

## Quantum dynamics and super-symmetric quantum mechanics.

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In my talk I will present an overview of our recent work involving the use of supersymmetric quantum mechanics (SUSY-QM). I begin by discussing the mathematical underpinnings of SUSY-QM and then discuss how we have used this for developing novel theoretical and numerical approaches suitable for studying molecular systems. I will conclude by discussing our attempt to extend SUSY-QM to multiple dimensions.

### I. A FIRST DATE

My introduction to supersymmetric quantum mechanics (SUSY) came quite by accident. I had heard of SUSY in the context of high-energy physics where the SUSY theory postulates that for every fermion there is boson of equal mass (i.e. energy). This comes about because for every quantum Hamiltonian there is a partner Hamiltonian that has the same energy spectrum above the ground-state of the original system. In other words, above the ground state of  $H_1$ , each higher-lying eigenstate is partnered with an eigenstate of  $H_2$ . In particle physics, the  $H_1$  “sector” is populated by bosons and the  $H_2$  sector by fermions and SUSY predicts that the lowest lying fermion state is energetically degenerate with the first excited boson state. Evidence for SUSY has proven to be elusive and it is now believed that SUSY is a broken symmetry.

Last January (Jan-09) at a conference dedicated to Bob Wyatt, my co-author suggested that we look at SUSY as a way to develop new computational methods and approaches. Up until now, SUSY has been more of a mathematical technique that has been used more or less as a way to obtain stationary solutions to the Schrödinger equation for the variety of one-dimensional potential systems. In this paper and in my talk, I will discuss some of the work we have been doing in developing “SUSY” inspired methods for performing quantum many-body

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calculations and quantum scattering calculations. I shall begin with a brief overview of the SUSY theory and some of its elementary results. I shall then discuss how we have used the approach to develop both analytical and numerical solutions of the stationary Schrödinger equation. I will conclude by discussing our recent extension of SUSY to higher dimensions and for scattering theory.

## II. MATHEMATICAL CONSIDERATIONS

Before discussing some of our recent results, it is important to introduce briefly the mathematical formulation of SUSY quantum mechanics.

### A. Hamiltonian formulation of SUSY

In quantum theory, there is a fundamental connection between a bound state and its potential. This is simple to demonstrate by writing the Schrödinger equation for the stationary states as

$$V_1(x) - E_n = -\frac{\hbar^2}{2m} \frac{1}{\psi_n} \partial_x^2 \psi_n = Q[\psi_n] \quad (1)$$

where we recognize the right-hand side as the Bohm quantum potential which will certainly be discussed repeatedly at this conference. One of the remarkable consequences of this equation is that every stationary state of a given potential has the same functional form for its quantum potential  $Q$ . Thus, knowing any bound state allows a global reconstruction of the potential,  $V(x)$  up to a constant energy shift.

SUSY is obtained by factoring the Schrödinger equation into the form [1–3]

$$H\psi = A^+ A\psi_o^{(1)} = 0 \quad (2)$$

using the operators

$$A = \frac{\hbar}{\sqrt{2m}} \partial_x + W \text{ and } A^+ = -\frac{\hbar}{\sqrt{2m}} \partial_x + W. \quad (3)$$

Since we can impose  $A\psi_o^{(1)} = 0$ , we can immediately write that

$$W(x) = -\frac{\hbar}{\sqrt{2m}} \partial_x \ln \psi_o. \quad (4)$$

$W(x)$  is the *superpotential* which is related to the physical potential by a Riccati equation.

$$V(x) = W^2(x) - \frac{\hbar}{\sqrt{2m}} W'(x). \quad (5)$$

The SUSY factorization of the Schrödinger equation can always be applied in one-dimension.

From this point on we label the original Hamiltonian operator and its associated potential, states, and energies as  $H_1$ ,  $V_1$ ,  $\psi_n^{(1)}$  and  $E_n^{(1)}$ . One can also define a partner Hamiltonian,  $H_2 = AA^+$  with a corresponding potential

$$V_2 = W^2 + \frac{\hbar}{\sqrt{2m}}W'(x). \quad (6)$$

All of this seems rather circular and pointless until one recognizes that  $V_1$  and its partner potential,  $V_2$ , give rise to a common set of energy eigenvalues. This principle result of SUSY can be seen by first considering an arbitrary stationary solution of  $H_1$ ,

$$H_1\psi_n^{(1)} = A^+A\psi_n = E_n^{(1)}\psi_n^{(1)}. \quad (7)$$

This implies that  $(A\psi_n^{(1)})$  is an eigenstate of  $H_2$  with energy  $E_n^{(1)}$  since

$$H_2(A\psi_n^{(1)}) = AA^+A\psi_n^{(1)} = E_n^{(1)}(A\psi_n^{(1)}). \quad (8)$$

Likewise, the Schrödinger equation involving the partner potential  $H_2\psi_n^{(2)} = E_n^{(2)}\psi_n^{(2)}$  implies that

$$A^+AA^+\psi_n^{(2)} = H_1(A^+\psi_n^{(2)}) = E_n^{(2)}(A^+\psi_n^{(2)}). \quad (9)$$

This (along with  $E_o^{(1)} = 0$ ) allows one to conclude that the eigenenergies and eigenfunctions of  $H_1$  and  $H_2$  are related in the following way:  $E_{n+1}^{(1)} = E_n^{(2)}$ ,

$$\psi_n^{(2)} = \frac{1}{\sqrt{E_{n+1}^{(1)}}}A\psi_{n+1}^{(1)}, \text{ and } \psi_{n+1}^{(1)} = \frac{1}{\sqrt{E_n^{(2)}}}A^+\psi_n^{(2)} \quad (10)$$

for  $n > 0$ . [51] Thus, the *ground state of  $H_2$  has the same energy as the first excited state of  $H_1$* . If this state  $\psi_o^{(2)}$  is assumed to be node-less, then  $\psi_1^{(1)} \propto A^+\psi_o^{(2)}$  will have a single node. We can repeat this analysis and show that  $H_2$  is partnered with another Hamiltonian,  $H_3$  whose ground state is isoenergetic with the first excited state of  $H_2$  and thus isoenergetic with the second excited state of the original  $H_1$ . This hierarchy of partners persists until all of the bound states of  $H_1$  are exhausted.

## B. SUSY algebra

We can connect the two partner Hamiltonians by constructing a matrix super-Hamiltonian operator

$$\mathbf{H} = \begin{pmatrix} H_1 & 0 \\ 0 & H_2 \end{pmatrix} \quad (11)$$

and two matrix “super-charge” operators

$$\mathbf{Q} = \begin{pmatrix} 0 & 0 \\ A & 0 \end{pmatrix} = A\sigma_- \quad (12)$$

and

$$\mathbf{Q}^+ = \begin{pmatrix} 0 & A^+ \\ 0 & 0 \end{pmatrix} = A^+\sigma_+ \quad (13)$$

where  $\sigma_{\pm}$  are  $2 \times 2$  Pauli spin matrices. Using these we can re-write the SUSY Hamiltonian as

$$\mathbf{H} = \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + W^2 \right) \sigma_o + W' \sigma_z \quad (14)$$

The operators  $\{\mathbf{H}, \mathbf{Q}, \mathbf{Q}^+\}$  form a closed algebra (termed the Witten superalgebra) with

$$[\mathbf{H}, \mathbf{Q}] = [\mathbf{H}, \mathbf{Q}^+] = 0 \quad (15)$$

$$\{\mathbf{Q}, \mathbf{Q}\} = \{\mathbf{Q}^+, \mathbf{Q}^+\} = 0 \quad (16)$$

$$\{\mathbf{Q}, \mathbf{Q}^+\} = \mathbf{H} \quad (17)$$

The first algebraic relation is responsible for the degeneracy of the spectra of  $H_1$  and  $H_2$  and the supercharges transform an eigenstate of one sector into an eigenstate of the other sector.

As an example and perhaps a better connection to the physics implied by this structure, consider the case of a one-dimensional particle with an internal spin degree of freedom and with  $[x, p] = i$  denoting the position and momentum of the particle. Conserved SUSY would imply that all non-diagonal coupling terms between the bosonic (coordinate) and fermionic (spin) degrees of freedom are exactly zero. This of course is equivalent to making the Born Oppenheimer approximation for a two-state system coupled to a continuous field  $x(t)$ . In this case, SUSY is preserved so long as  $d_t \psi(x(t), t) = \partial_t \psi(x(t), t)$ . SUSY is broken when  $\dot{x}(t) \partial_x \psi(x(t), t) \neq 0$  which would lift the degeneracy between the states of  $H_1$  and  $H_2$ .

### C. Scattering in one dimension

The SUSY approach is not limited to bound-state problems. For a one-dimensional scattering system, it is straightforward to apply the SUSY theory to determine a relation between the transmission and reflection coefficients of the supersymmetric partners. Asymptotically, we can assume that  $W(x) \rightarrow W_{\pm}$  as  $x \rightarrow \pm\infty$ . In the same limit, the partner potentials become

$V_{1,2} \rightarrow W_{\pm}^2$ . For a plane wave incident from the left with energy  $E$  scattering from  $V_{1,2}$ , we require the following asymptotic forms:

$$\lim_{x \rightarrow -\infty} \psi^{(1,2)}(k, x) \sim e^{ikx} + R^{(1,2)} e^{-ikx} \quad (18)$$

$$\lim_{x \rightarrow +\infty} \psi^{(1,2)}(k', x) \sim T^{(1,2)} e^{ik'x} \quad (19)$$

We can derive a relation between the two scattering states by using the relation  $\psi^{(1)}(k, x) = N A^+ \psi_2(k', x)$ . For the left-hand components ( $x \rightarrow -\infty$ ).

$$e^{ikx} + R^{(1)} e^{-ikx} = N \left[ (-ik + \tilde{W}_-) e^{ikx} + (ik + \tilde{W}_-) e^{-ikx} \right] \quad (20)$$

where in the last line we have incorporated the  $\hbar/\sqrt{2m}$  in to the normalization and wrote  $\tilde{W}_{\pm} = W_{\pm} \sqrt{2m}/\hbar$ . Likewise for the transmitted coefficients ( $x \rightarrow +\infty$ ).

$$T^{(1)} e^{ik'x} = N(-ik' + \tilde{W}_+) T^{(2)} e^{ik'x} \quad (21)$$

Eliminating the common normalization factor and using the fact that  $k = \sqrt{2m(E - W_-)}/\hbar$  and  $k' = \sqrt{2m(E - W_+)}/\hbar$  from the Schrödinger equation we can arrive at

$$R^{(1)}(k) = \frac{W_- + ik}{W_- - ik} R^{(2)}(k) \quad (22)$$

$$T^{(1)}(k) = \frac{W_+ - ik'}{W_- - ik} T^{(2)}(k). \quad (23)$$

Consequently, knowledge of the scattering states of  $V_1$  allows one to easily construct scattering states for the partner potential.

#### D. Non-stationary states

Finally, one can use the SUSY approach in a time-dependent context by writing

$$i\hbar \partial_t \psi^{(1)} = H_1 \psi^{(1)} = A^+ A \psi^{(1)}$$

where  $\psi^{(1)}$  is a non-stationary state in the first sector. If  $V_1$  is independent of time, then the superpotential must also be independent of time and so we can write

$$i\hbar A \partial_t \psi^{(1)} = i\hbar \partial_t (A \psi^{(1)}) = A A^+ (A \psi^{(1)})$$

In other words, we have the time-dependent Schrödinger equation for the partner potential

$$i\hbar\partial_t\psi^{(2)} = H_2\psi^{(2)}.$$

The two non-stationary states are partnered,  $\psi^{(2)} \propto A^+\psi^{(1)}$ . We also note that these states satisfy

$$\psi^{(1)}(t) = e^{-iA^+At/\hbar}\psi(0)$$

and

$$\psi^{(2)}(t) = e^{-iAA^+t/\hbar}\psi(0)$$

for some initial state  $\psi(0)$ . Using the charge operators we can show that

$$A\psi^{(1)}(t) = e^{-iAA^+t/\hbar}(A\psi(0)).$$

As above in the scattering example, one can use the dynamics of one sector to determine the dynamics in the other sector.

The partnering scheme presents a powerful prescription for developing novel approaches for solving a wide variety of quantum mechanical problems. This allows one to use analytical or numerical solutions of one problem to determine either approximate or exact solutions to some new problem. In the sections that follow, I present some of our attempt to use SUSY in a numerical context. At the moment our numerical results are limited to one spatial dimension. As I shall discuss, extending SUSY to multiple dimensions has proven to be problematic. However, in Sec. V we present our extension using a vector-SUSY approach we are developing.

### III. USING SUSY TO OBTAIN EXCITATION ENERGIES AND EXCITED STATES

The SUSY hierarchy also provides a useful prescription for determining the excited states of  $H_1$  (which may represent the physical problem of interest.) The first excited state of  $H_1$  is isoenergetic with the ground state of  $H_2$ . Since this state is node-less, one can use either Ritz variational approaches or Monte Carlo approaches to determine this state to very high accuracy.

Two basic tools used in computational chemistry are the Quantum Monte Carlo (QMC) and the Rayleigh-Ritz variational approaches. Both approaches yield their best and most accurate results for ground state energies and wave functions. Although the variational method also gives bounds for the excited state energies as well as the ground state (the Hylleraas-Undheim theorem [4]), it is well known that their accuracy is significantly lower than that of the ground

state. Even more serious, the wave functions are known to converge much more slowly than the energies.

In the case of the QMC[5–10], there are additional difficulties associated with the presence of nodes in the excited state wave functions [11]. While some progress has been made in dealing with this issue (e.g., the “fixed node” or “guide wave” techniques)[8–12] the computational effort required is greater and the accuracy is lower and in fact, no general solution to the difficulty has been found for reducing the computational effort and increasing the accuracy for excited state calculations in QMC to the same level as is attained for the ground state. In fact, it is very likely the presence and effects of nodes in the excited states that is largely responsible for the lower accuracy and slower convergence of excited state results in the variational method. The precise determination of nodal surfaces is expected to play a crucial role since they reflect changes in the relative phase of the wave function. Because of the ubiquitous importance of both the variational and QMC methods, solving the so-called “node problem” will have enormous impact on computational chemistry.

#### A. Using SUSY to improve quality of variational calculations

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[4]. 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 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 the potential

$$V_1(x) = x^6 + 4x^4 + x^2 - 2. \quad (24)$$

exact solutions are known for all states of  $H_1$ . We use the exact results to assess the accuracy of the variational calculations. Here we employed a  $n$ -point discrete variable representation (DVR) based upon the Tchebchev polynomials to compute the eigenspectra of the first and second sectors.[13, 14] In Fig. 1 we show the numerical error in the first excitation energy by comparing  $E_1^1(n)$  and  $E_0^2(n)$  from an  $n$  point DVR to the numerically “exact” value corresponding to

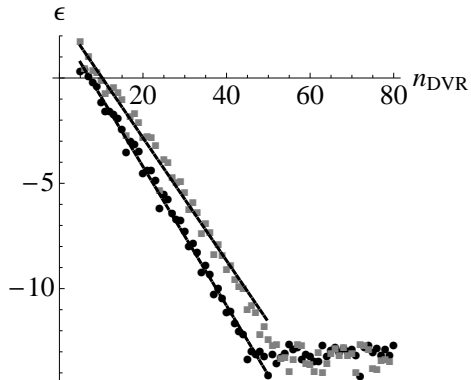


FIG. 1: Convergence of first excitation energy  $E_1^1$  for model potential  $V_1 = x^6 + 4x^4 + x^2 - 2$  using a  $n$ -point discrete variable representation (DVR). Gray squares:  $\epsilon = \log_{10} |E_1^1(n) - E_1^1(\text{exact})|$ , Black squares:  $\epsilon = \log_{10} |E_0^2(n) - E_1^1(\text{exact})|$ . Dashed lines are linear fits. (From Ref[15].)

a 100 point DVR,

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

Likewise,

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

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.

## B. Monte Carlo SUSY

Having defined the basic terms of SUSY quantum mechanics, let us presume that one can determine an accurate approximation to the ground state density  $\rho_o^{(1)}(x)$  of Hamiltonian  $H_1$ . One can then use this to determine the superpotential using the Riccati transform

$$W_o^{(1)} = -\frac{1}{2} \frac{\hbar}{\sqrt{2m}} \frac{\partial \ln \rho_o^{(1)}}{\partial x} \quad (25)$$



and the partner potential

$$V_2 = V_1 - \frac{\hbar^2}{2m} \frac{\partial^2 \ln \rho_o^{(1)}}{\partial x^2}. \quad (26)$$

Certainly, our ability to compute the energy of the ground state of the partner potential  $V_2$  depends on having first obtained an accurate estimate of the ground-state density associated with the original  $V_1$ .

For this we turn to an adaptive Monte Carlo-like approach developed by Maddox and Bittner.[16] Here, we assume we can write the trial density as a sum over  $N$  Gaussian approximate functions

$$\rho_T(x) = \sum_n G_n(x, \mathbf{c}_n). \quad (27)$$

parameterized by their amplitude, center, and width.

$$G_n(x, \{\mathbf{c}_n\}) = c_{no} e^{-c_{n2}(x-c_{n3})^2} \quad (28)$$

This trial density then is used to compute the energy

$$E[\rho_T] = \langle V_1 \rangle + \langle Q[\rho_T] \rangle \quad (29)$$

where  $Q[\rho_T]$  is the Bohm quantum potential,

$$Q[\rho_T] = -\frac{\hbar^2}{2m} \frac{1}{\sqrt{\rho_T}} \frac{\partial^2}{\partial x^2} \sqrt{\rho_T}. \quad (30)$$

The energy average is computed by sampling  $\rho_T(x)$  over a set of trial points  $\{x_i\}$  and then moving the trial points along the conjugate gradient of

$$E(x) = V_1(x) + Q[\rho_T](x). \quad (31)$$

After each conjugate gradient step, a new set of  $\mathbf{c}_n$  coefficients are determined according to an expectation maximization criteria such that the new trial density provides the best  $N$ -Gaussian approximation to the actual probability distribution function sampled by the new set of trial points. The procedure is repeated until  $\delta\langle E \rangle = 0$ . In doing so, we simultaneously minimize the energy and optimize the trial function. Since the ground state is assumed to be node-less, we will not encounter the singularities and numerical instabilities associated with other Bohmian equations of motion based approaches. [16–21] Moreover, the approach has been extended to very high-dimensions and to finite temperature by Derrickson and Bittner in their studies of the structure and thermodynamics of rare gas clusters with up to 130 atoms. [22, 23]

#### IV. TEST CASE: TUNNELING IN A DOUBLE WELL POTENTIAL

As a non-trivial test case, consider the tunneling of a particle between two minima of a symmetric double potential well. One can estimate the tunneling splitting using semi-classical techniques by assuming that the ground and excited states are given by the approximate form

$$\psi_{\pm} = \frac{1}{\sqrt{2}}(\phi_o(x) \pm \phi_o(-x)) \quad (32)$$

where  $\phi_o$  is the lowest energy state in the right-hand well in the limit the wells are infinitely far apart. From this, one can easily estimate the splitting as [24]

$$\delta = 4 \frac{\hbar^2}{m} \phi_o(0) \phi_o'(0) \quad (33)$$

If we assume the localized states ( $\phi_o$ ) to be gaussian, then

$$\psi_{\pm} \propto \frac{1}{\sqrt{2}}(e^{-\beta(x-x_o)^2} \pm e^{-\beta(x+x_o)^2}) \quad (34)$$

and we can write the superpotential as

$$W = \sqrt{\frac{2}{m}} \hbar \beta (x - x_o \tanh(2xx_o\beta)). \quad (35)$$

From this, one can easily determine both the original potential and the partner potential as

$$V_{1,2} = W^2 \pm \frac{\hbar}{\sqrt{2m}} W' \quad (36)$$

$$\begin{aligned} &= \frac{\beta^2 \hbar^2}{m} (2(x - x_o \tanh(2xx_o\beta))^2 \\ &\pm (2x_o^2 \operatorname{sech}^2(2xx_o\beta) - 1)) \end{aligned} \quad (37)$$

While the  $V_1$  potential has the characteristic double minima giving rise to a tunneling doublet, the SUSY partner potential  $V_2$  has a central dimple which in the limit of  $x_o \rightarrow \infty$  becomes a  $\delta$ -function which produces an unpaired and node-less ground state. [3] Using Eq. 9, one obtains  $\psi_1^{(1)} = \psi_- \propto A^\dagger \psi_o^{(2)}$  which now has a single node at  $x = 0$ .

For a computational example, we take the double well potential to be of the form

$$V_1(x) = ax^4 + bx^2 + E_o. \quad (38)$$

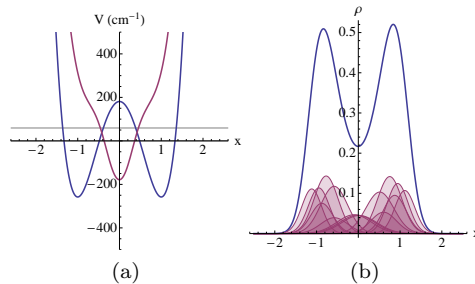


FIG. 2: (a) Model double well potential(blue) and partner potential (purple). The energies of the tunneling doublets are indicated by the horizontal lines at  $V = 0 \text{ cm}^{-1}$  and  $V = 59.32 \text{ cm}^{-1}$  indicating the positions of the sub-barrier tunneling doublet. (b) Final ground state density (blue) superimposed over the Gaussians used in its expansion. (purple) (From Ref.[25])

with  $a = 438.9 \text{ cm}^{-1}/(\text{bohr}^2)$ ,  $b = 877.8 \text{ cm}^{-1}/(\text{bohr})^4$ , and  $E_o = -181.1 \text{ cm}^{-1}$  which (for  $m = m_H$ ) gives rise to exactly two states at below the barrier separating the two minima with a tunneling splitting of  $59.32 \text{ cm}^{-1}$  as computed using a discrete variable representation (DVR) approach.[26] For the calculations reported here, we used  $n_p = 1000$  sample points and  $N = 15$  Gaussians and in the expansion of  $\rho_T(x)$  to converge the ground state. This converged the ground state to  $1 : 10^{-8}$  in terms of the energy. This is certainly a bit of an overkill in the number of points and number of gaussians since far fewer DVR points were required to achieve comparable accuracy (and a manifold of excited states). The numerical results, however, are encouraging since the accuracy of generic Monte Carlo evaluation would be  $1/\sqrt{n_p} \approx 3\%$  in terms of the energy. [52] Plots of  $V_1$  and the converged ground state is shown in 2.

The partner potential  $V_2 = W^2 + \hbar W'/\sqrt{2m}$ , can be constructed once we know the superpotential,  $W(x)$ . Here, we require an accurate evaluation of the ground state density and its first two log-derivatives. The advantage of our computational scheme is that one can evaluate these analytically for a given set of coefficients. In 2a we show the partner potential derived from the ground-state density. Whereas the original  $V_1$  potential exhibits the double well structure with minima near  $x_o = \pm 1$ , the  $V_2$  partner potential has a pronounced dip about  $x = 0$ . Consequently, its ground-state should have a simple “gaussian”-like form peaked about the origin.

Once we determined an accurate representation of the partner potential, it is now a trivial matter to re-introduce the partner potential into the optimization routines. The ground state converges easily and is shown in 3a along with its gaussians. After 1000 CG steps, the converged energy is within 0.1% of the exact tunneling splitting for this model system. Again, this is an order of

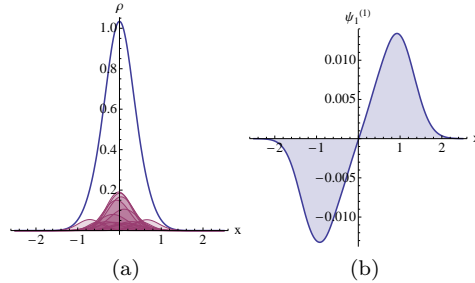


FIG. 3: (a) Ground state density of the partner Hamiltonian  $H_2$  (blue) superimposed over its individual Gaussian components. (b) Excited state  $\psi_1^{(1)}$  derived from the ground state of the partner potential,  $\psi_o^{(2)}$ . (From Ref.[25])

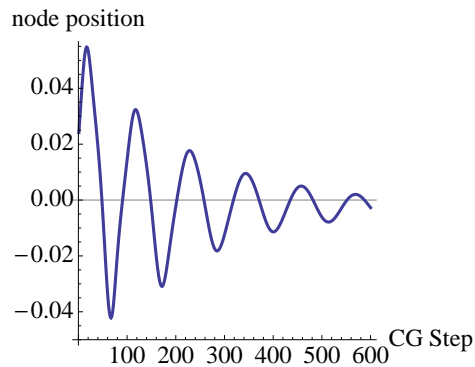


FIG. 4: Location of excited state node for the last 600 CG steps. (From Ref.[25])

magnitude better than the  $1/\sqrt{n_p}$  error associated with a simple Monte Carlo sampling. Furthermore, 3b shows  $\psi_1^{(1)} \propto A^\dagger \psi_o^{(2)}$  computed using the converged  $\rho_0^{(2)}$  density. As anticipated, it shows the proper symmetry and nodal position.

By symmetry, one expects the node to lie precisely at the origin. However, since we have not imposed any symmetry restriction or bias on our numerical method, the position of the node provides a sensitive test of the convergence of the trial density for  $\rho_0^{(2)}$ . In the example shown in Fig.4, the location of the node oscillates about the origin and appears to converge exponentially with number of CG steps. This is remarkably good considering that this is ultimately determined by the quality of the 3rd and 4th derivatives of  $\rho_o^{(1)}$  that appear when computing the conjugate gradient of  $V_2$ . We have tested this approach on a number of other one-dimensional bound-state problems with similar success.

## V. EXTENSION OF SUSY TO MULTIPLE DIMENSIONS.

While SUSY-QM has also been explored for one dimensional, non-relativistic quantum mechanical problems[3, 27–31], thus far these studies have focused on the formal aspects and on obtaining exact, analytical solutions for the ground state for specific classes of problems. In several recent papers[15, 25, 32, 33], we have begun exploring the SUSY-QM approach as the basis of a general computational scheme for bound state problems. Our initial studies have been restricted to one dimensional systems (for which there are, obviously, many powerful computational methods). In our first paper, we found that SUSY-QM (combined with a new periodic version of the Heisenberg-Weyl algebra) yields a robust, natural way to treat an infinite family of hindered rotors.[33] Next we showed that the SUSY-QM leads to a general treatment of an infinite family of anharmonic oscillators, such that highly accurate excited state energies and wave functions could be obtained variationally using significantly smaller basis sets than a traditional variational approach requires[15]. Most recently , we have considered a 1-D double well potential in which we solved for the ground state energy and wave function using a VQMC approach. Then using SUSY-QM, we (numerically) generated an auxiliary Hamiltonian whose *nodeless* ground state is iso-spectral (degenerate) with the first excited state of the original system Hamiltonian. This ground state was also easily determined by VQMC, yielding excellent accuracy for the first excited state energy. [25] Even more significant, by using the charge operators naturally generated in the SUSY-QM approach, we also obtained excellent accuracy for the first excited state wave function. Furthermore, at no point did impose a fixed node or symmetry on the excited state wave function and our calculation only involved working with a nodeless ground state.

Of course, all this begs the question: Can this approach be generalized to higher numbers of dimensions and to more than a single particle? There has been substantial effort in the past to do just this.[3, 28–30, 34–45] However, to date, no such generalization has been found that is able to generate all the excited states and energies even for so simple a system as a pair of separable, 1-D harmonic oscillators (HO) or equivalently, for a separable 2-D single HO. In our most recent, unpublished work [32], we have succeeded in obtaining such a generalization and showed that it does, in fact, yield the correct analytical results for separable and non-separable problems. In the next section, we present a succinct summary of our approach. The major question now is whether this formalism provides a basis for a robust, computational method for determining excited state energies and wave functions for large, strongly correlated systems using either QMC or variational algorithms applied solely to nodeless ground state problems.

### A. Difficulties in extending beyond one dimension

To move beyond one dimensional SUSY, Ioffe and coworkers have explored the use of higher-order charge operators [42, 43, 46, 47], and Kravchenko has explored the use of Clifford algebras[48]. Unfortunately, this is difficult to do in general. The reason being that the Riccati factorization of the one-dimensional Schrödinger equation does not extend easily to higher dimensions. One remedy is write the charge operators as vectors  $\vec{A} = (+\vec{\partial} + \vec{W})$  and with  $\vec{A}^\dagger = (-\vec{\partial} + \vec{W})^\dagger$  as the adjoint charge operator. The original Schrödinger operator is then constructed as an inner-product

$$H_1 = \vec{A}^\dagger \cdot \vec{A}. \quad (39)$$

Working through the vector product produces the Schrödinger equation

$$H_1\phi = (-\nabla^2 + W^2 - (\vec{\nabla} \cdot \vec{W}))\phi = 0 \quad (40)$$

and a Riccati equation of the form

$$U(x) = W^2 - \vec{\nabla} \cdot \vec{W}. \quad (41)$$

For a 2d harmonic oscillator, we would obtain a vector superpotential of the form

$$\vec{W} = -\frac{1}{\psi_0^{(1)}} \vec{\nabla} \psi_0^{(1)} = (x, y) = (W_x, W_y) \quad (42)$$

Let us look more closely at the  $\vec{\nabla} \cdot \vec{W}$  part. If we use the form that  $\vec{W} = -\vec{\nabla} \ln \psi$ , then  $-\vec{\nabla} \cdot \vec{\nabla} \ln \psi = -\nabla^2 \ln \psi$  which for the 2D oscillator results in  $\vec{\nabla} \cdot \vec{W} = 2$ . Thus,

$$W^2 - \vec{\nabla} \cdot \vec{W} = (x^2 + y^2) - 2 \quad (43)$$

which agrees with the original symmetric harmonic potential. Now, we write the scaled partner potential as

$$U_2 = W^2 + \vec{\nabla} \cdot \vec{W} = (x^2 + y^2) + 2. \quad (44)$$

This is equivalent to the original potential shifted by a constant amount.

$$U_2 = U_1 + 4. \quad (45)$$

The ground state in this potential would be have the same energy as the states of the original potential with quantum numbers  $n + m = 2$ . Consequently, even with the this naïve factorization, one can in principle obtain excitation energies

for higher dimensional systems, but there is no assurance that one can reproduce the entire spectrum of states.

The problem lies in the fact that neither Hamiltonian  $H_2$  nor its associated potential  $U_2$  is given correctly by the form implied by Eq. 40 and Eq. 44. Rather, the correct approach is to write the  $H_2$  Hamiltonian as a *tensor* by taking the outer product of the charges  $\vec{H}_2 = \vec{A}\vec{A}^+$  rather than as a scalar  $\vec{A} \cdot \vec{A}^+$ . At first this seems unwieldy and unlikely to lead anywhere since the wave function solutions of

$$\vec{H}_2\vec{\psi} = E\vec{\psi} \quad (46)$$

are now vectors rather than scalars. However, rather than adding an undue complexity to the problem, it actually simplifies matters considerably. As we demonstrate in a forthcoming paper, this tensor factorization preserves the SUSY algebraic structure and produces excitation energies for any  $n$ -dimensional SUSY system. Moreover, this produces a scalar  $\mapsto$  tensor  $\mapsto$  scalar hierarchy as one moves to higher excitations.[32]

## B. Vector SUSY

We now give a brief summary of our new generalization of SUSY-QM to treat higher dimensionality and more than one particle. Previous attempts generally involved introducing additional, “spin-like” degrees of freedom.[29, 30, 37–40, 42, 43, 46, 47, 49] In our approach, we make use of a vectorial technique that can deal simultaneously with either higher dimensions or more than one particle. In fact, the two problems are dealt with in exactly the same manner. Therefore, for simplicity, we consider a general  $n$ -dimensional distinguishable particle system with orthogonal coordinates  $\{x_\mu\}$ . The Hamiltonian is given by [53]

$$H = -\nabla^2 + V_0(x_1, \dots, x_n) \quad (47)$$

and the nodeless ground state satisfies the Schrödinger equation,

$$H\psi_0^{(1)} = E_0^{(1)}\psi_0^{(1)}. \quad (48)$$

We now define a “vector super-potential”,  $\vec{W}_1$ , with components

$$W_{1\mu} = -\frac{\partial}{\partial x_\mu} \ln \psi_0^{(1)}. \quad (49)$$

Then it is easily seen that the original Hamiltonian can be recast as

$$H_1 = (-\nabla + \vec{W}_1) \cdot (\nabla + \vec{W}_1) = \vec{Q}_1^+ \cdot \vec{Q}_1 \quad (50)$$

where the  $\vec{Q}_1$  and  $\vec{Q}_1^+$  are multi-dimensional generalizations of the SUSY charge operators from Eq. ???. This defines our “sector-1” (or “boson”) Hamiltonian and Eq.(48) can be written as [54]

$$H_1\psi_0^{(1)} = E_0^{(1)}\psi_0^{(1)} \quad (51)$$

One can show that the vector superpotential is related to the original (scalar) potential via:

$$V_0 = \vec{W}_1 \cdot \vec{W}_1 - \nabla \cdot \vec{W}_1. \quad (52)$$

The various components of the charge operators,  $\vec{A}_1$  and  $\vec{A}_1^+$  are defined by

$$A_{1\mu} = \frac{\partial}{\partial x_\mu} + W_{1\mu} \quad \& \quad A_{1\mu}^+ = -\frac{\partial}{\partial x_\mu} + W_{1\mu}. \quad (53)$$

Note that since these are associated with orthogonal degrees of freedom, the charge operators can be applied either by individual components or in vector form.

Next, consider the Schrödinger equation for the first excited state of  $H$ . We can write this using the charge operators as

$$H_1\psi_1^{(1)} = E_1^{(1)}\psi_1^{(1)} = (\vec{A}_1^+ \cdot \vec{A}_1 + E_0^{(1)})\psi_1^{(1)} \quad (54)$$

We apply  $\vec{A}_1$  to Equation (9):

$$(\vec{A}_1\vec{A}_1^+) \cdot \vec{A}_1\psi_1^{(1)} = (E_1^{(1)} - E_1^{(0)})\vec{A}_1\psi_1^{(1)} \quad (55)$$

Here we identify  $(\vec{A}_1\vec{A}_1^+)$  as a new, auxiliary Hamiltonian. It is important to note that this is constructed from the outer or tensor product of the charge operators rather than from inner or dot product as used in constructing  $H_1$ . Its eigenvector,  $\vec{A}_1\psi_1^{(1)}$ , is isospectral with the excited state,  $\psi_1^{(1)}$  of  $H_1$  ( since  $E_0^{(1)}$  is known, determining  $(E_1^{(1)} - E_1^{(0)})$  yields  $E_1^{(1)}$  ). We therefore define the **tensor** Hamiltonian for the second sector as

$$\overleftrightarrow{H}_2 = \vec{A}_1\vec{A}_1^+ \quad (56)$$

and **vector** state function as

$$\vec{\psi}_0^{(2)} = \frac{1}{(E_1^{(1)} - E_1^{(0)})}\vec{A}_1\psi_1^{(1)}. \quad (57)$$

It is easy to show that the ground state energy of  $\overleftrightarrow{H}_2$  is related to the first excitation energy of the original Hamiltonian

$$E_0^{(2)} = E_1^{(1)} - E_1^{(0)}. \quad (58)$$



Furthermore, the ground state of  $\overleftarrow{H}_2$  is also **nodeless**. This has been explicitly shown to be true for the separable 2-particle HOs considered earlier[32]. Therefore, we propose to apply both the VQMC and the standard variational methods to determine  $E_0^{(2)}$  and  $\vec{\psi}_0^{(2)}$ . Of course, knowing the second sector ground state energy also gives us the first excited state energy of the original Hamiltonian (Eq. (58)). Furthermore, we form the scalar product of

$$\overleftarrow{H}_2 \cdot \vec{\psi}_0^{(2)} = E_0^{(2)} \vec{\psi}_0^{(2)} \quad (59)$$

with  $\vec{A}_1^+$  obtaining

$$(\vec{A}_1^+ \cdot \vec{A}_1) \vec{A}_1^+ \vec{\psi}_0^{(2)} = E_0^{(2)} \vec{A}_1^+ \cdot \vec{\psi}_0^{(2)} \quad (60)$$

Clearly, this is exactly

$$H_1(\vec{A}_1^+ \cdot \vec{\psi}_0^{(2)}) = E_1^{(1)}(\vec{A}_1^+ \cdot \vec{\psi}_0^{(2)}) \quad (61)$$

so we can conclude that

$$\psi_1^{(1)} = \frac{1}{\sqrt{E_0^{(2)}}} (\vec{A}_1^+ \cdot \vec{\psi}_0^{(2)}) \quad (62)$$

Thus we also obtain the excited state wave function without any significant additional computational effort. This is because applying the charge operator is much simpler than solving an eigenvalue problem (it is a strictly linear operation). Evidence from our 1-D studies indicates that the accuracy of the excited states obtained using the SUSY-QM charge operator is significantly higher, for a given basis set, than what is obtained variationally (or with QMC) from the original Hamiltonian[15, 32]. This procedure can be continued as follows. We define a sector-2 vector super-potential with components

$$W_{2\mu} = \frac{\partial}{\partial x_\mu} \ln \psi_{0\mu}^{(2)} \quad (63)$$

Then it follows that

$$\vec{A}_2 \cdot \vec{\psi}_0^{(2)} = (\nabla + \vec{W}_2) \cdot \psi_0^{(2)} = 0 \quad (64)$$

so we can write

$$\overleftarrow{H}_2 = \vec{A}_2^+ \vec{A}_2 + E_0^{(2)} \mathbf{I} \quad (65)$$

and Eq. (59) is still satisfied. We form the scalar product of  $\vec{A}_2$  with the first excited state Schrödinger equation to obtain

$$(\vec{A}_2 \cdot \vec{A}_2^+) \vec{A}_2 \cdot \vec{\psi}_1^{(2)} = E_1^{(2)} \vec{A}_2 \cdot \vec{\psi}_1^{(2)} \quad (66)$$

Then we define the sector 3 *scalar* Hamiltonian by

$$H_3 = \vec{A}_2 \cdot \vec{A}_2^+ + E_0^{(2)} \quad (67)$$

with the ground state wave equation

$$H_3 \psi_0^{(3)} = E_0^{(3)} \psi_0^{(3)}. \quad (68)$$

It is easily seen that  $E_0^{(3)} = E_1^{(2)} - E_0^2$ . This procedure continues until all bound states of the original Hamiltonian are exhausted. It should also be clear that the sector 2 excited state wave function is obtained from the nodeless sector 3 ground state by applying  $\vec{A}_2^+$  to it. Then the second excited state for sector 1 results from taking the scalar product of  $\vec{A}_1^+$  with  $\vec{\psi}_1^{(2)}$ . The approach thus leads to an alternating sequence of scalar and tensor Hamiltonians, *but in all cases we need only determine nodeless ground states.*

There are two additional aspects of the tensor sector problem that require discussion. First we consider the validity of the Rayleigh-Ritz variational principle. It is easily seen from Eq. (56) that  $\overleftrightarrow{H}_2$  is a Hermitian operator. Therefore, its eigenspectrum is real and its eigenvectors are complete. With these facts in hand, the proof of the variational principle follows the standard one in every detail. This is also true for the Hylleraas-Undheim theorem.

Second, the QMC method is also directly applicable to the tensor sector problem. For the example discussed above, we note that the energy is given by

$$E_{trial} = \frac{\int d\tau \vec{\psi}_{trial} \cdot \overleftrightarrow{H}_2 \cdot \vec{\psi}_{trial}}{\int d\tau \vec{\psi}_{trial} \cdot \vec{\psi}_{trial}} \quad (69)$$

We next note that the integral can be expanded in terms of its components as

$$E_{trial} = \frac{\sum_{\mu\nu} \int d\tau (\psi_{\mu,trial} H_{2,\mu\nu} \psi_{\nu,trial})}{\sum_{\mu} \int d\tau (\psi_{\mu,trial})^2}. \quad (70)$$

It is then clear that each separate integral can be evaluated by QMC. For example, the  $\mu \neq \nu$  cross term is divided and multiplied by

$$\psi_{\mu,trial} \int d\tau \psi_{\nu,trial} \psi_{\mu,trial}. \quad (71)$$

Then the sampling is done relative to the mixed probability distribution,

$$P_{\mu\nu} = \frac{\psi_{\mu,trial} \psi_{\nu,trial}}{\int d\tau \psi_{\mu,trial} \psi_{\nu,trial}}. \quad (72)$$

A similar expression applies to each term in the energy expression and the evaluation would need to be performed self-consistently.

Thus far, we have developed a formalism that appears to be suitable for extending the SUSY-QM technique to higher dimensional systems. We believe the approach we have outlined above will provide the mathematical basis for a number of potentially interesting theoretical results. Moreover, we anticipate that when combined with either variational or Monte Carlo methods, our multi-dimensional extension of SUSY-QM will facilitate the calculation of accurate excitation energies and excited state wave functions.

## VI. OUTLOOK

I presented a number of avenues we are actively pursuing with the goal of using SUSY-QM or SUSY-inspired-QM to solve problems that are difficult to solve using more conventional approaches. In addition to what I have discussed here we are exploring the use of the Riccati equation to solve quantum scattering problems. It is as if one of the co-authors of this paper (DJK) has come full-circle since one of his first papers concerned solving the Hamilton-Jacobi for the action integral in quantum scattering, [50][55]

$$iS/\hbar = - \int_{r_o}^r W(r') dr'.$$

The integrand in this last equation is the SUSY super-potential. Furthermore, there is a connection between our work and the complex-valued quantum trajectories studied by Wyatt and Tannor and their respective co-workers.

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- [51] Our notation from here on is that  $\psi_n^{(m)}$  denotes the  $n$ th state associated with the  $m$ th partner Hamiltonian with similar notion for related quantities such as energies and superpotentials.
- [52] In our implementation, the sampling points are only used to evaluate the requisite integrals and they themselves are adjusted along a conjugate gradient rather than by resampling. One could in principle forego this step entirely and optimize the parameters describing the gaussians directly.
- [53] Our units are such that  $\hbar^2/2m = 1$ .
- [54] In analogy with the original descriptions of SUSY, we refer to the partner pairs as “boson” and “fermion” sectors or less poetically as “sector-1”, “sector 2”, and so forth.

[55] Coincidentally, Ref. [50] appeared in the J. Chem. Phys. issue immediately before the birthday of the other author of this paper. There appears to be some interesting Karma at work here.