

Supersymmetric Quantum Mechanics for a General Family of Anharmonic Oscillator Models

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In this paper we consider a general family of anharmonic oscillator models. Using the supersymmetric (SUSY) form of quantum mechanics, we obtain the exact, analytic ground states for a general family of anharmonic systems. We give the general, factorized form of the Hamiltonian for the hierarchy that arises in SUSY theory. The sector or “charge” operators convert states among the sectors. We illustrate the approach with two specific anharmonic oscillator models. Using the ground states of the second and third sector Hamiltonians, we show that the corresponding excited states and wave functions of the first sector are accurately obtained by applying the charge operators, using significantly smaller basis sets than are required in a standard variational approach applied to the original Schrödinger equation.

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I. INTRODUCTION

One-dimensional, anharmonic oscillator models are useful for a variety of problems in chemistry and physics. Examples include intra-molecular vibration [1] and oscillators in solid state physics [2]. Many such systems are modeled using polynomial potentials[3-4] and the eigenstates and eigenenergies are typically computed using the variational principle or perturbation theory. There is also a long history of using the ladder operator techniques for solving quantum mechanics problems (e.g. the harmonic oscillator, the hydrogen atom, angular momentum[5-12], etc). Some years ago, a systematic study of this approach to quantum mechanics led to a general formulation known as “supersymmetric” quantum mechanics

(SUSY-QM)[13-17]. In this approach, a so-called “superpotential” was introduced, in terms of which the Hamiltonian could be factored, leading to the SUSY generalization of the ladder operators. The approach has proved useful in many areas of theoretical physics [13-17]; however, so far as we are aware, it has not been applied in theoretical chemistry. In recent papers, we have explored consequences of minimizing the Heisenberg uncertainty product subject to the constraints of periodicity[18]. Most recently, we have considered this for periodic systems. This led us to a natural SUSY-QM approach to hindered rotor systems. Of course, hindered rotation is similar to anharmonic vibration, and consequently we explore the SUSY-QM technique for such systems in this paper.

This paper is organized as follows. In section II, we present a brief introduction to SUSY-QM. In section III, we formulate a general treatment of a family of anharmonic oscillators. In section IV, we specialize to two specific examples of anharmonic oscillator models in order to illustrate the approach. In section V we examine these systems computationally and compare our results with the standard, variational QM approach solutions.

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Finally, in section VI we present our conclusions.

II. INTRODUCTION TO THE HIERARCHICAL HAMILTONIAN FORMULATION OF SUSY QUANTUM MECHANICS

In SUSY quantum mechanics (QM), one introduces operators that result in a factored Hamiltonian [13]. In certain cases, these correspond to raising (or “creation”) and lowering (or annihilation) operators, but in general, the charge operators transfer among sets of isospectral eigenstates. In fact, it is possible to develop a hierarchy of factored Hamiltonians (one for each bound state of the original system). It is this aspect of SUSY QM that we shall take advantage of for a variational approach to determine accurate excited state energies and wave functions.

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 [13]:

$$\psi_0^1(x) = N e^{-\int_0^x W(x) dx}. \quad (\text{II.1})$$

The relationship between the superpotential W and the physical interaction $V(x)$ results from assuming that Eq(II.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,

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_0^1}{dx^2} + V_1 \psi_0^1 = 0 \quad (\text{II.2})$$

We easily see that

$$W_1 = -\frac{\frac{d\psi_0^1}{dx}}{\psi_0^1} = -\frac{d}{dx} \ln \psi_0^1 \quad (\text{II.3})$$

It is readily verified that the Riccati equation for W_1 is

$$-\frac{\hbar^2}{2m} \left[W_1^2(x) - \frac{dW_1}{dx} \right] + V_1 = 0 \quad (\text{II.4})$$

and, if W_1 is known, V_1 is given by

$$V_1(x) = \frac{\hbar^2}{2m} \left(W_1^2(x) - \frac{dW_1}{dx} \right) \quad (\text{II.5})$$

It is then evident that

$$-\frac{d^2 \psi_0^1}{dx^2} + \left(W_1^2(x) - \frac{dW_1}{dx} \right) \psi_0^1 = 0 \quad (\text{II.6})$$

However, the Hamiltonian operator now can be factored in the form

$$-\frac{d^2}{dx^2} + W_1^2(x) - \frac{dW_1}{dx} = \left[-\frac{d}{dx} + W_1(x) \right] \left[\frac{d}{dx} + W_1(x) \right] \quad (\text{II.7})$$

We define the “charge” operator

$$Q_1 = \frac{d}{dx} + W_1 \quad (\text{II.8})$$

and its adjoint is then given by (assuming W_1 is hermitian)

$$Q_1^\dagger = -\frac{d}{dx} + W_1 \quad (\text{II.9})$$

Then the “first sector” Hamiltonian is defined as

$$H_1 = Q_1^\dagger Q_1 \quad (\text{II.10})$$

A “second sector” Hamiltonian is defined as

$$H_2 = Q_1 Q_1^\dagger \quad (\text{II.11})$$

We note that in principle, one might expect the ground state of H_2 to be given by $\psi_0^1(x) = N e^{+\int_0^x W_1(x) dx}$. For an unbounded domain, this will not be normalizable, since we already know that $\psi_0^1(x) = N e^{-\int_0^x W_1(x) dx}$ is L^2 . The eigenspectra of H_1 and H_2 are positive semi-definite.

Let ψ_n^1 be an eigenstate of H_1 with energy $E_n \neq 0$. Then it follows that for $n > 0$, (since for $n = 0$, $E_0 = 0$),

$$Q_1^\dagger Q_1 \psi_n^1 = E_n^1 \psi_n^1 \quad (\text{II.12})$$

We then apply Q_1 to the equation, to obtain

$$Q_1 Q_1^\dagger (Q_1 \psi_n^1) = E_n^1 Q_1 \psi_n^1 \quad (\text{II.13})$$

Thus, $Q_1 \psi_n^1$ is an eigenstate of H_2 with the same energy, E_n^1 , as the state ψ_n^1 . Similarly, consider the eigenstates of H_2 :

$$H_2 \psi_n^2 = Q_1 Q_1^\dagger \psi_n^2 = E_n^2 \psi_n^2, \quad (\text{II.14})$$

which implies that $Q_1^\dagger \psi_n^2$ is an eigenstate of H_1 :

$$(Q_1^\dagger Q_1)(Q_1^\dagger \psi_n^2) = E_n^2 Q_1^\dagger \psi_n^2 \quad (\text{II.15})$$

It follows that the hamiltonians H_1 and H_2 have identical

spectra (with the possible 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

$$Q_1^\dagger Q_1 \psi_0^1 = 0 \quad (\text{II.16})$$

which shows that the quantity

$$Q_1 \psi_0^1 \quad (\text{II.17})$$

cannot be used to generate the ground state of the second sector. Indeed, Eq II.16 indicates that ψ_0^2 vanishes 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

$$Q_1 Q_1^\dagger \psi_n^2 = E_n^2 \psi_n^2 \quad (\text{II.18})$$

Then

$$Q_1^\dagger Q_1 (Q_1^\dagger \psi_{n+1}^1) = E_{n+1}^1 (Q_1^\dagger \psi_{n+1}^1) \quad (\text{II.19})$$

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

So

$$E_n^2 = E_{n+1}^1 \quad (\text{II.20})$$

and we conclude that

$$\psi_n^2 = \frac{Q_1 \psi_{n+1}^1}{\sqrt{E_{n+1}^1}} \quad (\text{II.21})$$

and

$$\psi_{n+1}^1 = \frac{Q_1^\dagger \psi_n^2}{\sqrt{E_n^2}} \quad (\text{II.22})$$

Then

$$Q_1 \psi_{n+1}^1 = \sqrt{E_{n+1}^1} \psi_n^2 \quad (\text{II.23})$$

From these expressions, it follows that

$$Q_1^\dagger Q_1 \psi_{n+1}^1 = \sqrt{E_{n+1}^1} Q_1^\dagger \psi_n^2 \quad (\text{II.24})$$

$$= \sqrt{E_{n+1}^1} \sqrt{E_n^2} \psi_n^1 \quad (\text{II.25})$$

$$= E_{n+1}^1 \psi_n^1 \quad (\text{II.26})$$

which shows again that

$$E_{n+1}^1 = E_n^2 \quad (\text{II.27})$$

The source of the degeneracy of H_1 and H_2 is the intertwining relation,

$$Q_1 H_1 = H_2 Q_1 \quad (\text{II.28})$$

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

$$W_2 = -\frac{d}{dx} \ln \psi_0^2 \quad (\text{II.29})$$

It is then clear that we can define an alternate form for H_2 , given by

$$H_2 = Q_2^\dagger Q_2 + E_0^2 \quad (\text{II.30})$$

Where

$$Q_2 = \frac{d}{dx} + W_2 \quad (\text{II.31})$$

We observe that ψ_0^2 is automatically an eigenstate of this form for H_2

$$H_2 \psi_0^2 = E_0^2 \psi_0^2 \quad (\text{II.32})$$

since

$$Q_2 \psi_0^2 \equiv 0. \quad (\text{II.33})$$

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

$$H_2 \psi_1^2 = E_1^2 \psi_1^2 \quad (\text{II.34})$$

We apply Q_2 to eq II.34 to find

$$(Q_2 Q_2^\dagger + E_0^2) Q_2 \psi_1^2 = E_n^2 Q_2 \psi_1^2 \quad (\text{II.35})$$

Then, by similar reasoning, we deduce that

$$Q_2 \psi_1^2 = \sqrt{E_1^2 - E_0^2} \psi_0^3. \quad (\text{II.36})$$

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

$$H_3 = Q_2 Q_2^\dagger + E_0^2, \quad (\text{II.37})$$

with ground state equation

$$H_3 \psi_0^3 = E_1^3 \psi_0^3 \quad (\text{II.38})$$

We then observe that by applying Q_2^\dagger to eq (II.38) gives

$$\left[(Q_2^\dagger Q_2 + E_0^2) \right] Q_2^\dagger \psi_0^3 = E_0^3 Q_2^\dagger \psi_0^3 \quad (\text{II.39})$$

We then conclude that Q_2^\dagger satisfies the intertwining relationship

$$Q_3^\dagger H_3 = H_2 Q_2^\dagger. \quad (\text{II.40})$$

It follows that

$$Q_2^\dagger \psi_0^3 = \sqrt{E_1^2 - E_0^2} \psi_1^2 \quad (\text{II.41})$$

and using (II.37),

$$Q_2 Q_2^\dagger \psi_0^3 = (E_1^2 - E_0^2) \psi_0^3 = E_0^3 \psi_0^3 \quad (\text{II.42})$$

Thus, we conclude that

$$E_0^3 = E_1^2 - E_0^2 \quad (\text{II.43})$$

This procedure can be continued by defining the third superpotential, W_3 , as

$$W_3 = -\frac{d}{dx} \ln \psi_0^3. \quad (\text{II.44})$$

The charge operators are

$$Q_3 = \frac{d}{dx} + W_3 \quad (\text{II.45})$$

and

$$Q_3^\dagger = -\frac{d}{dx} + W_3. \quad (\text{II.46})$$

It is then easy to express H_3 in terms of the third sector charge operators:

$$H_3 = Q_3^\dagger Q_3 + E_0^3 \quad (\text{II.47})$$

The first excited state equation for the third sector is then

$$H_3 \psi_1^3 = E_1^3 \psi_1^3 \quad (\text{II.48})$$

so that

$$Q_3 Q_3^\dagger \psi_1^3 = (E_1^3 - E_0^3) \psi_1^3. \quad (\text{II.49})$$

We then apply Q_3 to the above equation to find

$$(Q_3 Q_3^\dagger) Q_3 \psi_1^3 = E_1^3 Q_3 \psi_1^3. \quad (\text{II.50})$$

Then the fourth sector Hamiltonian is defined as

$$H_4 = Q_3 Q_3^\dagger + E_0^3 \quad (\text{II.51})$$

and the groundstate equation for sector four is

$$H_4 \psi_0^4 = E_0^4 \psi_0^4 = (E_1^3 - E_0^3) \psi_0^4. \quad (\text{II.52})$$

One deduces also the next intertwining relation

$$Q_3 H_3 = H_4 Q_3 \quad (\text{II.53})$$

with the isospectral relation being

$$E_0^4 = E_1^3 - E_0^3. \quad (\text{II.54})$$

Clearly, the different sector wave functions result from the application of the charge operators:

$$Q_3 \psi_1^3 = \sqrt{E_1^3 - E_0^3} \psi_0^4, \quad (\text{II.55})$$

$$Q_3^\dagger \psi_0^4 = \sqrt{E_0^4} \psi_1^3. \quad (\text{II.56})$$

It is clear that this procedure can be continued until one exhausts the number of bound states supported by H_1 . We also see that determining the excited state energies and wave functions for H_1 involves solving for the ground state energies and wave functions for each sector Hamiltonian, H_j , $j > 1$

III. A SUSY QM FAMILY OF ANHARMONIC OSCILLATORS

The main system of interest in this paper is the anharmonic oscillator which is ubiquitous in chemistry. For

example, all nuclear vibrations in molecules are anharmonic, with the effect increasing as the vibrational energy gets closer to the dissociation limit [REFS]. Anharmonicity also results from 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

$$W(x) = \sum_{j=0}^J d_j x^{2j+1} \quad (\text{III.1})$$

Then the corresponding sector 1 potential, $V_1(x)$, is

$$V_1(x) = \sum_{j=0}^J \sum_{j'=0}^J d_j d_{j'} x^{2(j+j'+1)} - \sum_{j=0}^J d_j (2j+1) x^{2j} \quad (\text{III.2})$$

The ‘‘charge’’ operators are given by

$$Q_1 = \frac{d}{dx} + W_1 \quad (\text{III.3})$$

and

$$Q_1^\dagger = -\frac{d}{dx} + W_1 \quad (\text{III.4})$$

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

$$\psi_0^+(x) = N e^{-\sum_{j=0}^J \frac{d_j x^{2j+1}}{(2j+1)}} \quad (\text{III.5})$$

We stress that contrary to the periodic case, the solution of the sector two equation,

$$Q_1^\dagger \psi_0^2(x) = 0 \quad (\text{III.6})$$

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

$$Q_1 Q_1^\dagger \psi_0^2(x) = E_0^2 \psi_0^2(x) = E_1^1 \psi_0^2(x) \quad (\text{III.7})$$

where

$$E_1^1 \neq 0 \quad (\text{III.8})$$

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

$$Q_1^\dagger \psi_0^2(x) = \sqrt{E_0^2} \psi_1^1(x) \quad (\text{III.9})$$

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 . Thus,

$$\psi_0^1(x) = N \prod_{j=0}^J e^{-\frac{d_j x^{2j+1}}{(2j+1)}}, \quad (\text{III.10})$$

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

$$d_j d_{j'} x^{2(j+j'+1)}, \quad j \neq j' \quad (\text{III.11})$$

In fact, even more general anharmonic oscillators can be dealt with. Thus, any function, $g(x)$ can be added to $W(x)$ in Eq (III.1), provided only that $e^{-\int_0^x g(x') dx'}$ is L^2 . Thus, not only polynomial anharmonic potentials can be treated but many others. Of course, the resulting potential will involve added terms such as $g^2(x)$, along with cross products of $g(x)$ with $W(x)$ of Eq. (III.1), and also $\frac{dg}{dx}$.

IV. TWO EXAMPLE ANHARMONIC OSCILLATOR SYSTEMS

We now consider two examples of anharmonic oscillators. In the following section we will explore the computational aspects of the anharmonic oscillator, using these systems. To illustrate this approach to polynomial anharmonic oscillation we define $W(\varphi)$ to be

$$W_1(x) = x^3 + 2x, \quad (\text{IV.1})$$

which obviously yields a potential for the first sector of

$$V_1(x) = x^6 + 4x^4 + x^2 - 2. \quad (\text{IV.2})$$

It should be noted that x is defined on the domain $-\infty < x < \infty$.

We can thus define H_1 as:

$$H_1 = \left[-\frac{d}{dx} + W_1(x) \right] \left[\frac{d}{dx} + W_1(x) \right] \quad (\text{IV.3})$$

which satisfies the equation

$$H_1 \psi(x)_0^{(1)} = 0 \quad (\text{IV.4})$$

and possesses an analytic ground state wave function of

$$\psi_0^{(1)} = N e^{-\left(\frac{x^4}{4} + x^2\right)}. \quad (\text{IV.5})$$

To get the second hamiltonian in the hierarchy we next define H_2 as

$$H_2 = \left[\frac{d}{dx} + W_1(x) \right] \left[-\frac{d}{dx} + W_1(x) \right] \quad (\text{IV.6})$$

so

$$V_2 = x^6 + 4x^4 + 7x^2 + 2 \quad (\text{IV.7})$$

and we must solve the equation

$$H_2\psi_0^{(2)} = E_0^{(2)}\psi_0^{(2)}. \quad (\text{IV.8})$$

Possessing $\psi_0^{(2)}$, we may develop the next hamiltonian in the hierarchy. To do so, we begin by expressing H_2 in the following form

$$H_2 = \left[-\frac{d}{dx} + W_2(x) \right] \left[\frac{d}{dx} + W_2(x) \right] + E_0^{(2)} \quad (\text{IV.9})$$

where

$$W_2(x) = -\frac{d}{dx} \ln \psi_0^{(2)}. \quad (\text{IV.10})$$

It should be obvious that

$$Q_2 H_2 \psi_1^{(2)} = E_1^{(2)} Q_2 \psi_1^{(2)} \quad (\text{IV.11})$$

leading to

$$Q_2 Q_2^\dagger Q_2 \psi_1^{(2)} = (E_1^{(2)} - E_0^{(2)}) Q_2 \psi_1^{(2)} \quad (\text{IV.12})$$

with

$$\psi_0^{(3)} = \frac{Q_2 \psi_1^{(2)}}{\sqrt{E_1^{(2)} - E_0^{(2)}}}. \quad (\text{IV.13})$$

It should be noted that from this point, one can obviously generate as many hamiltonians as needed. It should also be noted that the excited states can be obtained by using the charge operators we have previously defined.

The second example results from taking

$$W(x) = x^3 + x + e^x. \quad (\text{IV.14})$$

In this case,

$$V_1(x) = x^6 + 2x^4 + 2x^3 e^x + 2x e^x + x^2 + e^{2x} - 3x^2 - e^x - 1 \quad (\text{IV.15})$$

Then

$$H_1 = \left[-\frac{d}{dx} + x^3 + x + e^x \right] \left[\frac{d}{dx} + x^3 + x + e^x \right] \quad (\text{IV.16})$$

with

$$H_1 \psi_0^1 = 0 \quad (\text{IV.17})$$

and the analytical ground state is

$$\psi_0^{(1)} = N e^{-\left(\frac{x^4}{4} + x^2 + e^x\right)}. \quad (\text{IV.18})$$

Then the second sector Hamiltonian is

$$H_1 = \left[\frac{d}{dx} + x^3 + x + e^x \right] \left[-\frac{d}{dx} + x^3 + x + e^x \right] \quad (\text{IV.19})$$

The ground state satisfies

$$H_2 \psi_0^2 = E_0^2 \psi_0^2 \quad (\text{IV.20})$$

which must be solved numerically. However, having ψ_0^2 , one then obtains

$$W_2(x) = -\frac{d}{dx} \ln \psi_0^{(2)}. \quad (\text{IV.21})$$

and

$$H_3 = \left[\frac{d}{dx} + W_2(x) \right] \left[-\frac{d}{dx} + W_2(x) \right] \quad (\text{IV.22})$$

This procedure is continued until the bound states of H_1 are exhausted.

V. COMPUTATIONAL CONSIDERATIONS FOR THE ANHARMONIC OSCILLATOR

We now turn to illustrate this approach as a computational scheme to obtain excited states of anharmonic oscillators. 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. This, however, is unattractive for higher energy states because they require a much larger basis to converge to the same error. To remedy this situation, we present a method to decrease the size of basis sets required in the sum for convergence via a hierarchy of hamiltonians.

To demonstrate our computational scheme, we investigate the first example system from the previous section. For this potential (Eq. IV.2), exact solutions are known for all states of H_1 . We use the exact results to assess the accuracy of the variational calculations. For all variational calculations, we use the harmonic oscillator basis functions where:

$$\phi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-\frac{x^2}{2}}, \quad (\text{V.1})$$

with each matrix element determined using

$$\int_{-\infty}^{\infty} \phi(x)_n x^j \phi(x)_n dx. \quad (\text{V.2})$$

Using the hierarchy of hamiltonians, we present the converged eigenvalues in Table I. In Table I, all energies were obtained for each of the Hamiltonians, H_1 , H_2 , and H_3 by standard variational calculations using a basis set of 75 ϕ_n 's. It is easily seen that the n-levels of H_2 are degenerate with the corresponding (n-1)-levels of H_1 , and the n-levels of H_3 are degenerate with the (n-1)-levels of H_2 and with the (n-2)-levels of H_1 . This results from the intertwining relations. The energies are accurate to five significant figures (here, $E_0^1 = 6.721e - 5$ is a "numerical zero"). 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 II. Clearly, excited state wave functions require substantially larger basis sets to achieve a high degree of accuracy. In Table III 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 H_2 and H_3 . Again, N denotes the basis set required, and ΔN is the reduction of basis set achieved by use of the charge operators.

To find the solutions we used both BLAS routines to find these eigenvalues and vectors and GSL routines for numerical integration. Clearly, the use of the hierarchy of hamiltonians and the use of charge operators provides rapid convergence. which provides us with better methods to calculate the excited states.

We performed the same 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

$$\int_{-\infty}^{\infty} |N\psi_n -_{N-1}\psi_n|^2 dx, \quad (\text{V.3})$$

where N is the basis size. This system is non-trivial since no analytic solutions are possible. In Table IV, we give the converged energy levels (again to 5 significant figures) obtained by standard variational calculations applied to H_1 , H_2 , and H_3 . In Table V, we show the basis set sizes needed in standard variational calculations to converge the wave functions for H_1 , H_2 , and H_3 . In Table V, we show the basis set sizes needed in standard variational calculations to converge the wave functions for H_1 , H_2 , and H_3 (again, the Cauchy criterion of convergence was used.) Finally, in Table VI, we show the results for excited states obtained using the charge operators applied to the ground states of H_2 and H_3 . Again, ΔN shows the reduction in the basis size gained by the charge operator approach.

VI. CONCLUSIONS

Because of the importance of anharmonic oscillator models to a wide variety of problems in both chemistry and physics, we sought to develop more efficient methods to solve for excited states of general families of both such systems. 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. The crucial feature of the approach is that via charge operators, we obtain accurate excited state wave functions from the ground states of the hierarchy Hamiltonians. 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 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.

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TABLE I: Energies for the Anharmonic Polynomic Oscillator using Hierarchy of Hamiltonians. N = 75

n	H_1	H_2	H_3
0	6.721e-05	5.0251	11.705
1	5.0251	11.705	19.520
2	11.705	19.520	28.344
3	19.520	28.344	40.384
4	28.344	40.384	56.627

TABLE II: Wave function errors for the Anharmonic Polynomic Oscillator using the standard variational method for each hierarchy Hamiltonian.

n	$N\psi_0^n$	L_2	L_∞
0	$61\psi_0^1$	5.859e-4	4.440e-16
1	$152\psi_1^1$	9.355e-4	6.661e-16
2	$261\psi_2^1$	9.627e-4	9.463e-16
0	$58\psi_0^2$	4.647e-4	7.77e-16
1	$133\psi_1^2$	3.077e-4	8.210e-16
0	$67\psi_0^3$	3.135e-4	2.220e-15

TABLE III: Wave function errors for the Anharmonic Polynomic Oscillator using Charge Operators to find excited states

n	ΔN	$N\psi_0^n$	L_2	L_∞
1	61	$91\psi_1^1$	9.507-4	7.768e-16
2	126	$135\psi_2^1$	4.657e-4	8.777e-16
1	45	$88\psi_1^2$	5.468e-4	6.789e-16

TABLE IV: Energies for the Anharmonic Non-Polynomic Oscillator using Hierarchy of Hamiltonians, determined variationally. N = 80

n	H_1	H_2	H_3
0	5.327e-05	5.2761	12.8341
1	5.2765	12.8341	24.484
2	12.833	24.484	54.2624
3	24.484	54.2624	101.685
4	54.2624	101.685	247.094

TABLE V: Errors for the Anharmonic Non-Polynomic Oscillator wave functions using Hierarchy of Hamiltonians all determined variationally.

n	$N\psi_0^n$	L_2	L_∞
0	$59\psi_0^1$	7.426e-4	6.661e-16
1	$168\psi_1^1$	9.355e-4	1.045e-16
2	$303\psi_2^1$	7.779e-4	1.758e-16
0	$61\psi_0^2$	4.364e-4	2.220e-16
1	$139\psi_1^2$	2.112e-4	1.636e-16
0	$79\psi_0^3$	7.257e-4	4.207e-15

TABLE VI: 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

n	ΔN	$N\psi_0^n$	L_2	L_∞
1	60	$108\psi_1^1$	5.263-4	7.768e-16
2	136	$167\psi_2^1$	9.776e-4	8.777e-16
1	40	$99\psi_1^2$	2.5264e-4	6.789e-16