

Multidimensional Supersymmetric Quantum Mechanics: Spurious States for the Tensor Sector Two Hamiltonian

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ABSTRACT: We show that there exist spurious states for the sector two tensor Hamiltonian in multidimensional supersymmetric quantum mechanics. For one-dimensional supersymmetric quantum mechanics on an infinite domain, the sector one and two Hamiltonians have identical spectra with the exception of the ground state of the sector one. For tensorial multidimensional supersymmetric quantum mechanics, there exist normalizable spurious states for the sector two Hamiltonian with energy equal to the ground state energy of the sector one. These spurious states are annihilated by the adjoint charge operator, and hence, they do not correspond to physical states for the original Hamiltonian. The Hermitian property of the sector two Hamiltonian implies the orthogonality between spurious and physical states. In addition, we develop a method for construction of a specific form of the spurious states for any quantum system and also generate several spurious states for a two-dimensional anharmonic oscillator system and for the hydrogen atom.

One-dimensional SUSY QM		Multidimensional SUSY QM	
H_1	H_2	H_1	\tilde{H}_2
$\psi_3^{(1)}$ —————	—————	$\psi_3^{(1)}$ —————	————— $\tilde{\psi}_2^{(2)}$
$\psi_2^{(1)}$ —————	—————	$\psi_2^{(1)}$ —————	————— $\tilde{\psi}_1^{(2)}$
$\psi_1^{(1)}$ —————	—————	$\psi_0^{(2)}$ —————	————— $\tilde{\psi}_0^{(2)}$
$\psi_0^{(1)}$ —————		$\psi_0^{(1)}$ ————— $\tilde{\psi}_{sp}$

I. INTRODUCTION

Supersymmetric quantum mechanics (SUSY-QM) has been developed as an elegant analytical approach to one-dimensional problems. The SUSY-QM formalism grew out of an effort to generalize the ladder operator approach used in the treatment of the harmonic oscillator. The ladder operator technique has been utilized to solve quantum mechanics problems including the Morse oscillator¹ and the radial hydrogen atom equation.² The result of a systematic study of this approach to quantum mechanics led to the SUSY-QM approach.^{3–7} In analogy with the harmonic oscillator Hamiltonian, the factorization of a one-dimensional Hamiltonian can be achieved by introducing charge operators. A hierarchy of isospectral sector Hamiltonians can be constructed using the charge operators. For example, the sector two Hamiltonian is isoenergetic with the spectrum of the original Hamiltonian except possibly for the original ground state. On infinite domains, the ground state of the sector two one-dimensional Hamiltonian is degenerate with the first excited state of the original Hamiltonian. The SUSY charge operators can be used to convert the ground state wave function of the sector two Hamiltonian into the first excited state wave function of the sector one Hamiltonian.

In our previous studies, we have explored the use of SUSY-QM as a computational tool for calculating accurate excited state energies and wave functions.^{8,9} Using the isospectral property of the SUSY sector Hamiltonians, we can apply

various methods specifically designed for the ground state to the SUSY sector Hamiltonians to obtain excited state energies and wave functions of the original Hamiltonian. For one-dimensional systems, the variational Monte Carlo scheme⁸ and the Rayleigh–Ritz variational method⁹ have been applied to the SUSY sector Hamiltonians to obtain higher accuracy and more rapid convergence for excited state energies and wave functions for the original Hamiltonian.

In addition, several studies have been devoted to the generalization of one-dimensional SUSY-QM to multidimensional systems. Ioffe and collaborators have explored the use of higher-order derivative charge operators,^{10–13} and Kravchenko has explored the use of Clifford algebras.¹⁴ For the most part, these methods have involved the introduction of new spin-like variables. Moreover, we provided a generalization of SUSY-QM to treat any number of dimensions or particles using a tensorial operator approach.¹⁵ We demonstrated that the structure of the degeneracies between sector Hamiltonians makes it possible to achieve progress in more accurate calculations of excited state energies and wave functions. Related issues associated with generating a SUSY-QM hierarchy beyond the tensor sector two Hamiltonian have been discussed.^{16,17} Stedman has described a

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similar treatment for multidimensional systems and presented his equations for the hydrogen atom, but he has not solved any of the higher sector equations, and his sector two Hamiltonian possesses spurious states that do not have any connection with the original physical Hamiltonian.¹⁸

For one-dimensional SUSY-QM on an infinite domain, the sector one and two Hamiltonians have identical spectra with the exception of the ground state of the sector one. For our tensorial approach to multidimensional SUSY-QM, the correspondence between the eigenstates of the sectors one and two except for the ground state of the sector one is established through the intertwining relations between the charge operators and the sector Hamiltonians. However, in the current study, we show that there exist spurious states for the sector two Hamiltonian with energy equal to the ground state energy of the sector one. Even for infinite domains, contrary to our previous intuition, these spurious states are normalizable! These normalizable spurious states are annihilated by the adjoint charge operator, and the corresponding sector one states vanish. Therefore, they do not correspond to physical states for the original Hamiltonian and are therefore spurious.

In addition, we prove the orthogonality between spurious and physical states due to the Hermitian property of the sector two Hamiltonian. Furthermore, we provide an explicit method for construction of the spurious states in a specific form for any quantum system. Several specific spurious states are constructed for a two-dimensional anharmonic oscillator system and for the hydrogen atom. It is emphasized that we do not prove that all possible spurious states can be expressed in the specific form. However, this specific expression provides a straightforward method to generate spurious states for any quantum system. Thus, there exists an infinite number of spurious states for the sector two tensor Hamiltonian.

The organization of the remainder of this study is as follows. In section II, we briefly review salient features of one-dimensional SUSY-QM and present our new formulation of the vectorial approach to multidimensional SUSY-QM. In section III, spurious states for the sector two Hamiltonian are discussed. In section IV, we develop an approach to construction of a specific form of the spurious states and generate several spurious states for a two-dimensional anharmonic oscillator system and for the hydrogen atom. In section V, we summarize our results and conclude with some comments.

II. THEORETICAL FORMULATION

A. One-Dimensional Supersymmetric Quantum Mechanics. For one-dimensional SUSY-QM, the superpotential W is defined in terms of the ground state wave function by the Riccati substitution

$$\psi_0^{(1)}(x) = C \exp\left[-\int_0^x W_1(x') dx'\right] \quad (1)$$

where C is the normalization constant. The superscript “(1)” on the wave function and the subscript “1” on the superpotential indicate that the ground state wave function and the superpotential are associated with the sector one Hamiltonian. It is assumed that eq 1 solves the Schrödinger equation with energy equal to zero

$$-\frac{d^2\psi_0^{(1)}}{dx^2} + V_1\psi_0^{(1)} = 0 \quad (2)$$

where, for convenience, we set $\hbar = 2m = 1$ throughout this study. Setting the ground state energy to zero does not impose any restriction since the energy can be changed by adding any constant to the Hamiltonian. From eq 1, the superpotential can be expressed in terms of the ground state wave function by

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

Substituting eq 1 into the Schrödinger equation in eq 2, we obtain the Riccati equation for the superpotential

$$\frac{dW_1(x)}{dx} - W_1^2(x) + V_1(x) = 0 \quad (4)$$

On the other hand, if W_1 is known, then V_1 is given by

$$V_1(x) = W_1(x)^2 - \frac{dW_1(x)}{dx} \quad (5)$$

Obviously, the Schrödinger equation in eq 2 is equivalent to

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

The Hamiltonian operator can be factorized by introducing the charge operator and its adjoint (assuming W_1 is hermitian; i.e., $\psi_0^{(1)}$ is real)

$$Q_1 = \frac{d}{dx} + W_1 \quad (7)$$

$$Q_1^\dagger = -\frac{d}{dx} + W_1 \quad (8)$$

Then, the sector one Hamiltonian is defined as $H_1 = Q_1^\dagger Q_1$. Since $E_0^{(1)} = 0$ for $n = 0$, it follows from the Schrödinger equation that for $n > 0$

$$Q_1^\dagger Q_1 \psi_n^{(1)} = E_n^{(1)} \psi_n^{(1)} \quad (9)$$

where $\psi_n^{(1)}$ is an eigenstate of H_1 with $E_n^{(1)} \neq 0$. Applying Q_1 to this equation, we obtain

$$H_2(Q_1 \psi_n^{(1)}) = Q_1 Q_1^\dagger (Q_1 \psi_n^{(1)}) = E_n^{(1)} (Q_1 \psi_n^{(1)}) \quad (10)$$

where the sector two Hamiltonian is defined as $H_2 = Q_1 Q_1^\dagger$. Thus, $Q_1 \psi_n^{(1)}$ is an eigenstate of H_2 with the same energy $E_n^{(1)}$ as the state $\psi_n^{(1)}$. Analogously, we consider the eigenstates of H_2

$$H_2 \psi_n^{(2)} = Q_1 Q_1^\dagger \psi_n^{(2)} = E_n^{(2)} \psi_n^{(2)} \quad (11)$$

Applying Q_1^\dagger to this equation, we notice that $Q_1^\dagger \psi_n^{(2)}$ is an eigenstate of H_1

$$H_1(Q_1^\dagger \psi_n^{(2)}) = (Q_1^\dagger Q_1)(Q_1^\dagger \psi_n^{(2)}) = E_n^{(2)} (Q_1^\dagger \psi_n^{(2)}) \quad (12)$$

It follows that the Hamiltonians H_1 and H_2 have identical spectra with the possible exception of the ground state with $E_0^{(1)} = 0$. Additionally, for the ground state, $Q_1 \psi_0^{(1)} = 0$, and this shows that the quantity $Q_1 \psi_0^{(1)}$ cannot be used to generate the ground state of the sector two Hamiltonian. Because of the uniqueness of the ground state with $E_0^{(1)} = 0$, the indexing of the first and second sector levels must be modified. It is clear that the eigenvalues and eigenfunctions of the two Hamiltonians H_1 and H_2 are related by

$$E_n^{(2)} = E_{n+1}^{(1)} \quad E_0^{(1)} = 0 \quad \psi_n^{(2)} = \frac{Q_1 \psi_{n+1}^{(1)}}{\sqrt{E_{n+1}^{(1)}}}$$

$$\psi_{n+1}^{(1)} = \frac{Q_1^\dagger \psi_n^{(2)}}{\sqrt{E_n^{(2)}}}$$

Analogously, starting from H_2 whose ground state energy is $E_0^{(2)} = E_1^{(1)}$, we can generate the sector three Hamiltonian H_3 as a SUSY partner of H_2 . This procedure can be continued until the number of bound excited states supported by H_1 is exhausted.

B. Multidimensional Supersymmetric Quantum Mechanics. In our previous studies,^{8,9,15} SUSY-QM has been extended to multidimensional systems involving any number of distinguishable particles. We employed a vectorial approach that simultaneously treats more than one dimension and any number of distinguishable particles. In our original formulation,¹⁵ we defined an orthogonal hyperspace of dimension $3n$ for a system of n particles in three-dimensional space. However, this formulation fails to treat multielectron systems correctly such as the helium atom. Thus, in the current study, we present a new formulation for generalization of SUSY to multidimensional systems, and the introduction of the hyper-dimensional coordinate frames has been completely eliminated.

The Hamiltonian of an N particle system is given by

$$H_1 = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 + V_1 \quad (13)$$

where one has a complete set of orthogonal eigenstates $\{\psi_n^{(1)}\}$ and energies $\{E_n^{(1)}\}$ for $n = 0, 1, 2, \dots$. For simplicity, we set the masses of the particles to be equal and use units such that $\hbar^2/2m = 1$. In order to factorize the Hamiltonian into the sector one SUSY form, we introduce a matrix notation so that the kinetic energy can be expressed as

$$-\sum_{i=1}^N \nabla_i^2 = (-\vec{\nabla}_1, -\vec{\nabla}_2, \dots, -\vec{\nabla}_N) \cdot \begin{pmatrix} \vec{\nabla}_1 \\ \vec{\nabla}_2 \\ \vdots \\ \vec{\nabla}_N \end{pmatrix} \equiv \vec{\nabla}^\dagger \cdot \vec{\nabla} \quad (14)$$

where

$$\vec{\nabla}_m = \hat{i} \frac{\partial}{\partial x_m} + \hat{j} \frac{\partial}{\partial y_m} + \hat{k} \frac{\partial}{\partial z_m}$$

for $m = 1, \dots, N$. Thus, the coordinates of all particles are referenced to a single three-dimensional Cartesian frame. This is a fundamental change from our original formulation,¹⁵ where we embedded a separate coordinate frame in each particle in the system. Now, all particle coordinates are measured relative to a single Cartesian reference frame.

In quantum mechanics, the ground-state wave function is a solution of the Schrödinger equation

$$H_1 \psi_0^{(1)} = E_0^{(0)} \psi_0^{(1)} \quad (15)$$

For a nodeless ground state, the exact ground state wave function can be written as

$$\psi_0^{(1)} = A e^{-S(\vec{u})} \quad (16)$$

where A is a normalization constant, $\vec{u} = (\vec{u}_1, \vec{u}_2, \dots, \vec{u}_N)$, and $\vec{u}_m = \hat{i}x_m + \hat{j}y_m + \hat{k}z_m$ for $m = 1, \dots, N$. Then, the vector superpotential \vec{W} can be defined by the exact differential

$$dS = \vec{W}(\vec{u}) \cdot d\vec{u} = (\vec{W}_1, \vec{W}_2, \dots, \vec{W}_N) \cdot \begin{pmatrix} d\vec{u}_1 \\ d\vec{u}_2 \\ \vdots \\ d\vec{u}_N \end{pmatrix} \quad (17)$$

We emphasize that it is crucial to define the superpotential \vec{W} in terms of a vector. It follows from this expression that the i th particle's superpotential is related to the ground state wave function by

$$\vec{W}_i = -\vec{\nabla}_i \ln \psi_0^{(1)} \quad (18)$$

Throughout this study, the ground state wave function is assumed to be purely real; hence, the superpotential components are real. From this equation, we can obtain $(\vec{\nabla} + \vec{W})\psi_0^{(1)} = 0$. In addition, the SUSY charge operator and its adjoint operator are defined by

$$\vec{Q} = \vec{\nabla} + \vec{W} = \begin{pmatrix} \vec{\nabla}_1 + \vec{W}_1 \\ \vdots \\ \vec{\nabla}_N + \vec{W}_N \end{pmatrix} \quad (19)$$

$$\vec{Q}^\dagger = (-\vec{\nabla}_1 + \vec{W}_1, \dots, -\vec{\nabla}_N + \vec{W}_N) \quad (20)$$

Then, we can write H_1 in terms of \vec{W} as

$$H_1 - E_0^{(1)} = \vec{Q}^\dagger \cdot \vec{Q} \quad (21)$$

Thus, the sector one Hamiltonian H_1 can be factorized by the SUSY charge operators

$$H_1 = \vec{Q}^\dagger \cdot \vec{Q} + E_0^{(1)} \quad (22)$$

It follows from eq 18 that the SUSY charge operator annihilates the ground state of the system, $\vec{Q}\psi_0^{(1)} = 0$, and this implies that $H_1\psi_0^{(1)} = E_0^{(1)}\psi_0^{(1)}$ as required.

Following the similar procedure in one-dimensional SUSY-QM, we can construct the sector two Hamiltonian such that it is isospectral with H_1 . For an excited state $\psi_n^{(1)}$ ($n \neq 0$) in the sector one satisfying the Schrödinger equation $H_1\psi_n^{(1)} = E_n^{(1)}\psi_n^{(1)}$, we write

$$[\vec{Q}^\dagger \cdot \vec{Q} + E_0^{(1)}]\psi_n^{(1)} = E_n^{(1)}\psi_n^{(1)} \quad (23)$$

Forming the tensor product by operating on the left with \vec{Q} , we obtain

$$[\vec{Q}\vec{Q}^\dagger + E_0^{(1)}\vec{1}]\vec{Q}\psi_n^{(1)} = E_n^{(1)}\vec{Q}\psi_n^{(1)} \quad (24)$$

It follows that $\vec{Q}\psi_n^{(1)}$ is an eigenstate of the sector two tensor Hamiltonian

$$\vec{H}_2 = \vec{Q}\vec{Q}^\dagger + E_0^{(1)}\vec{1} \quad (25)$$

with energy equal to $E_n^{(1)}$. Hence, for any of the excited states in the sector one Hamiltonian, $\vec{Q}\psi_n^{(1)}$ generates an eigenstate of the sector two Hamiltonian with the same energy. In particular, $\vec{Q}\psi_0^{(1)}$ cannot give an eigenstate with energy equal to the ground state energy $E_0^{(1)}$ because the SUSY charge operator annihilates the ground state, $\vec{Q}\psi_0^{(1)} = 0$.

On the other hand, we consider the eigen-equation for the sector two Hamiltonian

$$\vec{H}_2 \cdot \vec{\psi}_\lambda^{(2)} = E_\lambda^{(2)} \vec{\psi}_\lambda^{(2)} \quad (26)$$

where $\vec{\psi}_\lambda^{(2)} = (\vec{\psi}_{\lambda_1}^{(2)}, \vec{\psi}_{\lambda_2}^{(2)}, \dots, \vec{\psi}_{\lambda_N}^{(2)})^T$ is any column vector eigenfunction. Forming the scalar product of the sector two Hamiltonian with \vec{Q}^\dagger , we obtain

$$\vec{Q}^\dagger \cdot [\vec{Q} \vec{Q}^\dagger + E_0^{(1)} \vec{1}] \cdot \vec{\psi}_\lambda^{(2)} = E_\lambda^{(2)} \vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)} \quad (27)$$

Rearranging this equation yields

$$[\vec{Q}^\dagger \cdot \vec{Q} + E_0^{(1)}] (\vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)}) = E_\lambda^{(2)} (\vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)}) \quad (28)$$

From eq 22, we obtain $H_1(\vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)}) = E_\lambda^{(2)}(\vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)})$. Thus, $\vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)}$ is an eigenstate of the sector one Hamiltonian H_1 with energy $E_\lambda^{(2)}$ (provided it is normalizable).

As shown in the above analysis, for any of the excited states in the sector one Hamiltonian, $\vec{Q}\psi_n^{(1)}$ generates an eigenstate of the sector two Hamiltonian with the same energy. Analogously, for any of the eigenstates in the sector two Hamiltonian, $\vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)}$ generates an eigenstate of the sector one Hamiltonian with the same energy provided it is normalizable. The eigenstates of these two sectors are connected by the SUSY charge operator and its adjoint. As demonstrated in ref 15, the correspondence between the eigenstates of the sector one and two Hamiltonians except for the ground state of the sector one is established through the intertwining relation and its adjoint

$$\vec{Q} H_1 = \vec{H}_2 \cdot \vec{Q} \quad (29)$$

$$\vec{Q}^\dagger \cdot \vec{H}_2 = H_1 \vec{Q}^\dagger \quad (30)$$

Since the SUSY charge operator annihilates the ground state, $\vec{Q}\psi_0^{(1)} = 0$, \vec{H}_2 is isospectral with H_1 above the ground state of H_1 . In the one-dimensional case, additional sector Hamiltonians, H_3 , etc., can be constructed until all of the states of H_1 have been exhausted. However, up to now, this has not been possible for multidimensions,¹⁵ so we must restrict our consideration to \vec{H}_2 and H_1 . Related issues concerning generation of higher sector Hamiltonians have been pointed out in ref 16 and responded to in ref 17.

III. SPURIOUS STATES FOR MULTIDIMENSIONAL SUPERSYMMETRIC QUANTUM MECHANICS

A. One-Dimensional Case. We now further explore the situation for sector two eigenstates with eigenvalues equal to the sector one ground state energy. For one-dimensional SUSY-QM, the sector one Hamiltonian is expressed in terms of the SUSY charge operators by $H_1 = \vec{Q}_1^\dagger \vec{Q}_1 + E_0^{(1)}$. As indicated in eq 3, the charge operator annihilates the ground state of the system, $\vec{Q}_1 \psi_0^{(1)} = 0$. From this equation, we can obtain the ground state wave function in eq 1. In principle, we might expect that the ground state of the sector two Hamiltonian $H_2 = \vec{Q}_2 \vec{Q}_1^\dagger + E_0^{(1)}$ is annihilated by the adjoint charge operator, $\vec{Q}_1^\dagger \psi_0^{(2)} = 0$. However, this equation implies that the ground state is expressed in terms of W_1 by

$$\psi_0^{(2)}(x) = N \exp\left[\int_0^x W_1(x') dx'\right] \quad (31)$$

If the domain of the position is finite, it is generally possible that the ground state of the sector two Hamiltonian satisfies $\vec{Q}_1^\dagger \psi_0^{(2)} = 0$ with $E_0^{(2)} = E_0^{(1)}$.¹⁹ However, for an unbounded domain, since the ground state of H_1 in eq 1 is square-

integrable, the expression above is not normalized. Therefore, on infinite domains, the Hamiltonians H_1 and H_2 have identical spectra with the exception of the ground state of H_1 .

B. Multidimensional Case. As shown in section II.B, for any of the eigenstates in the sector two Hamiltonian $\vec{H}_2 = \vec{Q} \vec{Q}^\dagger + E_0^{(1)} \vec{1}$, $\vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)}$ generates an apparent eigenstate of the sector one Hamiltonian with the same energy. In particular, if there exists a normalizable vector function $\vec{\psi}$ such that $\vec{Q}^\dagger \cdot \vec{\psi} = 0$, then this function satisfies the vector Schrödinger equation for the sector two Hamiltonian

$$\vec{H}_2 \cdot \vec{\psi} = \vec{Q} \vec{Q}^\dagger \cdot \vec{\psi} + E_0^{(1)} \vec{1} \cdot \vec{\psi} = E_0^{(1)} \vec{\psi} \quad (32)$$

This equation indicates that the vector function $\vec{\psi}$ is an eigenstate of \vec{H}_2 with energy equal to the ground state of H_1 . Analogous to one-dimensional SUSY-QM, we might think that functions satisfying $\vec{Q}^\dagger \cdot \vec{\psi} = 0$ cannot be normalized, so that the ground state of \vec{H}_2 has the same energy as the first-excited state of H_1 . However, this is not the case for multidimensional SUSY-QM. Actually, there exist such vector functions that not only satisfy $\vec{Q}^\dagger \cdot \vec{\psi} = 0$ but that are also normalizable. The normalizable vector function $\vec{\psi}$ with N vector components implies that the sum of the integrals of the square of the absolute value for each component is finite

$$\int \vec{\psi}^* \cdot \vec{\psi} d\tau = \sum_{i=1}^N \int |\vec{\psi}_i|^2 d\tau < \infty \quad (33)$$

As an example, we consider a two-dimensional separable harmonic oscillator system, and the sector one Hamiltonian is given by eq 13 with $V(x,y) = x^2 + y^2 - 2$. For simplicity, we denote the coordinates by x and y instead of u_1 and u_2 . The analytical expression of the sector one ground state wave function with $E_0^{(1)} = 0$ is given by

$$\psi_0^{(1)}(x, y) = C \exp\left[-\frac{1}{2}(x^2 + y^2)\right] \quad (34)$$

where C is a normalization constant. Substituting this expression into eq 18 gives the corresponding vector superpotential, $W_1 = x$ and $W_2 = y$. Then, the sector two Hamiltonian is constructed from the charge operators in eqs 19 and 20

$$\begin{aligned} \vec{H}_2 &= \vec{Q} \vec{Q}^\dagger + E_0^{(1)} \vec{1} \\ &= \begin{pmatrix} -\frac{\partial^2}{\partial x^2} + x^2 + 1 & -\frac{\partial^2}{\partial x \partial y} + xy - x \frac{\partial}{\partial y} + y \frac{\partial}{\partial x} \\ -\frac{\partial^2}{\partial x \partial y} + xy - y \frac{\partial}{\partial x} + x \frac{\partial}{\partial y} & -\frac{\partial^2}{\partial y^2} + y^2 + 1 \end{pmatrix} \end{aligned} \quad (35)$$

For the sector one Hamiltonian H_1 , there are two degenerate first-excited states with $E_1^{(1)} = 2$

$$\psi_{(1,0)}^{(1)} \propto x e^{-(x^2+y^2)/2} \quad (36)$$

$$\psi_{(0,1)}^{(1)} \propto y e^{-(x^2+y^2)/2} \quad (37)$$

Applying the charge operator \vec{Q} to these two states, we obtain the doubly degenerate states for the sector two Hamiltonian \vec{H}_2

$$\vec{\psi}_{(0,1)}^{(2)} = \vec{Q} \psi_{(1,0)}^{(1)} \propto (e^{-(x^2+y^2)/2}, 0)^T \quad (38)$$

$$\vec{\psi}_{(0,2)}^{(2)} = \vec{Q} \psi_{(0,1)}^{(1)} \propto (0, e^{-(x^2+y^2)/2})^T \quad (39)$$

It is straightforward to show that $\vec{H}_2 \cdot \vec{\psi}_{(0)k}^{(2)} = E_0^{(2)} \vec{\psi}_{(0)k}^{(2)}$ with $E_0^{(2)} = 2$ where $k = 1$ or 2 . Originally, we expected that these two doubly degenerate states are the ground states of \vec{H}_2 because the charge operator annihilates the ground state of the sector one Hamiltonian $\vec{Q}\psi_0^{(1)} = 0$. However, if we consider a normalizable vector function

$$\vec{\psi} = (-y e^{-(x^2+y^2)/2}, x e^{-(x^2+y^2)/2})^T \quad (40)$$

then we find from eq 35 that $\vec{H}_2 \cdot \vec{\psi} = E_0^{(1)} \vec{\psi}$ because of $\vec{Q}^\dagger \cdot \vec{\psi} = 0$. This implies that the vector function is an eigenstate of the sector two Hamiltonian with energy equal to $E_0^{(1)} = 0$, which is lower than $E_0^{(2)} = 2$. Additionally, it is interesting to notice that both of the two components for this vector function have nodes. Thus, the two doubly degenerate states $\vec{\psi}_{(0)1}^{(2)}$ and $\vec{\psi}_{(0)2}^{(2)}$ are not the ground states of the sector two Hamiltonian. Furthermore, since the adjoint charge operator annihilates the vector function $\vec{Q}^\dagger \cdot \vec{\psi} = 0$, this function does not produce a corresponding physically allowed state for H_1 .

C. Orthogonality between Spurious and Physical States. Because the sector two Hamiltonian is Hermitian, eigenstates with different eigenvalues are orthogonal to each other. All the spurious states have lowest energy equal to the ground state energy of the sector one Hamiltonian, and hence they are orthogonal to all the physical states. We can explicitly prove the orthogonality between spurious and physical states of the sector two Hamiltonian. We consider the inner product of a spurious state with a physical state

$$I_{n,\lambda} = \int \vec{\psi}_n^{(2)} \cdot \vec{\psi}_\lambda^{(2)} d\tau \quad (41)$$

where n and λ denote the physical state and the spurious state, respectively. Expressing the physical state in terms of the sector one state and using the integration by parts, we obtain

$$I_{n,\lambda} = \int \vec{Q}\psi_{n+1}^{(1)} \cdot \vec{\psi}_\lambda^{(2)} d\tau = \int \psi_{n+1}^{(1)} \vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)} d\tau = 0 \quad (42)$$

where $\vec{Q}^\dagger \cdot \vec{\psi}_\lambda^{(2)} = 0$ has been used. Therefore, the vanishing inner product indicates that spurious states are orthogonal to physical states.

IV. SPURIOUS STATES OF A SPECIFIC FORM

A. Spurious States for Two-Dimensional Systems.

Although any normalizable vector function satisfying $\vec{Q}^\dagger \cdot \vec{\psi} = 0 = \psi^{(1)}$ is an eigenstate of \vec{H}_2 with energy equal to the ground state energy of H_1 , these vector functions do not yield corresponding normalizable, physically allowed states for H_1 . Hence, these functions are called spurious states. As shown in section III.B, the vector function in eq 40 is a spurious state of \vec{H}_2 for the two-dimensional separable harmonic oscillator system.

Actually, there exists a trivial spurious state for any two-dimensional system. We consider a two-dimensional system with the ground state wave function $\psi_0(x,y)$. From eq 18, we can obtain the two components of the superpotential $W_1 = -\partial \ln \psi_0 / \partial x$ and $W_2 = -\partial \ln \psi_0 / \partial y$. The trivial spurious state is given by

$$\vec{\psi}_{\text{sp}} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} -W_2 \psi_0 \\ W_1 \psi_0 \end{pmatrix} \quad (43)$$

Applying the adjoint charge operator to this state, we have

$$\begin{aligned} \vec{Q}^\dagger \cdot \vec{\psi}_{\text{sp}} &= -\frac{\partial}{\partial x}(-W_2 \psi_0) - W_1 W_2 \psi_0 - \frac{\partial}{\partial y}(W_1 \psi_0) + W_1 W_2 \psi_0 \\ &= \frac{\partial}{\partial x}(W_2 \psi_0) - \frac{\partial}{\partial y}(W_1 \psi_0) = -\frac{\partial^2}{\partial x \partial y} \psi_0 + \frac{\partial^2}{\partial x \partial y} \psi_0 = 0 \end{aligned} \quad (44)$$

where the relationship between the ground state wave function and the superpotential in eq 18 has been used. Therefore, we have shown that there exists a trivial spurious state in eq 43 for any two-dimensional system. In fact, the spurious state in eq 40 for the two-dimensional separable harmonic oscillator system is the trivial spurious state with $W_1 = x$ and $W_2 = y$.

Furthermore, we can construct an infinite family of spurious states for any two-dimensional system. We suppose a spurious state of the specific form

$$\vec{\psi}_{\text{sp}}(x, y) = \begin{pmatrix} \psi_1(x, y) \\ \psi_2(x, y) \end{pmatrix} = \begin{pmatrix} -f(x, y) \psi_0(x, y)^n \\ g(x, y) \psi_0(x, y)^n \end{pmatrix} \quad (45)$$

where n is a positive integer. Given arbitrary $u(x)$ and $v(y)$, $f(x,y)$ and $g(x,y)$ are determined by

$$f(x, y) = u(x) \left[(n+1)v(y)W_2(x, y) - \frac{\partial v(y)}{\partial y} \right] \quad (46)$$

$$g(x, y) = v(y) \left[(n+1)u(x)W_1(x, y) - \frac{\partial u(x)}{\partial x} \right] \quad (47)$$

It is straightforward to show that the spurious state expressed in this specific form satisfies the equation $\vec{Q}^\dagger \cdot \vec{\psi}_{\text{sp}} = 0$. Thus, we can easily construct a spurious state by assigning appropriate $u(x)$ and $v(y)$ to the specific expression in eq 45, so that the resulting spurious state is normalizable. As a special case, if we choose $n = 1$ and $u(x) = v(y) = 1/\sqrt{2}$, we recover the trivial spurious state in eq 43. In fact, we do not need to require n in eq 45 to be a positive integer. The number n can be any real, positive number such that the spurious state in eq 45 is normalizable.

As an example, we consider a two-dimensional nonseparable nondegenerate system with the ground state wave function given by

$$\psi_0(x, y) = C \exp[-2x^2y^2 - x^2 - x - \sqrt{2}y^2 - \sqrt{2}y] \quad (48)$$

where C is a normalization constant. The superpotential is given by

$$W_1(x, y) = 4xy^2 + 2x + 1 \quad (49)$$

$$W_2(x, y) = 4x^2y + 2\sqrt{2}y + \sqrt{2} \quad (50)$$

In this case, we choose $n = 2$, $u(x) = x^2$, and $v(y) = e^y$, and the two components for the spurious state in eq 45 become

$$\psi_1(x, y) = -x^2 e^y (12x^2y + 6\sqrt{2}y + 3\sqrt{2} - 1) \psi_0(x, y)^2 \quad (51)$$

$$\psi_2(x, y) = x e^y (12x^2y^2 + 6x^2 + 3x - 2) \psi_0(x, y)^2 \quad (52)$$

It is straightforward to check that the spurious state is normalizable and satisfies $\vec{Q}^\dagger \cdot \vec{\psi}_{\text{sp}} = 0$. Thus, more complicated spurious states can be readily constructed by assigning $u(x)$ and $v(y)$.

B. Spurious States in Higher Dimensions. Analogous to the two-dimensional case, trivial spurious states can be readily

constructed for three-dimensional systems. For a three-dimensional system with the ground state wave function $\psi_0(x,y,z)$, it follows from eq 18 that the three components of the superpotential are given by $W_1 = -\partial \ln \psi_0 / \partial x$, $W_2 = -\partial \ln \psi_0 / \partial y$, and $W_3 = -\partial \ln \psi_0 / \partial z$. The trivial spurious states for the three-dimensional system are expressed by

$$\vec{\psi}_{sp1} = (-W_2\psi_0, W_1\psi_0, 0)^T \quad (53)$$

$$\vec{\psi}_{sp2} = (-W_3\psi_0, 0, W_1\psi_0)^T \quad (54)$$

$$\vec{\psi}_{sp3} = (0, -W_3\psi_0, W_2\psi_0)^T \quad (55)$$

In a similar manner to eq 44, we can show that these states satisfy $\vec{Q}^\dagger \cdot \vec{\psi}_{sp} = 0$. Obviously, since \vec{Q}^\dagger is linear, any linear combination of spurious states yields another spurious state. Let $\vec{\psi}' = \vec{\psi}_{sp1} + \vec{\psi}_{sp2}$, and we obtain $\vec{Q}^\dagger \cdot \vec{\psi}' = \vec{Q}^\dagger \cdot \vec{\psi}_{sp1} + \vec{Q}^\dagger \cdot \vec{\psi}_{sp2} = 0$. Thus, $\vec{\psi}'$ is also a spurious state. Moreover, the specific expression in eq 45 used to construct spurious states for two-dimensional systems can also be employed to construct spurious states for three-dimensional systems. For example, we can obtain a spurious state by assigning $u(x)$ and $w(z)$

$$\vec{\psi}'(x, y, z) = \begin{pmatrix} \psi_1(x, y, z) \\ \psi_2(x, y, z) \\ \psi_3(x, y, z) \end{pmatrix} = \begin{pmatrix} -f(x, y, z)\psi_0(x, y, z)^n \\ 0 \\ h(x, y, z)\psi_0(x, y, z)^n \end{pmatrix} \quad (56)$$

where $f(x,y,z)$ and $h(x,y,z)$ are given by

$$f(x, y, z) = u(x) \left[(n+1)w(z)W_3(x, y, z) - \frac{\partial w(z)}{\partial z} \right] \quad (57)$$

$$h(x, y, z) = w(z) \left[(n+1)u(x)W_1(x, y, z) - \frac{\partial u(x)}{\partial x} \right] \quad (58)$$

We simply need to ensure that the spurious state is normalizable by choosing appropriate $u(x)$ and $w(z)$.

As an example, we consider the hydrogen atom, which is nonseparable in Cartesian coordinates. The ground state wave function is given by $\psi_0(x,y,z) = e^{-r}$ where $r = (x^2 + y^2 + z^2)^{1/2}$. Substituting the wave function into eq 18 gives the superpotential $W = (W_1, W_2, W_3) = (x/r, y/r, z/r)$. From eqs 53 and 54, we obtain several spurious states for the hydrogen atom

$$\vec{\psi}_{sp1} = \begin{pmatrix} -\frac{y}{r}e^{-r} \\ \frac{x}{r}e^{-r} \\ 0 \end{pmatrix}, \quad \vec{\psi}_{sp2} = \begin{pmatrix} -\frac{z}{r}e^{-r} \\ 0 \\ \frac{x}{r}e^{-r} \end{pmatrix},$$

$$\vec{\psi}' = \begin{pmatrix} -\frac{y+z}{r}e^{-r} \\ \frac{x}{r}e^{-r} \\ \frac{x}{r}e^{-r} \end{pmatrix}$$

where $\vec{\psi}' = \vec{\psi}_{sp1} + \vec{\psi}_{sp2}$. It is easy to show that these states satisfy the equation $\vec{Q}^\dagger \cdot \vec{\psi}_{sp} = 0$. Actually, more spurious states for the hydrogen atom can be obtained, and the method used in the

construction of spurious states can be extended to higher dimensions. As shown in Figure 1, for one-dimensional infinite

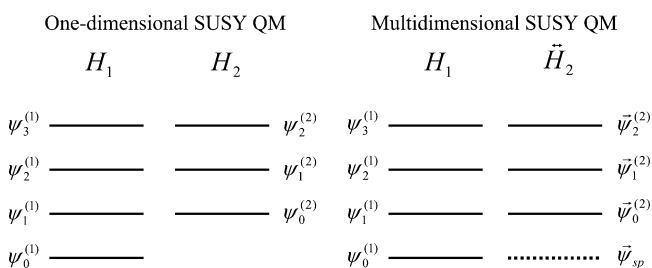


Figure 1. Comparison of one-dimensional and multidimensional SUSY-QM for the sector one and two Hamiltonians. For one-dimensional SUSY-QM, the sector one and two Hamiltonians have identical spectra with the exception of the ground state of the sector one. For multidimensional SUSY-QM, there are an infinite number of spurious states for the sector two Hamiltonian with energy equal to the ground state energy of the sector one Hamiltonian.

domain SUSY-QM, H_1 and H_2 have identical spectra with the exception of the ground state $\psi_0^{(1)}$. However, for infinite domain multidimensional SUSY-QM, there are an infinite number of spurious states for the sector two Hamiltonian \tilde{H}_2 with energy equal to the ground state energy of H_1 . In addition, we emphasize that it is not proved that all possible spurious states can be expressed in the specific form in eq 45. On the contrary, the expression in eq 45 provides one approach to the construction of the spurious states.

V. DISCUSSION AND CONCLUSIONS

We briefly reviewed one-dimensional SUSY-QM and presented our new formulation of the vector approach to multidimensional SUSY-QM. For one-dimensional infinite domain SUSY-QM, the sector one and two Hamiltonians have identical spectra with the exception of the ground state of the sector one. For multidimensional infinite domain SUSY-QM, the correspondence between the eigenstates of the sectors one and two except for the ground state of the sector one is established through the intertwining relations between the charge operators and the sector Hamiltonians. However, there exist spurious states for the sector two Hamiltonian with energy equal to the ground state energy of the sector one Hamiltonian. These normalizable spurious states are annihilated by the adjoint charge operator, and hence, these states do not generate normalizable, physical states for the sector one Hamiltonian. In addition, because the sector two Hamiltonian is Hermitian, all the spurious states are orthogonal to physical states.

Moreover, we presented a method for construction of the spurious states of a specific form for any quantum system. Several spurious states were constructed for a two-dimensional anharmonic oscillator system and for the hydrogen atom. Although it was not proved that all possible spurious states can be expressed in the specific form, this specific expression provides a straightforward method to generate spurious states for any quantum system. Thus, there exists an infinite family of spurious states for the sector two Hamiltonian.

In the companion article,²⁰ we show how one may avoid SUSY calculations in the tensor sector completely, so that all calculations are done using a scalar sector one SUSY Hamiltonian. In addition, the new approach totally eliminates any potential problems due to spurious sector two states.

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Notes

The authors declare no competing financial interest.

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REFERENCES

- (1) Jafarpour, M.; Afshar, D. Calculation of Energy Eigenvalues for the Quantum Anharmonic Oscillator with a Polynomial Potential. *J. Phys. A: Math. Gen.* **2002**, *35*, 87.
- (2) Liu, Y.; Lei, Y.; Zeng, J. Factorization of the Radial Schrödinger Equation and Four Kinds of Raising and Lowering Operators of Hydrogen Atoms and Isotropic Harmonic Oscillators. *Phys. Lett. A* **1997**, *231*, 9–22.
- (3) Infeld, L.; Hull, T. E. The Factorization Method. *Rev. Mod. Phys.* **1951**, *23*, 21–68.
- (4) Fernández C, D. J.; Hussin, V.; Nieto, L. M. Coherent States for Isospectral Oscillator Hamiltonians. *J. Phys. A: Math. Gen.* **1994**, *27*, 3547.
- (5) Mielnik, B. Factorization Method and New Potentials with Theoscillator Spectrum. *J. Math. Phys.* **1984**, *25*, 3387–3389.
- (6) Cooper, F.; Khare, A.; Sukhatme, U. *Supersymmetry in Quantum Mechanics*; World Scientific: Danvers, MA, 2002.
- (7) Gangopadhyaya, A.; Mallow, J. V.; Rasinariu, C. *Supersymmetric Quantum Mechanics: An Introduction*; World Scientific: Danvers, MA, 2010.
- (8) Kouri, D. J.; Markovich, T.; Maxwell, N.; Bittner, E. R. Supersymmetric Quantum Mechanics, Excited State Energies and Wave Functions, and the Rayleigh–Ritz Variational Principle: A Proof of Principle Study. *J. Phys. Chem. A* **2009**, *113*, 15257–15264.
- (9) Bittner, E. R.; Maddox, J. B.; Kouri, D. J. Supersymmetric Approach to Excited States. *J. Phys. Chem. A* **2009**, *113*, 15276–15280.
- (10) Andrianov, A. A.; Ioffe, M. V.; Spiridonov, V. P. Higher-Derivative Supersymmetry and the Witten Index. *Phys. Lett. A* **1993**, *174*, 273–279.
- (11) Andrianov, A. A.; Ioffe, M. V.; Nishnianidze, D. N. Polynomial SUSY in Quantum Mechanics and Second Derivative Darboux Transformations. *Phys. Lett. A* **1995**, *201*, 103–110.
- (12) Andrianov, A. A.; Ioffe, M. V.; Nishnianidze, D. N. Polynomial Supersymmetry and Dynamical Symmetries in Quantum Mechanics. *Theor. Math. Phys.* **1995**, *104*, 1129–1140.
- (13) Cannata, F.; Ioffe, M. V.; Nishnianidze, D. N. New methods for the Two-Dimensional Schrödinger Equation: SUSY-Separation of Variables and Shape Invariance. *J. Phys. A: Math. Gen.* **2002**, *35*, 1389–1404.
- (14) Kravchenko, V. V. On the Reduction of the Multidimensional Stationary Schrödinger Equation to a First-Order Equation and Its Relation to the Pseudoanalytic Function Theory. *J. Phys. A: Math. Gen.* **2005**, *38*, 851.
- (15) Kouri, D. J.; Maji, K.; Markovich, T.; Bittner, E. R. New Generalization of Supersymmetric Quantum Mechanics to Arbitrary Dimensionality or Number of Distinguishable Particles. *J. Phys. Chem. A* **2010**, *114*, 8202–8216.
- (16) Mandelshtam, V. A. Comment on “New Generalization of Supersymmetric Quantum Mechanics to Arbitrary Dimensionality or Number of Distinguishable Particles”. *J. Phys. Chem. A* **2011**, *115*, 948–949.
- (17) Kouri, D. J.; Maji, K.; Markovich, T.; Bittner, E. R. Reply to “Comment on ‘New Generalization of Supersymmetric Quantum Mechanics to Arbitrary Dimensionality or Number of Distinguishable Particles’”. *J. Phys. Chem. A* **2011**, *115*, 950.
- (18) Stedman, G. E. Simple Supersymmetry: II. Factorisation Method in Quantum Mechanics. *Eur. J. Phys.* **1985**, *6*, 225–231.

(19) Kouri, D. J.; Markovich, T.; Maxwell, N.; Bodmann, B. G. The Heisenberg–Weyl Algebra on the Circle and a Related Quantum Mechanical Model for Hindered Rotation. *J. Phys. Chem. A* **2009**, *113*, 7698–7705.

(20) Chou, C.-C.; Kouri, D. J. *J. Phys. Chem. A* **2013**, DOI: 10.1021/jp401068w.