmonic oscillator basis.

We have calculated energies and wave functions of the Hamiltonian in Equation (5.3) for sectors one and two using the variational approach we just described. In all calculations, we use the exact $\psi_0^{(1)}$ to generate $\vec{W}_1$ and $\overleftrightarrow{\mathcal{H}}_2$ exactly. In Table 11 we compare sector one and sector two energies for different harmonic oscillator basis set sizes. The notation N_{u_1}, N_{u_2} gives the number of basis functions for the variable u_1, u_2, respectively. The first row gives the approximate results for $E_0^{(1)}$. The next is the doubly degenerate first excited state energy, $E_1^{(1)}$ followed by the sector two ground state energy, $E_0^{(2)}$. The third row contains $E_2^{(1)}$ and $E_1^{(2)}$, for different basis sets. It is easily seen that the doubly degenerate ground state of sector two is also isospectral with the doubly degenerate first excited state of sector one. This correspondence is clearly in accordance with the general SUSY prediction about the eigenstates for the two supersymmetric partner potentials. For the higher excited states this precise correspondence between the two sectors breaks down when we use a small number of basis functions (*i.e.*, there appear some "spurious" solutions) but it is gradually restored by increasing the basis size. We attribute this apparent breakdown of the SUSY-correspondence for higher states to the error that arises in the calculation due to the truncation of an infinite basis to a finite one. Essentially, some "spurious" eigenvalues appear in the SUSY-QM sector two spectrum, but they disappear as the basis size is increased. This may raise a question regarding the precise nature of the Hylleraas-Undheim theorem for the SUSY sector two tensor Hamiltonian.

The accuracy of the variational results are known for the ground state of sector one, since we know the exact energy is $E_0^{(1)} = 0$. Thus, the (10, 10) basis gives an error of 9×10^{-3} while the (60, 60) basis gives an error of 4.9×10^{-9}. In the case of the first excited state of sector one, the error for the (10, 10) basis (computed relative to (60, 60) basis result) is 0.0634. By contrast, the error in the (10, 10) basis result for the sector two ground state (again, relative to the (60, 60) basis result) is 2.2×10^{-4}. Consequently, the use of the sector two Hamiltonian for a ground state calculation enables us to obtain much improved accuracy for the first excitation energy of sector one. Basically, we estimate an increase in accuracy (defined as the ratio of the accuracy of the sector one result to that of the sector two result) to be a factor of 280. Our exploratory calculation thus clearly reveals that for the calculation of excited state energies, the SUSY-variational method requires a smaller number of basis functions to achieve the same order of accuracy. Of course, this level of accuracy resulted in part because we have used the exact $\overleftrightarrow{\mathcal{H}}_2$.

As this model problem has no analytical solution for the excited states, we have taken the results of the $(60, 60)$ basis set calculation as the reference result for both sectors in order to check the convergence in wave functions. In Tables 12 and 13 we compare the $\mathcal{L}_\infty$ and $\mathcal{L}_2$ error of the first excited states of the sector one that we have obtained by the SUSY-variational calculation and the simple variational calculation. The $\mathcal{L}_\infty$ error is defined as the absolute maximum difference between the solution computed with an infinite basis set $(\psi^{(1)}(\infty))$ which we approximate with the (60,60) basis, and a smaller finite (n, n) basis set $(\psi^{(1)}(n))$

$$\mathcal{L}_\infty = Max\{|\psi^{(1)}(\infty) - \psi^{(1)}(n)|\}.$$

The $\mathcal{L}_2$ error is defined by

$$\mathcal{L}_2 = \int_{-\infty}^{\infty} du_1 \int_{-\infty}^{\infty} du_2 |\psi^{(1)}(\infty) - \psi^{(1)}(n)|^2.$$

In the first column of Table 12 we show the difference in the number of basis states used (in each degree of freedom) and the maximum, $N_{u_1} = N_{u_2} = 60$, used for the reference result. Since $\mathcal{L}_2$ and L_∞ are computed relative to the N_{u_1}, $N_{u_2} = 60$, 60 basis, they measure the degree of convergence of the calculations. It is clear from Tables 13 and 13 that the state obtained from the SUSY relation $\psi^{(1)}_{(1,0)} = \vec{Q}_1^{\dagger}.\vec{\psi}^{(2)}_{(0)}$ converges more rapidly than the result obtained directly from the variational solution for sector one. We note that the same level of convergence is obtained for both of the degenerate wave functions. Since the analytical solution for the ground state wave function of the sector one is known, we also have calculated the $\mathcal{L}_2$ and $\mathcal{L}_\infty$ error for this wave function, comparing the analytical and variational wave function of sector one for different numbers of basis states to determine a basis size which gives a satisfactory convergence. The results are given in Table 14. It is again clear that the variational results for the sector one ground state wave function are very well converged.

sector one $N_{u_1}, N_{u_2} = 10$ (in a.u.)	sector two $N_{u_1}, N_{u_2} = 10$ (in a.u.)	sector one $N_{u_1}, N_{u_2} = 40$ (in a.u.)	sector two $N_{u_1}, N_{u_2} = 40$ (in a.u.)	sector one $N_{u_1}, N_{u_2} = 60$ (in a.u.)	sector two $N_{u_1}, N_{u_2} = 60$ (in a.u.)
9.0×10^{-3}	-	4.0×10^{-7}	-	5.0×10^{-9}	-
4.6	4.5849	4.58473	4.5847275	4.5847275	4.58472742
8.3	8.005	8.00007	8.0000005	8.000001	8.000000005

Table 11. Comparison of energy eigenvalues of sector one and sector two for different number of basis functions (N_{u_1}, N_{u_2}).

$\Delta N = N_{ref} - n$	Error	$\psi^{(1)}_{(1,0)} = \vec{Q}_1^{\dagger}.\vec{\psi}^{(2)}_{(0)}$	$\psi^{(1)}_{(1,0)}$
40 = 60 - 20	$\mathcal{L}_\infty$	1.1×10^{-4}	4.9×10^{-4}
30 = 60 - 30	$\mathcal{L}_\infty$	2.2×10^{-5}	8.5×10^{-5}
20 = 60 - 40	$\mathcal{L}_\infty$	5.3×10^{-6}	1.9×10^{-5}
10 = 60 - 50	$\mathcal{L}_\infty$	1.6×10^{-6}	3.9×10^{-6}

Table 12. Comparison between wave-function $\mathcal{L}_\infty$ -Error for the doubly-degenerate sector one excited state, (1, 0) generated by standard variational calculation of the sector one and variational SUSY calculation for sector two ground state, followed by application of the SUSY Charge Operator for different number of basis($n = N_{u_1}, N_{u_2}$). ($N_{ref} = (N_{u_1} = 60, N_{u_2} = 60)$).

In Figures 3(a-b) we show the two components of one of the degenerate sector two ground state wave functions and in Figures 3(c-d) we show the two components for the other degenerate sector two ground state wave function. It may seem problematic that the components $\psi^{(2)}_{(0)1}$ and $\psi^{(2)}_{(0')2}$ for the pair of sector two ground state wave functions have nodes. We shall see below that these nodes can be eliminated in a very simple manner. However, we stress that for each of the degenerate sector two ground state wave functions, there is a large and small component. Unlike the two dimensional separable harmonic oscillator case,

$\Delta N = N_{ref} - n$	Error	$\psi^{(1)}_{(1,0)} = \vec{Q}^{\dagger}_1.\vec{\psi}^{(2)}_{(0)}$	$\psi^{(1)}_{(1,0)}$
40 = 60 - 20	$\mathcal{L}_2$	3.0×10^{-6}	1.8×10^{-5}
30 = 60 - 30	$\mathcal{L}_2$	1.1×10^{-7}	5.7×10^{-7}
20 = 60 - 40	$\mathcal{L}_2$	6.2×10^{-9}	3.0×10^{-8}
10 = 60 - 50	$\mathcal{L}_2$	3.5×10^{-10}	1.5×10^{-9}

Table 13. Comparison between wave-function $\mathcal{L}_2$-Error for the doubly-degenerate sector one Excited state, (1, 0) generated by standard variational calculation of the sector one and variational SUSY calculation for the sector two ground state, followed by application of the SUSY charge operator for different size basis($n = N_{u_1}, N_{u_2}$). ($N_{ref} = (N_{u_1} = 60, N_{u_2} = 60)$).

N_{u_1}, N_{u_2}	$\mathcal{L}_\infty$	$\mathcal{L}_2$
20, 20	9.3×10^{-5}	1.5×10^{-6}
30, 30	1.5×10^{-5}	3.9×10^{-8}
40, 40	3.4×10^{-6}	2.0×10^{-9}
50, 50	9.1×10^{-7}	1.4×10^{-10}
60, 60	2.8×10^{-7}	1.3×10^{-11}

Table 14. Comparison between wave-function $\mathcal{L}_2$ and L_∞ -Error for the 1^{st} sector exact ground state wave function $\psi^{(1)}_{(0,0)}(\infty)$ and variationally calculated ground state wave function $\psi^{(1)}_{(0,0)}(n)$ for different number of basis states($n = N_{u_1}, N_{u_2}$).

the small component is not only non-zero but it has nodes. It is roughly ten times smaller in magnitude than the large component. The two degenerate states are 90^o out of phase so far as their signs. In Figures 4(a-b) we show the first excited states $\psi^{(1)}_{(0,1)}$ and $\psi^{(1)}_{(1,0)}$ of the sector one that we have obtained after applying the SUSY charge operator to the sector two ground states and Figures 4(c-d) present the same states that were found variationally from the sector one Hamiltonian. The similarity of Figure 4a to 4c and 4b to 4d clearly reflects the correctness of our method. To eliminate the nodes in the components of $\vec{\psi}^{(2)}_{(0)}$ and $\vec{\psi}^{(2)}_{(0')}$, we note that since they are degenerate, any linear combination of them is also a valid wave function. Accordingly, in analogy to the separable two dimensional harmonic oscillator considered previously we can define $\vec{\phi}^{(2)}_{(0)}$ and $\vec{\phi}^{(2)}_{(0')}$ by combining the components of $\vec{\psi}^{(2)}_{(0)}$ and $\vec{\psi}^{(2)}_{(0')}$ according to

$$\phi^{(2)}_{(0)1} = \psi^{(2)}_{(0)1} + \psi^{(2)}_{(0')1} \tag{5.8}$$

$$\phi^{(2)}_{(0)2} = \psi^{(2)}_{(0)2} + \psi^{(2)}_{(0')2} \tag{5.9}$$

$$\phi^{(2)}_{(0')1} = \psi^{(2)}_{(0)1)} - \psi^{(2)}_{(0')1} \tag{5.10}$$

$$\phi^{(2)}_{(0')2} = \psi^{(2)}_{(0)2} - \psi^{(2)}_{(0')2}. \tag{5.11}$$

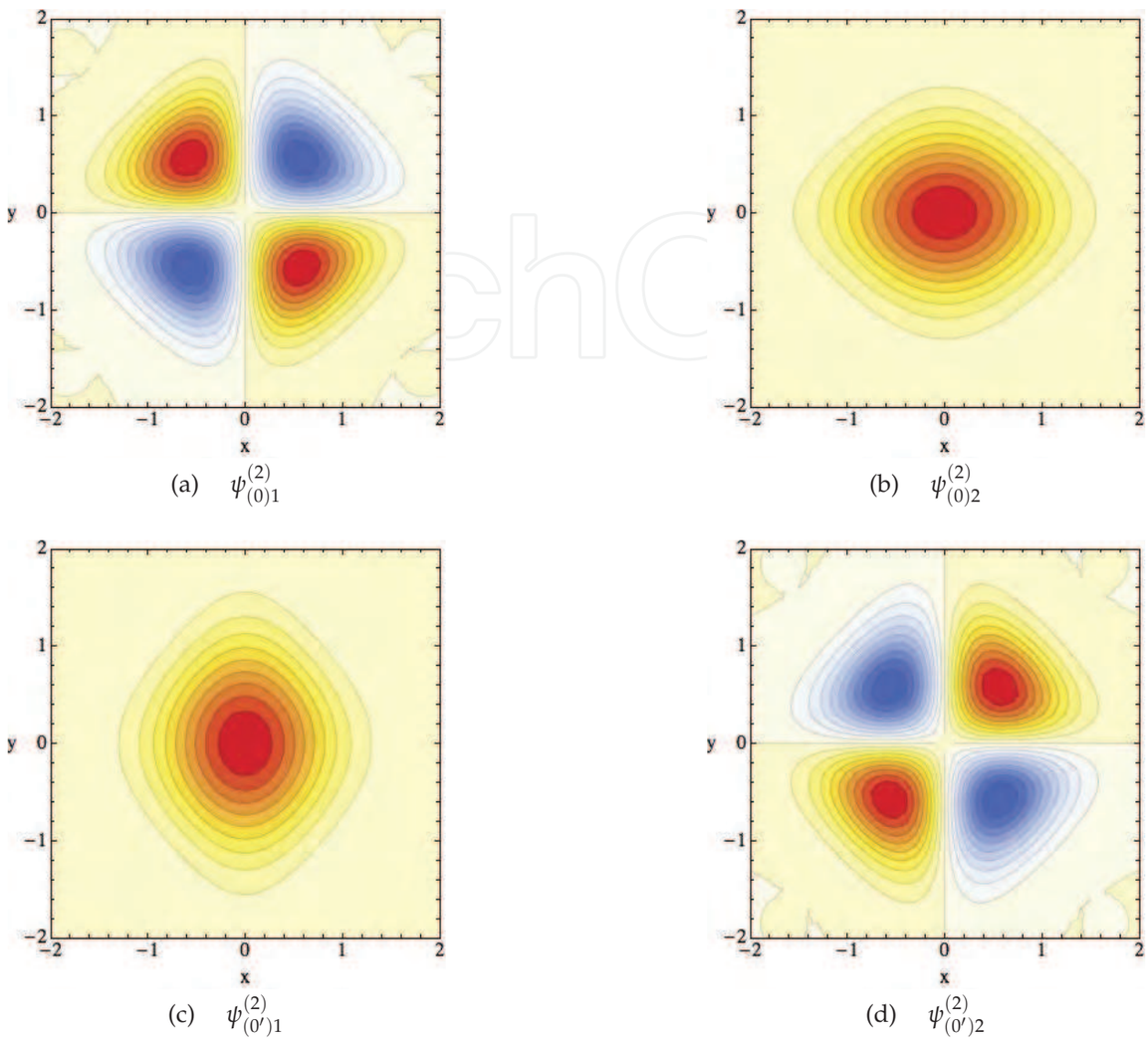
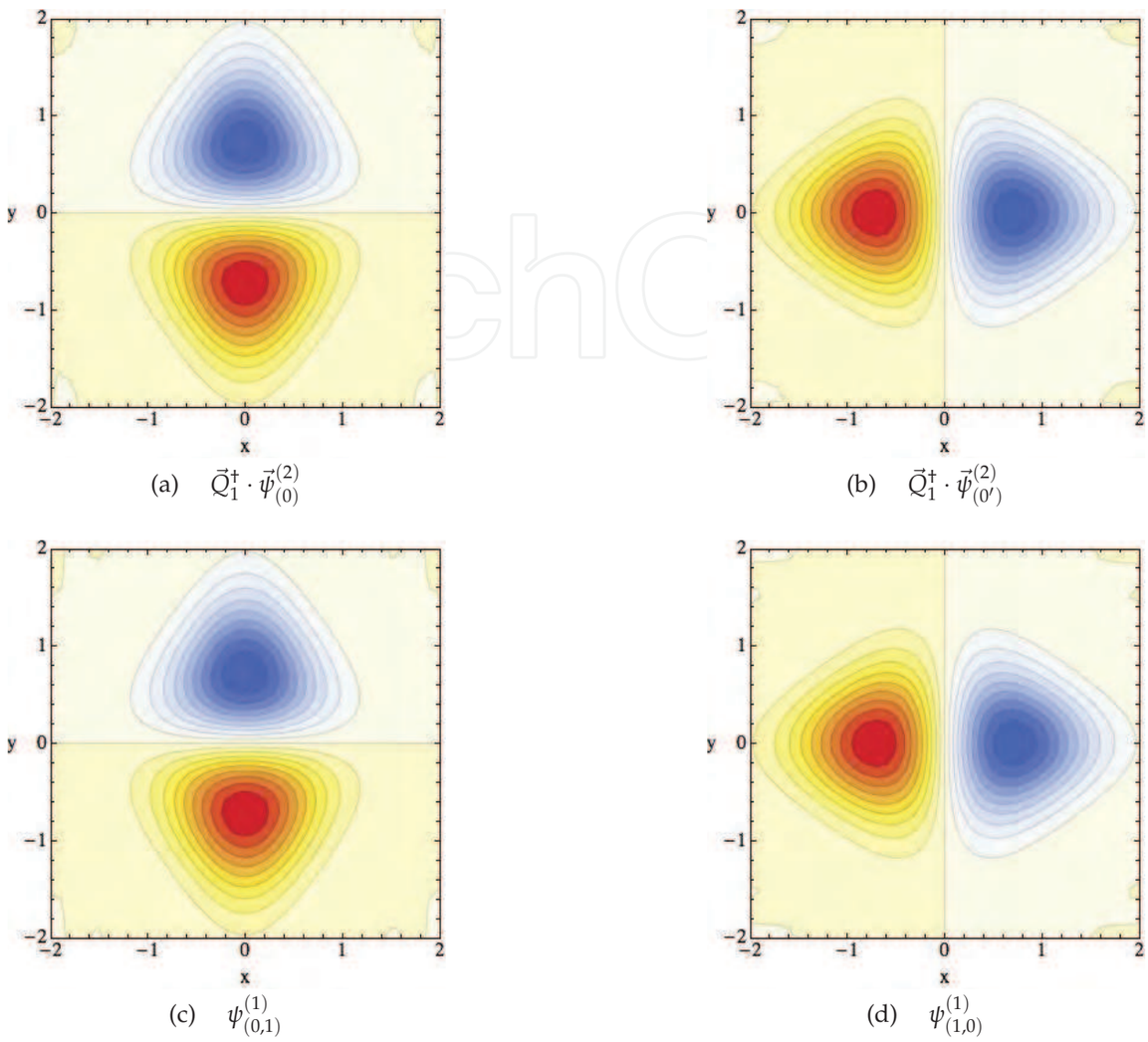


Fig. 3. (a-b) represent the two components of one of the degenerate sector two ground states. (c-d) represent the same for the other sector two ground state. Contour shading is such that red indicates positive amplitude and blue indicates negative amplitude. The prime on the quantum number "0" denotes the second of the 2 degenerate ground states.

In Figures 5(a-d) we show the components of $\vec{\phi}^{(2)}_{(0)}$ and $\vec{\phi}^{(2)}_{(0')}$. These combinations are nodeless and have definite symmetry. We stress that the forms of the above $\vec{\phi}^{(2)}_{(0)}$ and $\vec{\phi}^{(2)}_{(0')}$ are analogous to the results in Equation (4.27), obtained for the degenerate separable two dimensional harmonic oscillator.

For sector two, in the case of a doubly degenerate first excited state of $\mathcal{H}_1$, we obtain a doubly degenerate ground state and the energies obtained by the Rayleigh-Ritz method are consistently lower for all the excited states of the sector one Hamiltonian, for the same basis size. In addition, the SUSY-QM sector two result for the first excited state energy is always several orders of magnitude more accurate than the Rayleigh-Ritz result for sector one for any given basis set size. Assessing the accuracy of the excited state wave functions is more

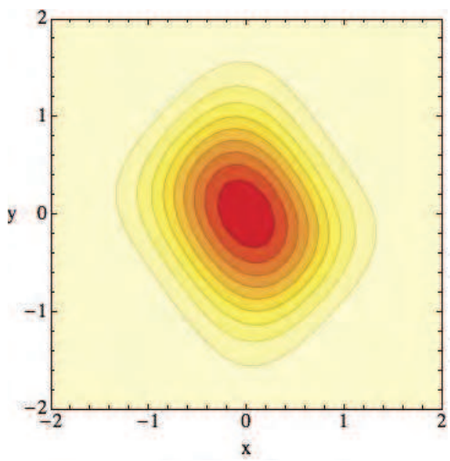


(a) $\vec{Q}_1^{\dagger} \cdot \vec{\psi}^{(2)}_{(0)}$ (b) $\vec{Q}_1^{\dagger} \cdot \vec{\psi}^{(2)}_{(0')}$

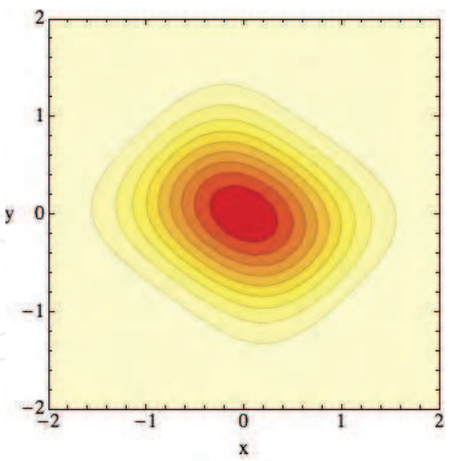
(c) $\psi^{(1)}_{(0,1)}$ (d) $\psi^{(1)}_{(1,0)}$

Fig. 4. (a-b) show the doubly degenerate 1^{st} excited states of the sector one. The two states are generated by the SUSY -variational method. (c-d) the corresponding states of the sector one Hamiltonian, which are generated variationally.

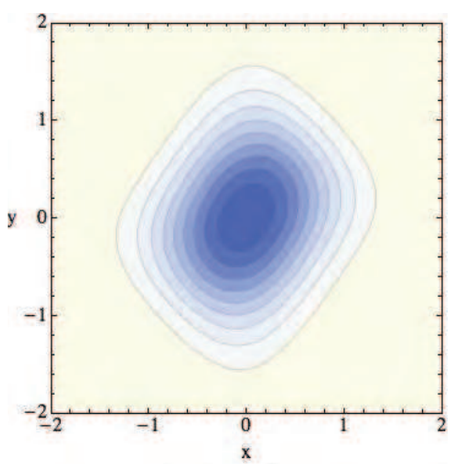
difficult. We chose to do this in terms of convergence of the wave functions relative to the largest basis set results. However, we are able to assess the accuracy of our variational results quantitatively in the case of the sector one ground state , since it is exactly known. We report our results in terms of $\mathcal{L}_2$ and $\mathcal{L}_\infty$ measures, as is typical for assessing convergence and accuracy of functions in a Hilbert space. We find that the $\mathcal{L}_2$ and $\mathcal{L}_\infty$ accuracies of the SUSY-QM results are consistently better than the Rayleigh-Ritz results for excited states of sector one. As a further proof of this, we also consider the accuracy for the ground state of sector one (where we have the exact wave function), with the variational result. In fact, we find that the convergence of the sector two ground state is consistently better than the convergence of the variationally obtained ground state wave function for sector one.



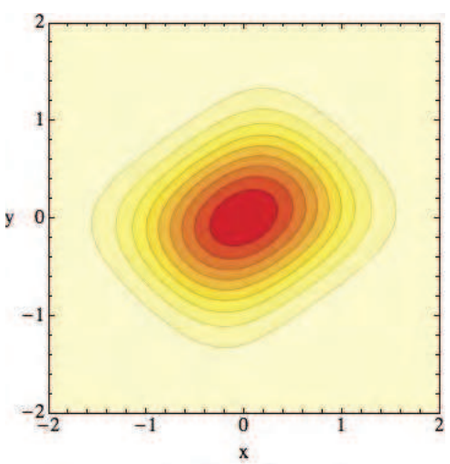
(a) $\phi^{(2)}_{(0)1} = \psi^{(2)}_{(0)1} + \psi^{(2)}_{(0')1}$



(b) $\phi^{(2)}_{(0)2} = \psi^{(2)}_{(0)2} + \psi^{(2)}_{(0')2}$



(c) $\phi^{(2)}_{(0')1} = \psi^{(2)}_{(0)1} - \psi^{(2)}_{(0')1}$



(d) $\phi^{(2)}_{(0')2} = \psi^{(2)}_{(0)2} - \psi^{(2)}_{(0')2}$

Fig. 5. Components of linear combinations of the two degenerate ground states of the sector two.

5.2 Non-degenerate case

For completeness of our presentation, we also consider a non-degenerate, two dimensional anharmonic oscillator model. To generate such a Hamiltonian, we modify the ground state in (5.1) to the form

$$\psi^{(1)}_{(0)}(u_1, u_2) = N \exp(-2u_1^2 u_2^2 - u_1^2 - \sqrt{2}u_2^2) \tag{5.12}$$

Then the exact Hamiltonians $\mathcal{H}_1$ and $\overleftrightarrow{\mathcal{H}}_2$ are readily generated. However, we also shall generate an approximate $\overleftrightarrow{\mathcal{H}}_2$ using the variationally determined, approximate ground state wave function. The formal structure of the equations is the same as that above. In the case

where $\psi^{(1)}_{0,approx}$ is used to develop $\vec{W}_1$ and $\overleftrightarrow{\mathcal{H}}_2$, we shall see that its accuracy is an extremely important consideration.

In the non-degenerate example, we have performed two distinct calculations. First we used the exact $\vec{W}_1$ to construct the exact $\overleftrightarrow{\mathcal{H}}_2$. The results are given in Tables 15 - 17. In Table 15, we see basically the same behavior as was obtained in the non-separable degenerate two dimensional example. The errors in the ground state energy are of similar size for both the degenerate and non-degenerate cases, with the same variation with basis set size. This behavior extends also to the first and second excited state energies. We conclude that the presence or absence of degeneracy does not affect the performance of our SUSY approach when the exact $\vec{W}_1$ is used.

In the case of the $\mathcal{L}_\infty$ and $\mathcal{L}_2$ errors obtained when using the exact $\vec{W}_1$, we again see the same basic behavior with regard to the convergence of the wave functions.

However, the situation is more interesting when we use the variationally obtained approximate ground state, $\psi^{(1)}_{0,approx}$ to generate $\vec{W}_1^{approx}$ and thereby $\overleftrightarrow{H}_{2,approx}$. These results are shown in Table 18 and are compared to the exact $\vec{W}_1$ results (the columns labeled $E_1^{(1)}$ and $E_0^{(2)}$). Results are shown for three different basis set sizes, (10,10), (20,20) , and (30,30). Now because we are using an approximate $\psi_0^{(1)}$ to generate $\vec{W}_1^{approx}$, it is important to note how the accuracy depends not only on basis size (which affects the accuracy of $\psi_0^{(1)}$) but also how the accuracy of $\vec{W}_1^{approx}$ is affected by errors in $\psi_0^{(1)}$. We have found that $\vec{W}_1^{approx}$ is most sensitive to errors in region where $\psi_0^{(1)}$ is small in magnitude. This is reasonable since $\vec{W}_1^{approx} = -\vec{\nabla} \ln \psi^{(1)}_{0,approx}$ and we expect that $(\partial\psi_0^{(1)}/\partial u_j)/\psi_0^{(1)}$ to be most sensitive to errors in regions where $\psi_0^{(1)}$ is smallest in magnitude. In view of this, we have introduced ψ_{cutoff} levels at which we cease calculating $\vec{W}_1$. These correspond to cutoff values of $\psi^{(1)}_{0,cutoff} = 10^{-10}$, 10^{-5}, 10^{-3} and 10^{-2}. Those results are in columns 4 - 7 in Table 18. It is clear that the SUSY result is always better than the sector one variational result, although this is only marginally the case with the very small cutoff values (i.e., $\psi^{(1)}_{0,cutoff} \leq 10^{-5}$). The best results are obtained with the 10^{-2} cutoff value. While obviously, this is a single computational example, it is encouraging. However, additional careful studies are underway.

sector one $N_{u_1}, N_{u_2} = 10$ (in a.u.)	sector two $N_{u_1}, N_{u_2} = 10$ (in a.u.)	sector one $N_{u_1}, N_{u_2} = 40$ (in a.u.)	sector two $N_{u_1}, N_{u_2} = 40$ (in a.u.)	sector one $N_{u_1}, N_{u_2} = 60$ (in a.u.)	sector two $N_{u_1}, N_{u_2} = 60$ (in a.u.)
6.4×10^{-3}	-	3.4×10^{-7}	-	3.6×10^{-9}	-
4.80	4.752	4.75181	4.75180771	4.75180778	4.75180770
6.70	6.65	6.64636	6.64634938	6.6463495	6.64634937

Table 15. Comparison of energy eigenvalues of sector one and sector two for different number of basis functions (N_{u_1}, N_{u_2}). Exact sector one and sector two Hamiltonians are used.

Finally, in Figures 6(a-b), we give the two components of the (non-degenerate) ground state, $\psi^{(2)}_{(0)1}$ and $\psi^{(2)}_{(0)2}$. In Figures 6(c-d), we display the components of the first excited state, $\psi^{(2)}_{(1)1}$ and $\psi^{(2)}_{(1)2}$. We note that they are qualitatively similar to the results obtained for the degenerate

$\Delta N = N_{ref} - n$	Error	$\psi^{(1)}_{(1)} = \vec{Q}^{\dagger}_1 . \vec{\psi}^{(2)}_{(0)}$	$\psi^{(1)}_{(1)}$
40 = 60 - 20	$\mathcal{L}_\infty$	9.5×10^{-5}	4.5×10^{-4}
30 = 60 - 30	$\mathcal{L}_\infty$	1.9×10^{-5}	7.5×10^{-5}
20 = 60 - 40	$\mathcal{L}_\infty$	4.5×10^{-6}	1.7×10^{-5}
10 = 60 - 50	$\mathcal{L}_\infty$	9.9×10^{-7}	4.3×10^{-6}

Table 16. Comparison between wave-function $\mathcal{L}_\infty$ -Error for the sector one excited state, generated by standard variational calculation of the sector one and variational SUSY calculation for sector two ground state, followed by application of the SUSY Charge Operator for different number of basis($n = N_{u_1}, N_{u_2}$). ($N_{ref} = (N_{u_1} = 60, N_{u_2} = 60)$). Exact sector one and sector two Hamiltonians are used.

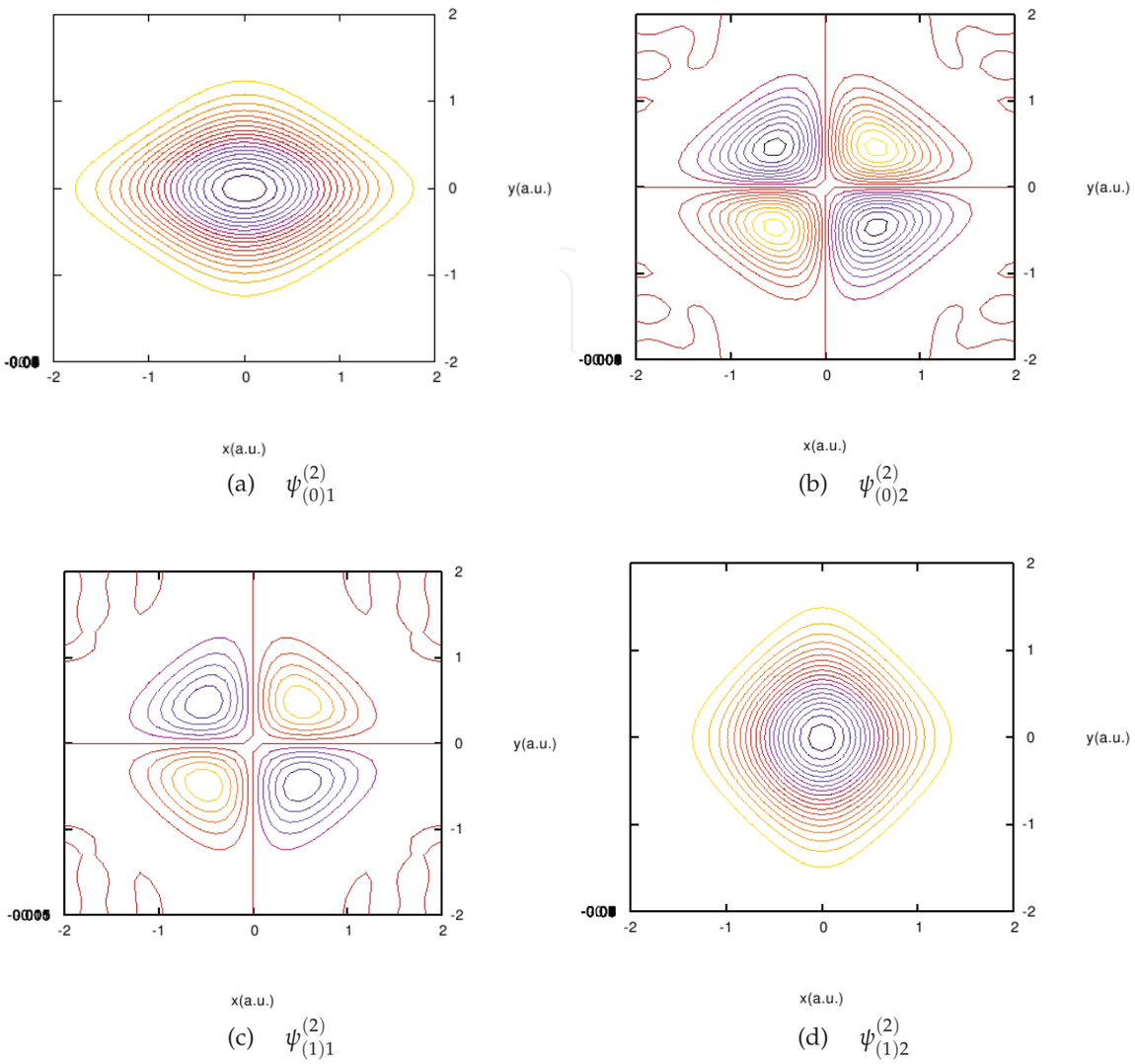
$\Delta N = N_{ref} - n$	Error	$\psi^{(1)}_{(1)} = \vec{Q}^{\dagger}_1 . \vec{\psi}^{(2)}_{(0)}$	$\psi^{(1)}_{(1)}$
40 = 60 - 20	$\mathcal{L}_2$	1.5×10^{-6}	8.9×10^{-6}
30 = 60 - 30	$\mathcal{L}_2$	5.8×10^{-8}	2.7×10^{-7}
20 = 60 - 40	$\mathcal{L}_2$	3.2×10^{-9}	1.5×10^{-8}
10 = 60 - 50	$\mathcal{L}_2$	1.8×10^{-10}	1.1×10^{-9}

Table 17. Comparison between wave-function $\mathcal{L}_2$ -Error for the sector one excited state, generated by standard variational calculation of the sector one and variational SUSY calculation for sector two ground state, followed by application of the SUSY Charge Operator for different number of basis($n = N_{u_1}, N_{u_2}$). ($N_{ref} = (N_{u_1} = 60, N_{u_2} = 60)$). Exact sector one and sector two Hamiltonians are used.

n	$E^{(1)}_1$	$E^{(2)}_0$	$\psi^{(1)}_{(0),cutoff}$ = 10^{-10}	$\psi^{(1)}_{(0),cutoff}$ = 10^{-5}	$\psi^{(1)}_{(0),cutoff}$ = 10^{-3}	$\psi^{(1)}_{(0),cutoff}$ = 10^{-2}
10, 10	4.80	4.752	4.794	4.791	4.78	4.756
20, 20	4.7532	4.75181	4.75317	4.75313	4.7526	4.75181
30, 30	4.752	4.751808	4.75187	4.75187	4.75186	4.751808

Table 18. Comparison among 1^{st} excited state energy of sector one (calculated using analytical $\vec{W}_1$), ground state energy of sector two (calculated using analytical $\vec{W}_1$) and different sector two ground state energy that we obtained using $\vec{W}^{approx}_1$ with different degrees of approximation for $\psi^{(1)}_{0,approx}$ for different basis size ($n = N_{u_1}, N_{u_2}$).

case (Figures 3(a-b) and (c-d))! This suggests to us that the non-degenerate and degenerate cases are very similar so far as the wave functions are concerned. Again, in all cases the large component is nodeless and the small component has nodes. In Figures 7(a-b) we show the first ($\psi^{(1)}_1$) and second excited state ($\psi^{(1)}_2$) , of the sector one that we have obtained after applying the SUSY charge operator to the sector two ground ($\vec{\psi}^{(2)}_0$) and first excited state ($\vec{\psi}^{(2)}_1$) and the Figures 7(c-d) presents the same states that were found variationally from the sector one Hamiltonian. These results also reflect the similarity between degenerate and non-degenerate case.



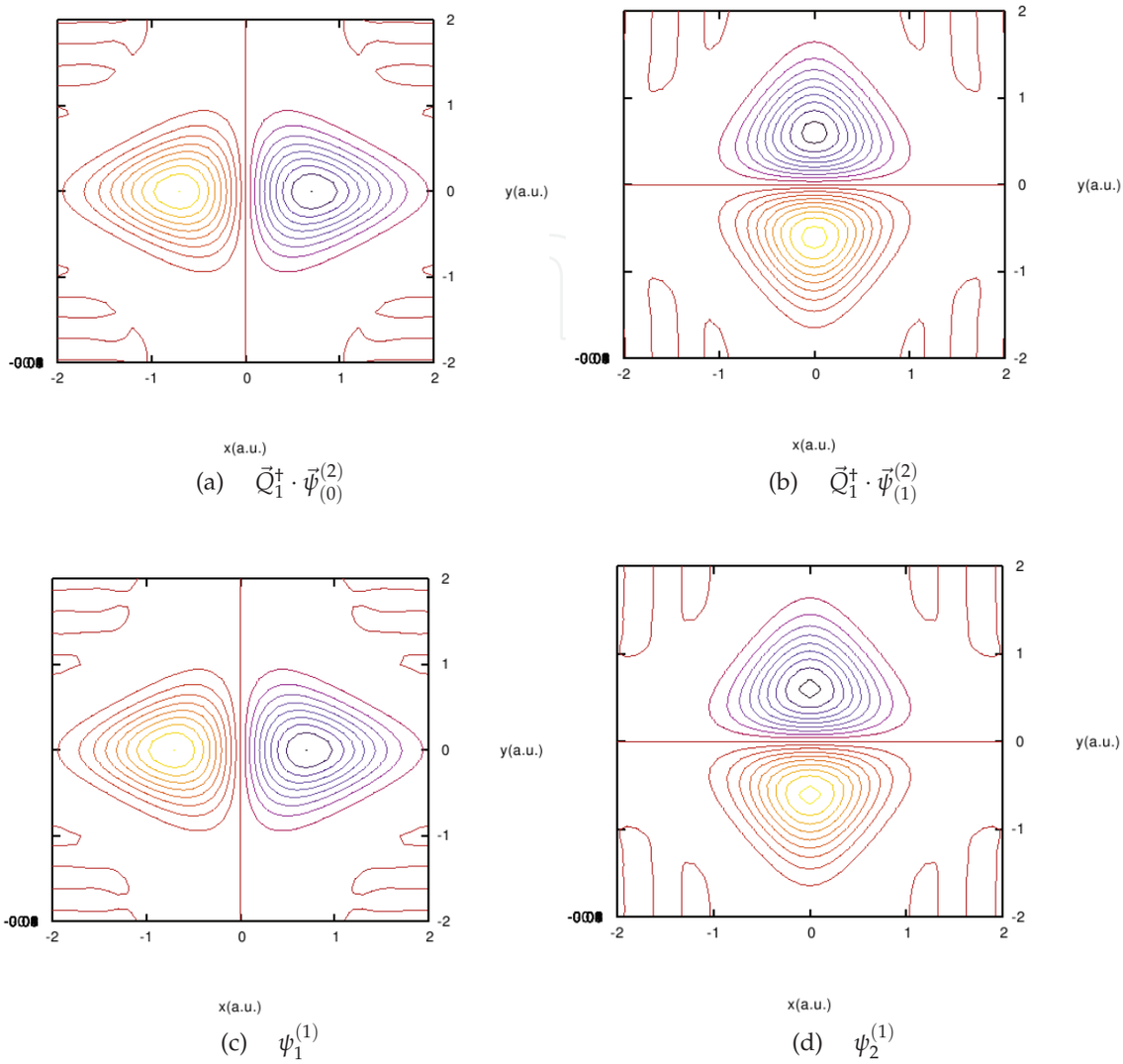
(a) $\psi^{(2)}_{(0)1}$ (b) $\psi^{(2)}_{(0)2}$

(c) $\psi^{(2)}_{(1)1}$ (d) $\psi^{(2)}_{(1)2}$

Fig. 6. (a-b) display the two components of the sector two ground state. (c-d) represent the two components for the sector two first excited state. Contour shading is such that red indicates positive amplitude and blue indicates negative amplitude.

For comparison, we display in Figures 8(a-b) the sum of $\vec{\psi}^{(2)}_0$ and $\vec{\psi}^{(2)}_1$ and in Figures 8(c-d) the difference of $\vec{\psi}^{(2)}_0$ and $\vec{\psi}^{(2)}_1$. The results are qualitatively the same as those in the two dimensional separable and two dimensional non-separable degenerate cases. That is, both linear combinations are nodeless and of definite sign.

The two dimensional non-seperable, non-degenerate case is interesting in that it appears that there is a similar relationship between $\vec{\psi}^{(2)}_0$ and $\vec{\psi}^{(2)}_1$ to that which was seen for the degenerate states $\vec{\psi}^{(2)}_{(0)}$ and $\vec{\psi}^{(2)}_{(0')}$. That is, one component is nodeless and large and the second component has nodes and is smaller in magnitude. As in the degenerate case, sums and differences yield states with both components being nodeless. In this case, however, the non degenerate character of the states precludes simply using two different nodeless, orthogonal $\vec{\phi}^{(2)}_{trial}$ states



(a) $\vec{Q}_1^{\dagger} \cdot \vec{\psi}_{(0)}^{(2)}$ (b) $\vec{Q}_1^{\dagger} \cdot \vec{\psi}_{(1)}^{(2)}$

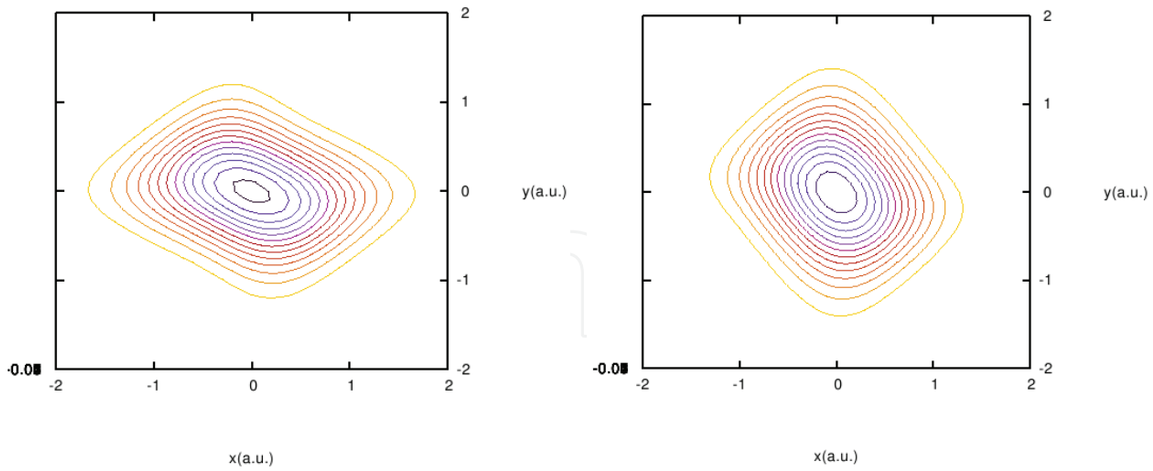
(c) $\psi_1^{(1)}$ (d) $\psi_2^{(1)}$

Fig. 7. (a-b) show the 1^{st} and 2^{nd} excited states of the sector one. The two states are generated by the SUSY -variational method. (c-d) the corresponding states of the sector one Hamiltonian, which are generated variationally. The exact $\vec{W}_1$ is used.

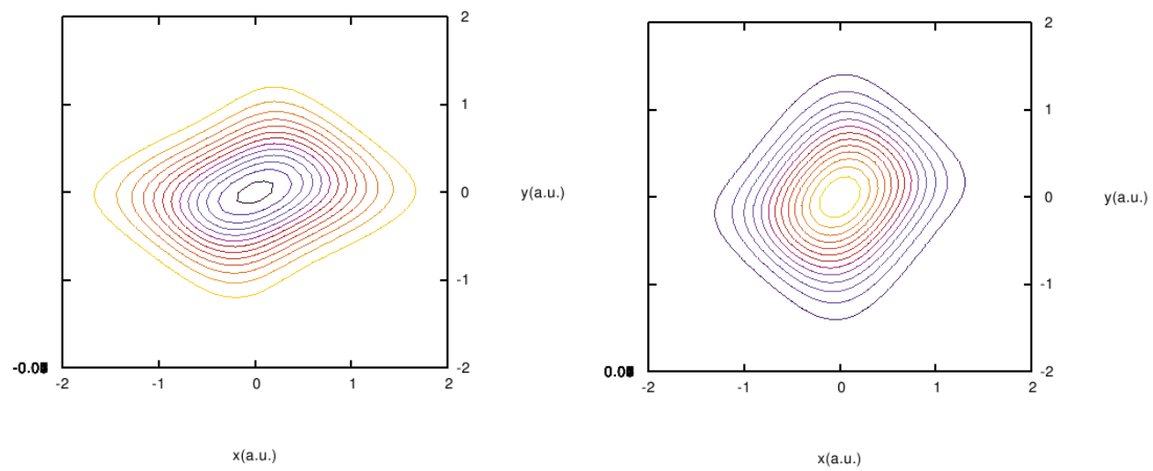
for the quantum Monte Carlo method. Thus, the implementation of the quantum Monte Carlo method in the non-degenerate case appears to require further consideration. We are currently exploring this aspect of our multi-dimensional SUSY approach.

It is important to stress that our basic strategy is to use *only* the ground state results of the higher SUSY sectors. We believe that this will allow us to obtain the best results for both excited state energies and wave functions of the sector one Hamiltonian, while requiring the least computational effort.

Our upcoming computational studies will be to apply the present approach to more interesting, non-separable higher dimensional systems such as rare-gas atomic clusters where the structure and thermodynamics seem to require a fully quantum many-body treatment.



(a) $\phi^{(2)}_{(0)1} = \psi^{(2)}_{(0)1} + \psi^{(2)}_{(1)1}$ (b) $\phi^{(2)}_{(0)2} = \psi^{(2)}_{(0)2} + \psi^{(2)}_{(1)2}$



(c) $\phi^{(2)}_{(1)1} = \psi^{(2)}_{(0)1} - \psi^{(2)}_{(1)1}$ (d) $\phi^{(2)}_{(1)2} = \psi^{(2)}_{(0)2} - \psi^{(2)}_{(1)2}$

Fig. 8. Components of linear combinations of non-degenerate ground and first excited state.

Chakravarty (1995a;b); Derrickson & Bittner (2006; 2007); Franke et al. (1993); Lynden-Bell & Wales (1994); Rick et al. (1991); Schmidt et al. (2001); Wales & Doye (1997) For systems composed of a single type atom or molecule, we expect to encounter degeneracies. Thus, we expect the situation to mirror the present two dimensional non-separable degenerate case.
In dealing with such systems, we anticipate that as the number of particles is increased, we will find that a Monte Carlo based approach may be preferred.
Finally, we stress that this is the first formulation of a general SUSY approach for multi-dimensional and/or multi-particle systems. There remain many formal and computational questions, which we are continuing to explore. Our main conclusion is that there is sufficient promise that such studies are justified.

6. Electronic structure of atoms: Hydrogen and helium

In the previous sections, we have provided a generalization of SUSY-QM to treat any number of dimensions or particles with a focus on its usefulness as a computational tool for calculating accurate excited state energies and wave functions.
Because of the significant analytical and computational ramifications, and motivated by the future study of more complex electronic systems, we here apply our multi-dimensional generalization of SUSY-QM to the hydrogen atom in full three-dimensional detail. This is of interest because, until now, the standard application of SUSY-QM to the hydrogen atom required that we first separate out the angular degrees of freedom – effectively reducing the problem to a one-dimensional treatment [Kirchberg et al. (2003); Lahiri et al. (1987); Tangerman & Tjon (1993)]. With our vector superpotential approach, one can deal with the full three-dimensional nature of the hydrogen atom.
Our approach provides, for the first time, a SUSY-QM framework that can be employed to treat non-hydrogenic atoms. For example, the standard SUSY-QM treatment of the hydrogen atom cannot be extended readily to the helium atom because it is impossible reduce it to a one-dimensional system. In addition, the form of the three-dimensional vector superpotential for the hydrogen atom is of interest in its own right. It is quite different from the radial superpotential obtained in earlier SUSY-QM studies of the hydrogen atom. The present study thus lays the groundwork for a systematic SUSY-QM study of excited state energies and wave functions of atoms.

6.1 SUSY-QM for the three-dimensional hydrogen atom

We now consider the hydrogen atom. We begin by noting that the ground state is exactly given by

$$\psi_{1,0,0} = \frac{e^{-r}}{\sqrt{\pi}}, \tag{6.1}$$

where we have set the Bohr radius equal to 1. The Hamiltonian (in atomic units) is simply

$$\mathcal{H} = -\frac{1}{2}\nabla^2 - \frac{1}{r}. \tag{6.2}$$

Then, the vector superpotential is given by

$$\vec{W} = -\nabla \ln \psi_{1,0,0} = \hat{r}, \tag{6.3}$$

where $\hat{r}$ is a unit vector in the direction of $\vec{r}$. This is an extremely interesting result. First, we see that the superpotential for the Coulomb interaction is, itself, non-singular. Second, in the standard approach, because the angular degrees of freedom have already been separated out, the superpotential is a scalar and it depends on the angular momentum squared (*i.e.* on $l(l+1)$). The precise form for the ground state ($l = 0$) is

$$W_{radial} = 1 \tag{6.4}$$

In three dimensions, we have

$$\vec{W} = \vec{\epsilon_x}\frac{x}{r} + \vec{\epsilon_y}\frac{y}{r} + \vec{\epsilon_z}\frac{z}{r} = \hat{r}. \tag{6.5}$$

The magnitude of $\vec{W}$ is equal to the radial superpotential, as one expects, but the individual components are radically different. Note that these components can also be written solely

in terms of angular functions (the direction cosines of $\vec{r}$). To obtain the atomic potential for hydrogen, we form

$$\vec{W}\cdot\vec{W}-\nabla\cdot\vec{W}=1-\left(\frac{3}{r}-\frac{x^2+y^2+z^2}{r^3}\right) \tag{6.6}$$

$$=1-\frac{2}{r}=-2E_0-\frac{2}{r}. \tag{6.7}$$

Now we recall that

$$H\psi_{m_l}=E_n\psi_{m_l} \tag{6.8}$$

and

$$-\frac{1}{2}\nabla^2\psi_{m_l}=\left[E_n+\frac{1}{r}\right]\psi_{m_l} \tag{6.9}$$

yields

$$\nabla^2\psi_{1,0,0}=-\left[2E_0+\frac{2}{r}\right]\psi_{1,0,0}. \tag{6.10}$$

Since the ground state energy of hydrogen in atomic units is -1/2, we find that Equations (6.7) and (6.10) are consistent and we have obtained the correct vector superpotential. Of great interest is the wave equation for the sector two problem. This Hamiltonian is given by

$$\overleftrightarrow{\mathcal{H}}_2=-\frac{1}{2}\nabla\nabla+\frac{1}{2}\left[\vec{W}\vec{W}+\nabla\vec{W}\right]. \tag{6.11}$$

In the case of the hydrogen atom, because we have exact analytical expressions for the excited states of $\mathcal{H}_1$, it is a simple matter to generate analytical expressions for all the states of the sector two Hamiltonian. It is convenient to label the sector two states with an index indicating the n^{th} energy state (i.e., we use the principle quantum number n = 1,2,...) along with the quantum numbers of the sector one excited state from which they are obtained. Thus, the four degenerate ground states of $\overleftrightarrow{\mathcal{H}}_2$ will be denoted by $\vec{\psi}^{(2)}_{1,2p_x}$, $\vec{\psi}^{(2)}_{1,2p_y}$, $\vec{\psi}^{(2)}_{1,2p_z}$, $\vec{\psi}^{(2)}_{1,2s}$. We choose here to use the real states rather than those labeled by $m_l=\pm1$ and $m_l=0$ values. We find that these solutions are given by

$$\vec{\psi}^{(2)}_{1,2p_x}=N\left[\hat{i}e^{-r/2}+\frac{x\hat{r}}{2}e^{-r/2}\right], \tag{6.12}$$

$$\vec{\psi}^{(2)}_{1,2p_y}=N\left[\hat{j}e^{-r/2}+\frac{y\hat{r}}{2}e^{-r/2}\right], \tag{6.13}$$

$$\vec{\psi}^{(2)}_{1,2p_z}=N\left[\hat{k}e^{-r/2}+\frac{z\hat{r}}{2}e^{-r/2}\right], \tag{6.14}$$

$$\vec{\psi}^{(2)}_{1,2s}=-N\frac{\vec{r}}{2}e^{-r/2}. \tag{6.15}$$

These equations can be verified by simply applying $\vec{Q}$ to the first excited state wave functions of sector one. It is also easily verified that $\vec{Q}^{\dagger}$ acting on these states regenerates the $\psi^{(1)}_{2p}$ and $\psi^{(1)}_{2s}$ states. Furthermore, in Figures 9 and 10, we provide plots of the $\vec{\psi}^{(2)}_{1,2s}$ and $\vec{\psi}^{(2)}_{1,2p_x}$. It is straight forward to see that $\vec{\psi}^{(2)}_{1,2p_y}$ and $\vec{\psi}^{(2)}_{1,2p_z}$ are both similar to $\vec{\psi}^{(2)}_{1,2p_x}$.

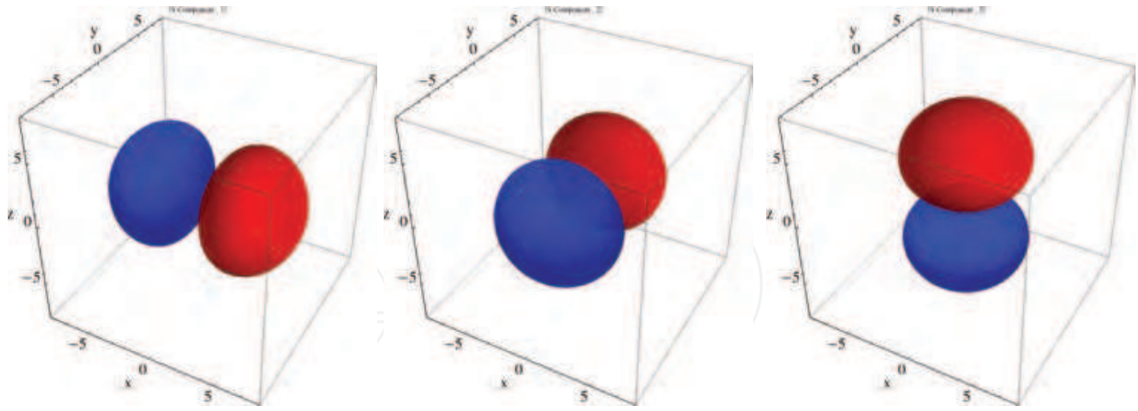


Fig. 9. The three components of the wave function for $\vec{\psi}^{(2)}_{1,S}$. Here, blue corresponds to positive values and red to negative.

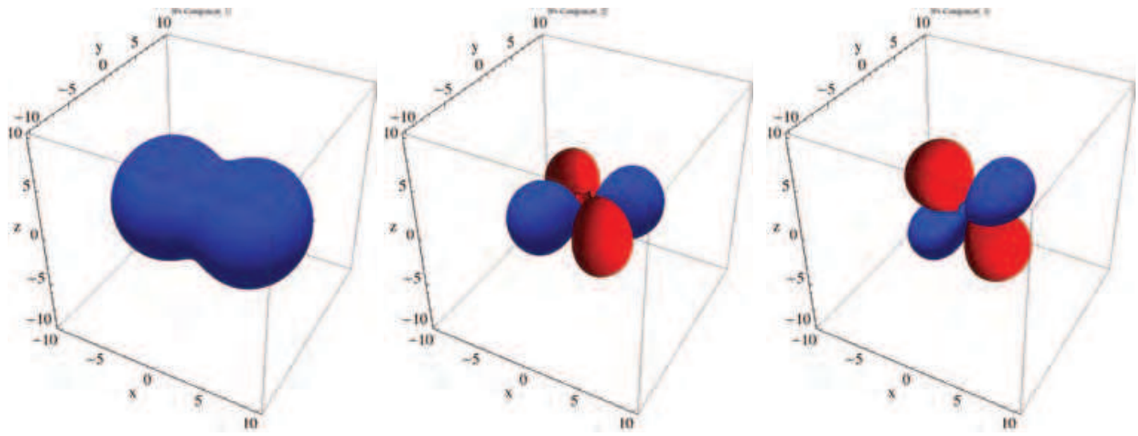


Fig. 10. The three components of the wave function for $\vec{\psi}^{(2)}_{1,p_x}$. Here, blue corresponds to positive values and red to negative.

6.2 An approximate superpotential for the helium atom

It is of interest to begin exploring how our approach to multidimensional SUSY-QM would deal with a two electron atom. It is clear that the usual radial (one-dimensional) hydrogen atom SUSY-QM treatment is not readily generalizable to deal with helium. We have carried out a Quantum Monte Carlo study of the sector one ground state of helium using the Padè Jastrow trial wave function Umrigar & Wilson (1988):

$$\psi^{(1)}_{T,\alpha} = e^{-2r_1} e^{-2r_2} e^{\frac{r_{12}}{2(1+\alpha r_{12})}}, \tag{6.16}$$

with the optimum α given by $\alpha = 0.353$. This yields an energy of $E^{(1)}_1 \approx 2.878$, which is in error by about 1%. This error is reasonable for a simple treatment neglecting relativistic interactions. The approximate $\vec{W}$ is generated from

$$\vec{W}(\vec{r}_1, \vec{r}_2) = -\vec{\nabla} \ln \psi^{(1)}_{T,\alpha} \tag{6.17}$$

$$= -\vec{\nabla}\left[-2r_1 - 2r_2 + \frac{r_{12}}{2(1+\alpha r_{12})}\right]. \tag{6.18}$$

Here,

$$\vec{\nabla} = \epsilon_{\hat{1}x}\frac{\partial}{\partial x_1} + \epsilon_{\hat{1}y}\frac{\partial}{\partial y_1} + \epsilon_{\hat{1}z}\frac{\partial}{\partial z_1} + \epsilon_{\hat{2}x}\frac{\partial}{\partial x_2} + \epsilon_{\hat{2}y}\frac{\partial}{\partial y_2} + \epsilon_{\hat{2}z}\frac{\partial}{\partial z_2}, \tag{6.19}$$

where the $\{\hat{\epsilon}_{ij}\}$ are orthonormal vectors. The resulting vector superpotential for the Padè-Jastrow trial function is readily found to be

$$\vec{W}_{He(PJ)} = 2\hat{r}_1 + 2\hat{r}_2 - \hat{r}_{12}\left[1 - \frac{\alpha}{(1+\alpha r_{12})}\right]. \tag{6.20}$$

Thus, the structure of $\vec{W}_{He(PJ)}$ is analogous to $\vec{W}_H$ in that Coulomb interactions generate vector superpotentials that involve unit vectors anti-parallel to the direction of the forces. This is true in general for Coulombic interactions. This emphasizes the important distinction between our three-dimensional SUSY-QM treatment of an atom and the standard hydrogen atom one-dimensional radial SUSY-QM.

7. Aufbau approach for excited states

For multielectron atoms, it becomes necessary to consider how the aufbau principle acts in the second sector to permit efficient calculations of sector one excited states. This is because we can use this principle to design reasonable trial wave functions for a variational approach to the sector two ground state. In this section, we consider a simple aufbau description of the sector one helium excited states in order to design an approximate sector two ground state of helium. We assume that in the first excited state of sector one, we have one electron in the $1S$ orbital, given by wave function α, and one electron in the $2S$ orbital, given by wave function β where

$$\alpha(r) = \frac{e^{-2r}}{\sqrt{\pi}} \text{ and } \beta(r) = \frac{e^{-r}}{4\sqrt{2\pi}}(1-r). \tag{7.1}$$

Then, it is of interest to take the product of these states such that we have $\alpha(r_1)\beta(r_2)$, to which we can apply our $\vec{Q}$ to find

$$\vec{Q}\left(\alpha(r_1)\beta(r_2)\right) = -e^{-2r_1-r_2}\left[2\hat{r}_1\left(1-r_2\right) + \hat{r}_2\right] \equiv \vec{\phi}_1^{(2)}. \tag{7.2}$$

The first excited sector one state of Helium is a triplet so the wave function is anti-symmetric under spatial electron exchange. It is clear that we require the second sector ground state also be anti-symmetric when we interchange labels 1 and 2. To obtain this, we apply P_{12} to Equation (7.2) to get

$$\vec{Q}\left(\alpha(r_2)\beta(r_1)\right) = -e^{-2r_2-r_1}\left[2\hat{r}_2\left(1-r_1\right) + \hat{r}_2\right] \equiv P_{12}\vec{\phi}_1^{(2)}, \tag{7.3}$$

where P_{12} exchanges the electron labels. Then, we can use Equations (7.2) and (7.3) as a "building blocks" to construct our ground state in the second sector by subtracting the first building block from the second. This gives us a second sector result of

$$\begin{aligned}\vec{\psi}_{1,triplet}^{(2)} = &- e^{-2r_1-r_2}\left[2\hat{r}_1\left(1-r_2\right) + \hat{r}_2\right] + \\ &e^{-2r_2-r_1}\left[2\hat{r}_2\left(1-r_1\right) + \hat{r}_1\right].\end{aligned} \tag{7.4}$$

And similarly, we can find the second sector first excited singlet state by simply adding the two building blocks as given below.

$$\begin{aligned}\vec{\psi}^{(2)}_{1,singlet} = &- e^{-2r_1-r_2}\left[2\hat{r}_1\left(1-r_2\right)+\hat{r}_2\right]- \\ &e^{-2r_2-r_1}\left[2\hat{r}_2\left(1-r_1\right)+\hat{r}_1\right].\end{aligned} \tag{7.5}$$

Indeed, by taking the scalar product with $\vec{Q}^{\dagger}$, we can verify that $\vec{\psi}^{(2)}_{1,triplet}$ and $\vec{\psi}^{(2)}_{1,singlet}$ give the appropriate spatial wave functions. This is to say that, to within a multiplicative constant, we get that

$$\vec{Q}^{\dagger}\cdot\vec{\psi}^{(2)}_{1,triplet} = \psi^{(1)}_1 = \alpha(r_1)\beta(r_2)-\alpha(r_2)\beta(r_1) \tag{7.6}$$

and

$$\vec{Q}^{\dagger}\cdot\vec{\psi}^{(2)}_{1,singlet} = \psi^{(1)}_2 = \alpha(r_1)\beta(r_2)+\alpha(r_2)\beta(r_1). \tag{7.7}$$

From this, we observe that the aufbau principle in the second sector is remarkably simple for Helium. We merely need to take the building block $\vec{\phi}^{(2)}_1$ and antisymmetrize or symmetrize appropriately. Of course our "building block", $\vec{\phi}^{(2)}_1$, is neither symmetric nor antisymmetric under particle exchange.

However, this basis doesn't include the correlation. To do this, we can multiply our antisymmetrized second sector wave function by a correlation function, given by the Padé-Jastrow function which only depends on r_{12}. It is clear, then, that because our correlation function is only a function of r_{12}, its symmetry will not be affected by the application of $\vec{Q}$ and, thus, we can simply multiply it by our second sector state of interest (where the minus corresponds to the triplet and the plus to the singlet):

$$\begin{aligned}\vec{\psi}^{(2)}_{1,triplet} = &e^{\frac{r_{12}}{2(1+\delta r_{12})}}\Big(-e^{-2r_1-r_2}\left[2\hat{r}_1\left(1-r_2\right)+\hat{r}_2\right]\mp \\ &e^{-2r_2-r_1}\left[2\hat{r}_2\left(1-r_1\right)+\hat{r}_1\right]\Big).\end{aligned} \tag{7.8}$$

Higher accuracy will result if we insert additional variational parameters (*e.g.*, effective charges, *etc.*) when doing computations.

8. Conclusions and perspectives

In this chapter, we began by presenting our computational approach to one dimensional systems. We showed with the anharmonic oscillator that we were able to achieve significant computational gains in a robust fashion, permitting more exact numerical solutions of one dimensional problems. Although anharmonic oscillator models are useful for a wide variety of problems in both chemistry and physics, it should be clear that other systems should show similar behaviour. The SUSY-QM approach enabled us to develop a hierarchy of isospectral Hamiltonians. This also led to the introduction of charge operators that transform wave functions between the various sectors, and the energies are always determined in a ground state setting. Because these are most easily and accurately obtained by the variational method, we realize a significant reduction in the basis size needed to yield accurate excited state wave functions. We then considered 2 specific examples of anharmonic oscillators. We concluded that using the SUSY hierarchy of hamiltonians and charge operators, provided faster convergence to the same level of accuracy and thus, provides a better method than the

standard variational approach. In most cases, only half as many basis functions were needed to generate the ground state wave function as were required for the first excited state of the same sector. As a result, the computational time for molecular models using anharmonic potentials will be significantly reduced, without sacrificing accuracy.

We also stress that our results do not depend on precisely what basis set is used for the calculations. Rather we are capitalizing on the general behavior of the Rayleigh-Ritz variational method with regard to accuracy and convergence rate for ground versus excited states of a given Hamiltonian.

We then presented our approach to generalizing SUSY-QM to deal with more than one dimension and more than one (distinguishable) particle. In general, previous attempts to do this have typically introduced Pauli spin matrices and so far as we are aware, none of these has been proved useful for the general case. Andrianov et al. (1985); Andrianov, Borisov & Ioffe (1984a;b;c); Andrianov et al. (1986); Andrianov, Borisov, Ioffe & Eides (1984); Andrianov & Ioffe (1988); Andrianov et al. (2002); Cannata et al. (2002); Das & Pernice (1996) One principle difficulty is that while the coordinates of different particles are independent variables, they are not defined relative to orthogonal axes. That is, there are only 3 independent, physical axes along which all particle positions are measured. Our approach introduces a higher dimensional vector space in which there is an orthonormal basis vector associated with each independent particle coordinate. This is analogous to the relativistic situation where each particle has its own coordinate system(and, of course, in the relativistic case, its own "proper time"). Here, however the device is a mathematical convenience (so far as we are currently aware) and it is, of course, non-relativistic. That is, we assume Gallilean transformations. The most striking consequence similar to relativistic quantum mechanics is that our second sector Hamiltonian becomes a tensor in the expanded space. This does *not* increase the number of independent variables (i.e., the wave function for the second sector is a vector in the new hyperspace). It is shown that this tensor character is then absent from the 3^{rd} sector Hamiltonian (which is once again a scalar operator). One in general obtains an alternating series of scalar and tensor Hamiltonians. *The occurrence of a tensor sector Hamiltonian is, of course, an added computational cost to the approach*. This is mitigated , to some degree, by the fact that we *never* must calculate an accurate wave function and energy except for *ground states* . It is this feature that makes the SUSY-QM approach attractive, since ground state energies and wave functions are the least computationally demanding of all and typically are obtained with the highest accuracy. Thus the computational effort of obtaining the second excited state energy and wave function again involves solving an equation comparable to that generated by the original H_1. A complication, however, arises due to the observed fact that for the ground state sector 2 wave function in both the degenerate and non-degenerate cases, one of the two components possesses nodes while the other component is nodeless. This is mitigated (in terms of accuracy of the sector 2 ground state calculation) by the fact that the component containing the node is (in the present computational examples) an order of magnitude smaller that the nodeless component. This appears to enable the variational evaluation of the ground state of the sector 2 to yield better accuracy for the first excited state energy and wave function than a comparable basis set calculation applied to H_1.

An extremely important question is, however, raised by the fact that the small component of $\vec{\psi}_0^{(2)}$ has nodes. This is whether the presence of nodes will prevent us from applying a simple variational quantum Monte-Carlo method to obtain $\vec{\psi}_0^{(2)}$. We are currently exploring this question. However, in the present context, it does not appear to create difficulties for the variational approach.

Finally, we have shown how our multi-dimensional generalization of SUSY-QM can be applied to the hydrogen atom. Previously, most detailed attempts to treat the hydrogen atom first separated the angular degrees of freedom, leaving a one-dimensional radial wave equation. It was then possible to obtain the SUSY-QM factorization, yielding a scalar superpotential that, for the $l = 0$ states, is simply $W = 1$. While these results are interesting, the one-dimensional radial SUSY-QM approach is not readily generalizable to treat even the helium atom.

In our approach, the full three-dimensional character of the hydrogen atom is considered, with the result being a vector-valued superpotential, $\vec{W}$, which for the hydrogen atom, is $\vec{W} = \hat{r}$. That is, the vector superpotential points in the opposite direction of the attractive Coulomb force between the electron and the nucleus. This is interesting also because, although the Coulomb potential is singular, its vector superpotential is not. It is important to note that such a superpotential was also obtained earlier by Stedman Stedman (1985). However, his sector two Hamiltonian differs from ours and produces "extra" states that are not degenerate with sector one.

The fact that $\vec{W}$ for the three-dimensional hydrogen atom is a vector does not, in any way, modify the sector one dynamical equation. However, the sector two situation is radically affected! In the one-dimensional SUSY-QM case, there is no significant change in the basic mathematical structure of the sector two partner Hamiltonian. In the multi-dimensional case, the sector two Hamiltonian is a tensor. However, we have shown in previous studies, that many of the standard computational techniques remain valid. Of particular interest is the Dirac-Frankel-McLachlan Variational Method, since this is known to deal better with higher-dimensional systemsRaab (2000).

In the case of the hydrogen atom, it is straight forward to generate all the sector two eigenstates. This is a consequence of the fact that exact analytical eigenstates of the three-dimensional hydrogen atom are known. It is then easy to apply the charge operator, $\vec{Q}$, to the excited hydrogen atom states and obtain sector two eigenstates. (We note that because of the four fold degeneracy for the sector two ground state, the resulting eigenstates can be super-posed in any manner convenient for the study at hand). It is of considerable interest to begin exploring how our multi-dimensional SUSY-QM treatment can be applied to the helium atom. In this case, the exact sector one ground state is, of course, unavailable. In our previous one and two-dimensional studies we have considered other systems for which an exact $\vec{W}$ was not possible. In the case of helium, we chose to examine an accurate Padè-Jastrow approximation to the sector one ground state. In this case, it is easy to obtain an analytical (albeit approximate) $\vec{W}$ that displays very reasonable intuitive character. In direct analogy with the exact hydrogen atom $\vec{W}$, we find that the $\vec{W}_{He(PJ)}$ vector superpotential consists of a combination of unit vectors that again, are anti-parallel to the Coulomb forces associated with the helium atom potential energy. The next step in our study will consist of computations of a sector two ground state, which will allow us to obtain an approximate helium atom sector one first excited state energy and wave function.

Future studies will explore extending the approach to more than two electron atoms. There, the issue will be taking account of the electrons' spin degrees of freedom. Our current plan is to employ the "spin-free" techniques of Matsen Matsen (1964; 1966; 1970); Matsen & Cantu (1968; 1969); Matsen et al. (1966); Matsen & Ellzey (1969); Matsen & Junker (1971); Matsen & Klein (1969; 1971); Matsen et al. (1971) and othersPauncz (1995).

We have also generalized the aufbau principle to work in the second sector Hamiltonian, demonstrating that we are able to produce reasonable forms of excited states by simply using

hydrogenic orbitals. The equations have a reasonable structure but variational computations are necessary. We shall report these results later.

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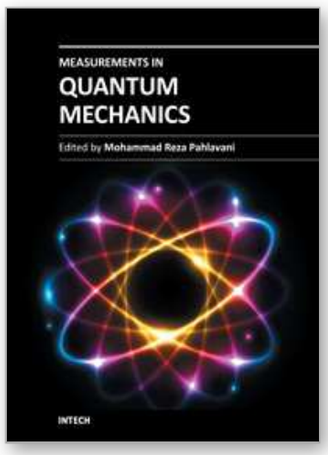

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