Chapter 21

New System-Specific Coherent States by Supersymmetric Quantum Mechanics for Bound State Calculations

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1. Introduction

Supersymmetric quantum mechanics (SUSY-QM) has been developed as an elegant analytical approach to one-dimensional problems. The SUSY-QM formalism generalizes the ladder operator approach used in the treatment of the harmonic oscillator. In analogy with the harmonic oscillator Hamiltonian, the factorization of a one-dimensional Hamiltonian can be achieved by introducing "charge operators". For the one-dimensional harmonic oscillator, the charge operators are the usual raising and lowering operators. The SUSY charge operators not only allow the factorization of a one-dimensional Hamiltonian but also form a Lie algebra structure. This structure leads to the generation of isospectral SUSY partner Hamiltonians. The eigenstates of the various partner Hamiltonians are connected by application of the charge operators. As an analytical approach, the SUSY-QM approach has been utilized to study a number of quantum mechanics problems including the Morse oscillator ([16]) and the radial hydrogen atom equation ([24]). In addition, SUSY-QM has been applied to the discovery of new exactly solvable potentials, the development of a more accurate WKB approximation, and the improvement of large N expansions and variational methods ([7, 11]). Developments and applications of one-dimensional SUSY-QM can be found in relevant reviews and books ([7, 9, 11, 15, 26, 32, 33]). Recently, SUSY-QM has been developed as a computational tool to provide much more accurate excitation energies using the standard Rayleigh-Ritz variational method ([5, 19, 20]).

The harmonic oscillator is fundamental to a wide range of physics, including the electromagnetic field, spectroscopy, solid state physics, coherent state theory, and SUSY-QM.

The broad application of the harmonic oscillator stems from the raising and lowering ladder operators which are used to factor the system Hamiltonian. For example, canonical coherent states are defined as the eigenstates of the lowering operator of the harmonic oscillator, and they are also minimum uncertainty states which minimize the Heisenberg uncertainty product for position and momentum. In addition, several different approaches have been employed to study generalized and approximate coherent states for systems other than the harmonic oscillator ([3, 12, 17, 18, 27–31, 34, 37]). Furthermore, algebraic treatments have been applied to the extension of coherent states for shape-invariant systems ([1, 4, 8, 10]).

The lowering operator of the harmonic oscillator annihilates the ground state, and the ground state minimizes the Heisenberg uncertainty product. Conventional harmonic oscillator coherent states correspond to those states which minimize the position-momentum uncertainty relation. However, these harmonic oscillator coherent states are also constructed by applying shift operators labeled with points of the discrete phase space to the ground state of the harmonic oscillator, termed the "fiducial state" ([18]). Indeed, Klauder and Skagerstam choose to define coherent states in the broadest sense in precisely this manner ([21]). Analogously, the charge operator in SUSY-QM annihilates the ground state of the corresponding system. We therefore expect that the ground state wave function should provide the ideal fiducial function for constructing efficient, overcomplete coherent states for computations of excited states of the system.

In our recent study ([6]), we construct system-specific coherent states for any bound quantum system by making use of the similarity between the treatment of the harmonic oscillator and SUSY-QM. First, since the charge operator annihilates the ground state, the superpotential that arises in SUSY-QM can be regarded as a SUSY-displacement operator or a generalized displacement variable. We show that the ground state for any bound quantum system minimizes the SUSY-displacement-standard momentum uncertainty product. Then, we use the ground state of the system as a fiducial function to generate new system-specific dynamically-adapted coherent states. Moreover, the discretized system-specific coherent states can be utilized as a dynamically-adapted basis for calculations of excited state energies and wave functions for bound quantum systems. Computational results demonstrate that these discretized system-specific coherent states provide more rapidly-converging expansions for excited state energies and wave functions than the conventional coherent states and the standard harmonic oscillator basis.

The organization of the remainder of this chapter is as follows. In Sec. 2, we briefly review the harmonic oscillator, conventional coherent states, and SUSY-QM. We also show that the ground state of a quantum system minimizes the SUSY-displacement-standard momentum uncertainty product. We then construct system-specific coherent states by applying shift operators to the ground state of the system. In Sec. 3, the discretized system-specific coherent state basis is developed for and applied to the Morse oscillator, the double well potential, and the two-dimensional anharmonic oscillator system for calculations of the excited state energies and wave functions. In Sec. 4, we summarize our results and conclude with some comments.

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2. Theoretical formulation

2.1. Harmonic oscillator and conventional coherent states

The Hamiltonian of the harmonic oscillator is expressed by

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2, \tag{1}$$

where m is the particle's mass, ω is the angular frequency of the oscillator. The Hamiltonian can be written in terms of the raising and lowering operators as

$$H = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \tag{2}$$

where $\hat{a}^\dagger$ is the raising operator and $\hat{a}$ is the lowering operator. These two operators can be expressed in terms of the position operator $\hat{x}$ and its canonically conjugate momentum operator $\hat{p}_x$ by

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i\hat{p}_x}{\sqrt{2m\hbar\omega}}, \tag{3}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i\hat{p}_x}{\sqrt{2m\hbar\omega}}. \tag{4}$$

Without loss of generality, we set $\hbar = 2m = 1$ throughout this study and $\omega = 2$ for this case. In particular, the ground state of the harmonic oscillator is annihilated by the lowering operator

$$\hat{a}\psi_0 = \frac{1}{\sqrt{2}}\left(\hat{x} + i\hat{p}_x\right)\psi_0 = 0. \tag{5}$$

By solving this differential equation in the position representation, we obtain the ground state wave function

$$\psi_0(x) = \langle x|0\rangle = Ne^{-x^2/2}, \tag{6}$$

where N is the normalization constant.

One of the important properties for the ground state of the harmonic oscillator is that the ground state is a minimum uncertainty state, which minimizes the Heisenberg uncertainty product $\Delta\hat{x}\Delta\hat{p}_x$. The usual derivation of the Heisenberg uncertainty principle makes use of Schwarz's inequality ([25])

$$\langle\psi|\hat{x}^2|\psi\rangle\langle\psi|\hat{p}_x^2|\psi\rangle \geq |\langle\psi|\hat{x}\hat{p}_x|\psi\rangle|^2, \tag{7}$$

where zero expectation values of the position and momentum operators are assumed for convenience. The equality holds for the state $|\psi\rangle$, which satisfies the condition

$$\hat{x}|\psi\rangle = -i\sigma^2\hat{p}_x|\psi\rangle, \tag{8}$$

where σ^2 is real and greater than zero. As noted in Eq. (5), the ground state of the harmonic oscillator satisfies the relation with $\sigma^2 = 1$, and hence it is a minimum uncertainty state . In fact, the ground state corresponds to a state centered in the phase space at $x = 0$ and $k = 0$. Harmonic oscillator coherent states can be constructed by applying shift operators labeled with points of the discrete phase space to a fiducial state, which is taken as the ground state of the harmonic oscillator ([18, 21]). In this sense, harmonic oscillator coherent states are generated by $|\alpha\rangle = \hat{D}(\alpha)|0\rangle$. The shift operator is given by

$$\hat{D}(\alpha) = e^{\alpha\hat{a}^\dagger - \alpha^*\hat{a}}, \tag{9}$$

where

$$\alpha = \frac{1}{\sqrt{2}}\left[\frac{x}{\sigma} + ik\sigma\right]. \tag{10}$$

Here α is a complex-number representation of the phase point x and k, and the quantity σ is a scaling parameter with the dimensions of length. Thus, the harmonic oscillator coherent states can be constructed by applying the shift operator to the ground state of the harmonic oscillator.

2.2. 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

$$\psi_0^{(1)}(x) = N\exp\left[-\int_0^x W_1(x')dx'\right], \tag{11}$$

where N is the normalization constant. The index "(1)" indicates that the ground state wave function and the superpotential are associated with the sector one Hamiltonian. It is assumed that Eq. (11) solves the Schrödinger equation with energy equal to zero

$$-\frac{d^2\psi_0^{(1)}}{dx^2} + V_1\psi_0^{(1)} = 0. \tag{12}$$

This does not impose any restriction since the energy can be changed by adding any constant to the Hamiltonian. From Eq. (11), the superpotential can be expressed in terms of the ground state wave function by

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$$W_1(x) = -\frac{d}{dx} \ln \psi_0^{(1)}(x). \tag{13}$$

Substituting Eq. (11) into the Schrödinger equation in Eq. (12), we obtain the Riccati equation for the superpotential

$$\frac{dW_1(x)}{dx} - W_1^2(x) + V_1(x) = 0. \tag{14}$$

On the other hand, if $W_1(x)$ is known, then $V_1(x)$ is given by

$$V_1(x) = \left(W_1(x)^2 - \frac{dW_1(x)}{dx} \right). \tag{15}$$

Obviously, the Schrödinger equation in Eq. (12) is equivalent to

$$-\frac{d^2\psi_0^{(1)}}{dx^2} + \left(W_1^2 - \frac{dW_1}{dx} \right) \psi_0^{(1)} = 0. \tag{16}$$

Analogous to the harmonic oscillator, the Hamiltonian operator can be factorized by introducing the "charge" operator and its adjoint

$$Q_1 = \frac{d}{dx} + W_1 = W_1 + i\hat{p}_x, \tag{17}$$

$$Q_1^\dagger = -\frac{d}{dx} + W_1 = W_1 - i\hat{p}_x, \tag{18}$$

where $\hat{p_x} = -i(d/dx)$ is the coordinate representation of the momentum operator. Throughout this study, the ground state wave function $\psi_0(x)$ is assumed to be purely real; hence, the superpotential $W(x)$ is self-adjoint. 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 $n > 0$

$$Q_1^\dagger Q_1 \psi_n^{(1)} = E_n^{(1)} \psi_n^{(1)}, \tag{19}$$

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

$$H_2 \left(Q_1 \psi_n^{(1)} \right) = Q_1 Q_1^\dagger \left(Q_1 \psi_n^{(1)} \right) = E_n^{(1)} \left(Q_1 \psi_n^{(1)} \right), \tag{20}$$

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

$$H_2\psi_n^{(2)} = Q_1 Q_1^\dagger \psi_n^{(2)} = E_n^{(2)}\psi_n^{(2)}. \tag{21}$$

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

$$H_1\left(Q_1^\dagger\psi_n^{(2)}\right) = \left(Q_1^\dagger Q_1\right)\left(Q_1^\dagger\psi_n^{(2)}\right) = E_n^{(2)}\left(Q_1^\dagger\psi_n^{(2)}\right). \tag{22}$$

It follows that the Hamiltonians H_1 and H_2 have identical spectra with the exception of the ground state with $E_0^{(1)} = 0$. 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

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

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.

2.3. SUSY Heisenberg uncertainty products

It follows from Eq. (13) that the charge operator annihilates the corresponding ground state

$$Q\psi_0 = \left(\hat{W} + i\hat{p}_x\right)\psi_0 = 0. \tag{23}$$

Because we concentrate only on the sector one Hamiltonian in the present study, we suppress the sector index. For the harmonic oscillator, the charge operators correspond to the raising and lowering operators for the harmonic oscillator with $W(x) = x$. From the similarity, the superpotential $\hat{W}$ can be regarded as a "SUSY-displacement" operator although such a displacement would, in general, not be generated by the standard momentum operator $\hat{p}_x$. In fact, $\hat{W}$ and $\hat{p}_x$ are not canonically conjugate variables.

The ground state of the harmonic oscillator is a minimum uncertainty state, which minimizes the Heisenberg uncertainty product $\Delta\hat{x}\Delta\hat{p}_x$. Analogously, it is expected that the ground state for a bound quantum system minimizes the SUSY Heisenberg uncertainty product

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$\Delta\hat{W}\Delta\hat{p}_x$. For an arbitrary normalized wave function, we consider the square of the SUSY-displacement-standard momentum uncertainty product

$$\left(\Delta\hat{W}\Delta\hat{p_x}\right)^2 = \langle\psi|\tilde{W}^2|\psi\rangle\langle\psi|\tilde{p}_x^2|\psi\rangle, \tag{24}$$

where $\tilde{W} = \hat{W} - W_0$ and $\tilde{p_x} = \hat{p}_x - p_0$. The quantities $W_0 = \langle W\rangle$ and $p_0 = \langle\hat{p}_x\rangle$ correspond to the averaged SUSY-displacement and momentum values, respectively. In order to obtain a lower bound on the uncertainty product in Eq. (24), we employ the Cauchy-Schwarz inequality

$$\langle\psi|\tilde{W}^2|\psi\rangle\langle\psi|\tilde{p}_x^2|\psi\rangle \geq |\langle\psi|\tilde{W}\tilde{p}_x|\psi\rangle|^2. \tag{25}$$

The equality is satisfied when the two vectors $\tilde{W}|\psi\rangle$ and $\tilde{p}_x|\psi\rangle$ are collinear. From this condition, we obtain $\tilde{W}|\psi\rangle = \lambda\tilde{p}_x|\psi\rangle$. Rearranging this equation yields

$$(\hat{W} - \lambda\hat{p}_x)|\psi\rangle = (W_0 - \lambda p_0)|\psi\rangle. \tag{26}$$

As a special case for $\lambda = -i$, this equation becomes

$$(\hat{W} + i\hat{p}_x)|\psi\rangle = (W_0 + ip_0)|\psi\rangle. \tag{27}$$

It follows from Eq. (23) that $(W_0 + ip_0) = \langle\psi_0|\hat{W} + i\hat{p}_x|\psi_0\rangle = 0$ for the ground state of the system. Thus, Eq. (23) implies that the ground state satisfies the condition in Eq. (27). Therefore, the ground state of a bound quantum system minimizes the SUSY-displacement-standard momentum uncertainty product $\Delta\hat{W}\Delta\hat{p}_x$.

We present some properties of the averaged SUSY-displacement and standard momentum values for the ground state. The averaged SUSY-displacement for the ground state is evaluated by

$$W_0 = \langle\psi_0|W|\psi_0\rangle = \int_{-\infty}^{\infty}\psi_0^*(x)W(x)\psi_0(x)dx = -\int_{-\infty}^{\infty}\psi_0^*(x)\frac{d\psi_0(x)}{dx}dx, \tag{28}$$

where Eq. (13) has been used. The averaged momentum for the ground state is given by

$$p_0 = \langle\psi_0|\hat{p}_x|\psi_0\rangle = -i\int_{-\infty}^{\infty}\psi_0^*(x)\frac{d\psi_0(x)}{dx}dx. \tag{29}$$

Again, from Eqs. (28) and (29), $W_0 + ip_0 = 0$ for the ground state of the system, as indicated in Eq. (23). Furthermore, when the ground state wave function is purely real, it follows from integration by parts that the integral in Eqs. (28) and (29) is equal to zero. Thus, the averaged SUSY-displacement and momentum values for the real-valued ground state wave function are equal to zero, $W_0 = p_0 = 0$.

The ground state of a quantum system is the minimizer of the SUSY Heisenberg uncertainty product. We can derive the minimum value for the SUSY Heisenberg uncertainty product

in Eq. (25). For the real-valued ground state wave function, $\tilde{W} = \hat{W} - W_0 = \hat{W}$ and $\tilde{p_x} = \hat{p}_x - p_0 = \hat{p}_x$. The right side of the uncertainty product in Eq. (25) becomes

$$\langle\psi_0|\hat{W}\hat{p}_x|\psi_0\rangle = i\langle\psi_0|\hat{W}^2|\psi_0\rangle, \tag{30}$$

where $\hat{p}_x|\psi_0\rangle = i\hat{W}|\psi_0\rangle$ from Eq. (23) has been used. Thus, the right side of the uncertainty product in Eq. (25) is given by

$$|\langle\psi_0|\hat{W}\hat{p}_x|\psi_0\rangle|^2 = \langle\hat{W}^2\rangle^2. \tag{31}$$

Similarly, the left side of the uncertainty product in Eq. (25) is given by

$$\langle\psi_0|\hat{W}^2|\psi_0\rangle\langle\psi_0|\hat{p}_x^2|\psi_0\rangle = \langle\hat{W}^2\rangle\langle\hat{W}^2\rangle. \tag{32}$$

Therefore, the equality in Eq. (25) holds for the ground state, and the SUSY Heisenberg uncertainty product is equal to $\Delta\hat{W}\Delta\hat{p_x} = \langle\hat{W}^2\rangle$.

The expectation value of $\hat{W}^2$ for the ground state is evaluated by

$$\langle\hat{W}^2\rangle = \int_{-\infty}^{\infty}\psi_0(x)W(x)^2\psi_0(x)dx = -\int_{-\infty}^{\infty}\psi_0(x)W(x)\frac{d\psi_0(x)}{dx}dx, \tag{33}$$

where Eq. (13) has been used. From integration by parts, the integral can be expressed by

$$\int_{-\infty}^{\infty}\psi_0(x)W(x)\frac{d\psi_0(x)}{dx}dx = -\frac{1}{2}\int_{-\infty}^{\infty}\psi_0(x)\frac{dW(x)}{dx}\psi_0(x)dx. \tag{34}$$

Thus, the expectation value of $\hat{W}^2$ for the ground state is equal to one half of the expectation value for the derivative of the superpotential

$$\langle\hat{W}^2\rangle = \frac{1}{2}\left\langle\frac{d\hat{W}}{dx}\right\rangle. \tag{35}$$

Moreover, the commutation relation of the SUSY-displacement and the momentum operator is given by

$$\left[\hat{W}, \hat{p}_x\right] = i\frac{d\hat{W}}{dx}. \tag{36}$$

Therefore, the SUSY Heisenberg uncertainty product for the ground state becomes

$$\Delta\hat{W}\Delta\hat{p_x} = \langle\hat{W}^2\rangle = \frac{1}{2}\left\langle\frac{d\hat{W}}{dx}\right\rangle = \frac{1}{2i}\left\langle\left[\hat{W}, \hat{p}_x\right]\right\rangle. \tag{37}$$

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For the harmonic oscillator, $W(x) = x$ and $dW/dx = 1$. We recover the conventional Heisenberg uncertainty product for the ground state $\Delta\hat{x}\Delta\hat{p_x} = 1/2$. As a special case, a similar derivation has been employed to determine exact minimum uncertainty coherent states for the Morse oscillator ([8]).

2.4. System-specific coherent states

Analogous to the harmonic oscillator coherent state, the analysis of a bound quantum system in terms of the SUSY Heisenberg uncertainty principle suggests the construction of system-specific coherent states based on the SUSY-QM ground state. Similarly, the procedure for creating an overcomplete set of such coherent states is to apply the shift operator to the ground state as a fiducial function ([18, 21])

$$\begin{aligned}\psi_\alpha(x) = \langle x|\alpha\rangle = \langle x|\hat{D}(\alpha)|\psi_0\rangle &= Ne^{ik_0(x-x_0)}e^{-x_0(d/dx)}\psi_0(x) \\ &= Ne^{ik_0(x-x_0)}\psi_0(x-x_0),\end{aligned} \tag{38}$$

where N is the normalization constant. The raising and lowering operators for the shift operator are given by $\hat{a}^\dagger = (\hat{x} - i\hat{p}_x)/\sqrt{2}$ and $\hat{a} = (\hat{x} + i\hat{p}_x)/\sqrt{2}$, respectively. The quantity $\alpha = (x_0 + ik_0)/\sqrt{2}$ is a point in the phase space which completely describes the coherent state. Thus, the functions ψ_α form an overcomplete set of the coherent states in the standard phase space which are specifically associated with the quantum-mechanical system described by the SUSY-displacement $W(x)$.

We now consider a coordinate transformation given by $x' = x - x_0$ for the system-specific coherent states in Eq. (38). The system-specific coherent state becomes

$$\psi_\alpha(x') = e^{ik_0x'}\psi_0(x'), \tag{39}$$

where $\psi_0(x')$ is the normalized real-valued ground state wave function, and thus $\psi_\alpha(x')$ is also normalized. The momentum operator is invariant under the coordinate transformation (i.e., $\hat{p}_{x'} = \hat{p}_x$). It is straightforward to show that

$$(\hat{W}(x') + i\hat{p}_{x'})|\psi_\alpha\rangle = ik_0|\psi_\alpha\rangle. \tag{40}$$

The averaged SUSY-displacement for the system-specific coherent state is given by

$$\begin{aligned}W_{0,\alpha} = \langle\psi_\alpha|W|\psi_\alpha\rangle &= \int_{-\infty}^{\infty}\psi_\alpha^*(x')W(x')\psi_\alpha(x')dx' \\ &= -\int_{-\infty}^{\infty}\psi_0(x')\frac{d\psi_0(x')}{dx'}dx'.\end{aligned} \tag{41}$$

Again, it follows from integration by parts that $W_{0,\alpha} = 0$ for all system-specific coherent states. Analogously, the averaged momentum for the system-specific coherent state is given by

$$p_{0,\alpha} = \langle \psi_\alpha | \hat{p}_{x'} | \psi_\alpha \rangle = k_0 - i \int_{-\infty}^{\infty} \psi_0(x') \frac{d\psi_0(x')}{dx'} dx'. \tag{42}$$

Because the integral is equal to zero, $p_{0,\alpha} = k_0$. Thus, Eq. (40) can be written as

$$(\hat{W}(x') + i\hat{p}_{x'})|\psi_\alpha\rangle = (W_{0,\alpha} + ip_{0,\alpha})|\psi_\alpha\rangle. \tag{43}$$

Analogous to the uncertainty condition for the ground state in Eq. (27), this equation implies that the system-specific coherent state $|\psi_\alpha\rangle$ minimizes the SUSY-displacement-momentum uncertainty product $\Delta\hat{W}\Delta\hat{p}_{x'}$ for the displaced coordinate $x' = x - x_0$.

2.5. Discretized system-specific coherent states

A discretized SUSY-QM coherent state basis can be constructed by discretizing the continuous label $\alpha = (q + ik)/\sqrt{2}$ and setting up a von Neumann lattice in phase space with an appropriate density D. The discretized system-specific coherent state basis is given by

$$\psi_{\alpha_i}(x) = \langle x|\alpha_i\rangle = Ne^{ik_i(x-q_i)} \exp\left[-\int_0^{x-q_i} W(x')dx'\right], \tag{44}$$

where $i = 1, \ldots, M$ and M is the number of basis functions. The phase space grid points are defined as ([2])

$$\{(q_i, k_i)\} = \left\{ \left(m\Delta x \sqrt{\frac{2\pi}{D}}, \frac{n}{\Delta x}\sqrt{\frac{2\pi}{D}} \right) \right\} \quad m, n \in \mathbb{Z} \tag{45}$$

where m and n run over all integers, hence i can be thought of as a joint index consisting of m and n. The quantity D is the density of grid points in units of $2\pi\hbar$. As discussed in Klauder and Skagerstam's book ([18]), generalized coherent states constructed by applying displacement operators to a fiducial state are overcomplete; however, completeness of the discretized system-specific coherent states in Eq. (44) has not been established here.

Since the ground state solves the time-independent Schrödinger equation for the corresponding Hamiltonian, the system-specific coherent states build in the dynamics of the system under investigation. This property leads to the expectation that these dynamically-adapted and system-specific coherent states will prove more rapidly convergent in calculations of the excited state energies and wave functions for quantum systems using variational methods.

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	E_0	E_1	E_2	E_3
Exact	**-56.25**	**-42.25**	**-30.25**	**-20.25**
SSCS ($M = 9$)	-56.25	-42.2499824	-30.2270611	-19.52261
SSCS ($M = 15$)	-56.25	-42.2499999	-30.2499343	-20.23502
HOCS ($M = 9$)	-54.95	-37.00	-21.08	-10.22
HOCS ($M = 15$)	-56.13	-41.62	-28.61	-17.62
HO ($M = 9$)	-53.79	-33.34	-16.45	-6.40
HO ($M = 15$)	-55.54	-39.03	-23.84	-12.30

Table 1. Comparison of the energy eigenvalues for the Morse oscillator obtained by the system-specific coherent states (SSCS), the harmonic oscillator coherent states (HOCS), and the harmonic oscillator basis functions (HO) with the exact results.

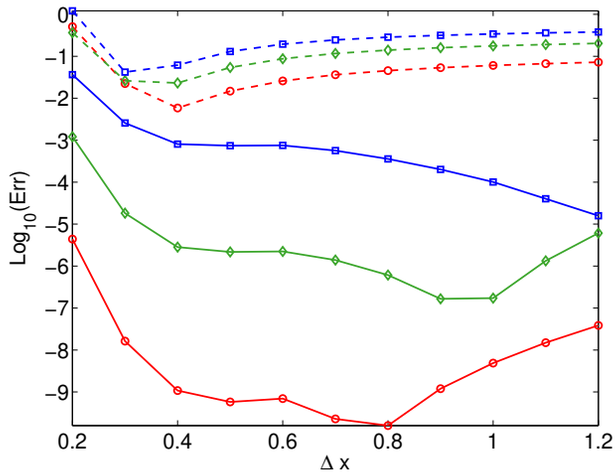

Figure 1. Logarithm of the relative error, versus grid spacing Δx, of the first (○), second (◇), and third (□) excited state energies for the Morse oscillator using the system-specific coherent states (—) and the harmonic oscillator coherent states (- - -) with 15 basis functions.

To use the Rayleigh-Ritz variational principle, we construct a trial wave function in terms of a linear combination of the system-specific coherent states

$$|\psi\rangle = \sum_{i=1}^{M} c_i |\alpha_i\rangle, \tag{46}$$

where c_i are the coefficients. Because of the non-orthogonality of the system-specific coherent states, the energy eigenvalues and wave functions are determined by solving the generalized eigenvalue problem ([36])

$$HC = ESC, \tag{47}$$

where$H_{ij} = \langle \alpha_i | H | \alpha_j \rangle$ is the matrix element of the Hamiltonian, $S_{ij} = \langle \alpha_i | \alpha_j \rangle$ is the overlap matrix, and C is a vector of linear combination coefficients for the eigenvector. Therefore, solving Eq. (47) yields the variational approximation to the eigenvalues and eigenvectors of the Hamiltonian operator.

3. Computational results

3.1. Morse oscillator

In order to demonstrate features of system-specific coherent states, computational results will be presented for three quantum systems. The first of these concerns the Morse oscillator. The Hamiltonian of the Morse oscillator is given by

$$H = -\frac{d^2}{dx^2} + V(x) = -\frac{d^2}{dx^2} + 64\left(e^{-2x} - 2e^{-x}\right). \tag{48}$$

The exact energy eigenvalues are $E_n = -(n - 15/2)^2$ where $n = 0, \ldots, 7$, and the analytical expression of the ground state wave function is given by

$$\psi_0(x) = N \exp\left[-8e^{-x} - \frac{15}{2}x\right], \tag{49}$$

where N is the normalization constant. In this case, the superpotential and its derivative are given by $W(x) = 15/2 - 8\exp(-x)$ and $dW/dx = 8\exp(-x)$, respectively. The minimum SUSY Heisenberg uncertainty product in Eq. (37) is equal to $\Delta\hat{W}\Delta\hat{p_x} = 15/4$. In addition, the discretized system-specific coherent state basis functions in Eq. (44) are expressed by

$$\psi_{\alpha_i}(x) = Ne^{ik_i(x-q_i)} \exp\left[-8e^{-(x-q_i)} - \frac{15}{2}(x - q_i)\right]. \tag{50}$$

The phase space grid in Eq. (45) used for the coherent states was $m = -1, 0, 1$ and $n = -1, 0, 1$ for $M = 9$ basis functions and $m = -1, 0, 1$ and $n = -2, \ldots, 2$ for $M = 15$ basis functions. The phase space density was set to be $D = 1$. In contrast with the present system-specific coherent states in Eq. (50), different coherent states for the Morse oscillator defined as eigenstates of the charge operator and minimum uncertainty states have been constructed ([8]).

Table 1 presents the computational results for the energy eigenvalues obtained by solving the generalized eigen-equation in Eq. (47) using the discretized system-specific coherent state basis functions with $\Delta x = 0.5$. Since the basis includes the exact ground state wave function, the computational result yields the exact ground state energy. As shown in this table, higher accuracy can be achieved when we increase the number of the basis functions from $M = 9$ to $M = 15$. In addition, Table 1 presents the computational results obtained using the harmonic oscillator coherent state basis and the standard harmonic oscillator basis. The discretized harmonic oscillator coherent state basis functions are readily determined by substituting $W(x) = x$ into Eq. (44)

$$\psi_{\alpha_i}(x) = Ne^{ik_i(x-q_i)}e^{-(x-q_i)^2/2}. \tag{51}$$

The standard harmonic oscillator basis is given by

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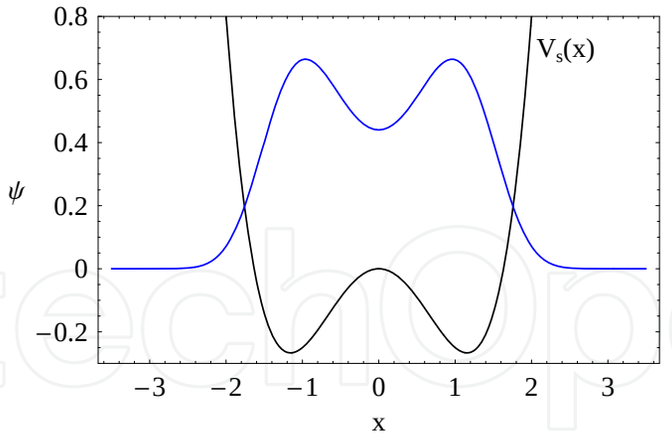

Figure 2. The ground state wave function of the double well potential obtained by the imaginary time propagation method is shown with the scaled potential $V_s(x) = V(x)/20$.

$$\phi_n(x) = \frac{1}{\sqrt{2^n n! \sqrt{\pi}}} H_n(x) e^{-x^2/2}, \tag{52}$$

where $H_n(x)$ is the Hermite polynomial. Compared with the results obtained from these two basis sets, the computational results from the system-specific coherent states achieve significantly higher accuracy using a small number of basis functions. Thus, the system-specific coherent states provide more accurate approximations of the excited state energies for the Morse oscillator.

Figure 1 displays the logarithm of the relative error of the excited state energies for the system-specific coherent states and the harmonic oscillator coherent states with different values for Δx with 15 basis functions. The relative error is defined by

$$Err = \frac{E_{numerical} - E_{exact}}{|E_{exact}|}. \tag{53}$$

As shown in this figure, the system-specific coherent states yield excellent results for the excited state energies. The relative error of the first-excited state energy can even reach 10^{-9} for a wide range of Δx. Additionally, compared with the harmonic oscillator coherent states, the system-specific coherent states give much more accurate results for the first three excited state energies. Also, the system-specific coherent states yield stable computational results for a wide range of Δx.

3.2. Double well potential

As an example of quantum systems without exact analytical solutions, we consider a symmetric double well potential given by

$$V(x) = 3x^4 - 8x^2. \tag{54}$$

	E_0	E_1	E_2	E_3
DVR	**-2.169693**	**-1.406472**	**3.102406**	**7.087930**
SSCS ($M = 9$)	-2.169697	-1.375254	3.106359	7.807534
SSCS ($M = 15$)	-2.169697	-1.406417	3.102440	7.088186
HOCS ($M = 9$)	-2.1223	-1.3214	3.3931	7.5166
HOCS ($M = 15$)	-2.1688	-1.4048	3.1088	7.0992
HO ($M = 9$)	-2.1246	-1.0650	3.5063	8.6640
HO ($M = 15$)	-2.1543	-1.3930	3.1555	7.4491

Table 2. Comparison of the energy eigenvalues for the double well potential obtained by the system-specific coherent states (SSCS), the harmonic oscillator coherent states (HOCS), and the harmonic oscillator basis functions (HO) with the discrete variable representation (DVR) results.

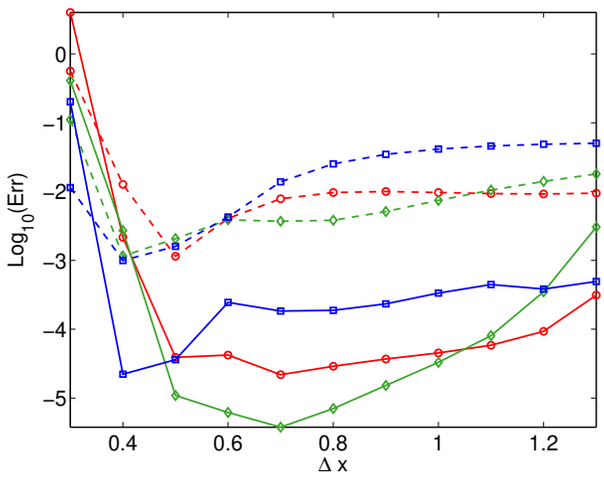

Figure 3. Logarithm of the relative error, versus grid spacing Δx, of the first (○), second (◇), and third (□) excited state energies for the double well potential using the system-specific coherent states (—) and the harmonic oscillator coherent states (- - -) with 15 basis functions.

In order to construct the discretized system-specific coherent state basis functions in Eq. (44), we numerically obtain the ground state wave function. We employed the split-operator method ([35]) to integrate the imaginary time Schrödinger equation from $t = 0$ to $t = 2$ ([36]). The computational grid extends from $x = -8$ to $x = 8$ with 2^{13} grid points, and the integration time step was $\Delta t = 0.01$. The initial state is a Gaussian wave packet given by

$$\psi(x) = \left(\frac{2}{\pi}\right)^{1/4} e^{-x^2}, \tag{55}$$

where the wave packet is centered at the origin. Figure 2 presents the resulting ground state wave function of the double well potential with the ground state energy $E_0 = -2.169694$.

From the computational result for the ground state, we can construct the approximate discretized system-specific coherent states in Eq. (44) used to determine the excited state energies of the double well potential by solving the generalized eigen-equation in Eq. (47). In order to assess the accuracy of the computational results, accurate results were obtained with a Chebyshev polynomial discrete variable representation (DVR) variational calculation

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	E_0	E_1	E_2	E_3
DVR	**0.000000**	**4.751807**	**6.646349**	**8.679575**
SSCS ($M = 81$)	0	4.754974	6.647358	8.684308
SSCS ($M = 225$)	0	4.751812	6.646353	8.679596
HOCS ($M = 81$)	0.0762	5.3029	6.9378	10.4334
HOCS ($M = 225$)	0.0029	4.7915	6.6554	8.8479
HO ($M = 81$)	0.0870	5.3587	7.0307	10.5626
HO ($M = 225$)	0.0144	4.8953	6.6967	9.2190

Table 3. Comparison of the energy eigenvalues for the two-dimensional anharmonic oscillator system obtained by the system-specific coherent states (SSCS), the harmonic oscillator coherent states (HOCS), and the harmonic oscillator basis functions (HO) with the discrete variable representation (DVR) results.

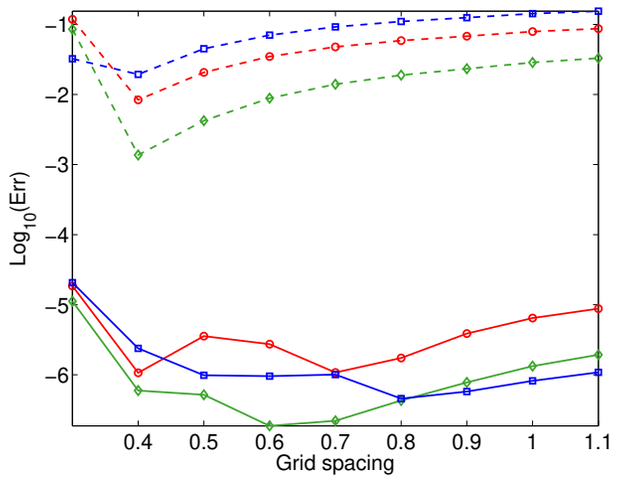

Figure 4. Logarithm of the relative error, versus grid spacing $\Delta x = \Delta y$, of the first (○), second (◇), and third (□) excited state energies for the two-dimensional anharmonic oscillator system using the system-specific coherent states (—) and the harmonic oscillator coherent states (- - -) with 225 basis functions.

using 1000 grid points on the computational domain extending from $x = -4$ to $x = 4$ ([23]). Table 2 presents the computational results for the energy eigenvalues with $\Delta x = 0.5$. Again, computational results for the first three excited state energies with significantly higher accuracy were achieved using a small number of the basis functions with $M = 15$. In addition, compared with the harmonic oscillator coherent state basis and the standard harmonic oscillator basis, the system-specific coherent states yields more accurate excited state energies for the double well potential. Moreover, Fig. 2 displays the logarithm of the relative error of the excited state energies for the system-specific coherent states and the harmonic oscillator coherent states with different values for Δx with 15 basis functions. As shown in this figure, the system-specific coherent states generally yield much more accurate results for the excited state energies than the harmonic oscillator coherent states except for small Δx.

3.3. Two-dimensional anharmonic oscillator system

As an example of multidimensional systems, we consider a nonseparable nondegenerate two-dimensional anharmonic oscillator system ([19]). The Hamiltonian is given by

$$\begin{aligned} H_1 &= -\nabla^2 + V(x,y) \\ &= -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \left(4xy^2 + 2x\right)^2 \\ &\quad + \left(4x^2y + 2\sqrt{2}y\right)^2 - 4\left(x^2 + y^2\right) - \left(2 + 2\sqrt{2}\right). \end{aligned} \tag{56}$$

The exact ground state energy of the system is zero and the analytical expression of the ground state wave function is given by

$$\psi_0^{(1)}(x,y) = N \exp\left(-2x^2y^2 - x^2 - \sqrt{2}y^2\right), \tag{57}$$

where N is a normalization constant. Analogous to the one-dimensional case, the discretized system-specific coherent state basis functions are expressed by

$$\psi_{\alpha_i}(x,y) = Ne^{ik_{xi}(x-q_{xi})}e^{ik_{yi}(y-q_{yi})}\psi_0(x-q_{xi}, y-q_{yi}). \tag{58}$$

In addition, the two-dimensional separable discretized harmonic oscillator coherent state basis functions are given by

$$\psi_{\alpha_i}(x,y) = Ne^{ik_{xi}(x-q_{xi})}e^{ik_{yi}(y-q_{yi})}e^{-(x-q_{xi})^2/2}e^{-(y-q_{yi})^2/2}. \tag{59}$$

The phase space grid points for these two basis sets are defined by

$$\{(q_{xi}, q_{yi}, k_{xi}, k_{yi})\} = \left\{\left(m\Delta x\sqrt{\frac{2\pi}{D}}, m\Delta y\sqrt{\frac{2\pi}{D}}, \frac{n}{\Delta x}\sqrt{\frac{2\pi}{D}}, \frac{n}{\Delta y}\sqrt{\frac{2\pi}{D}}\right)\right\} \quad m,n \in \mathbb{Z} \tag{60}$$

where m and n are integers. For computational results, we chose $m = -1, 0, 1$ and $n = -1, 0, 1$ for $M = 81$ basis functions and $m = -1, 0, 1$ and $n = -2, \ldots, 2$ for $M = 225$ basis functions. The phase space density was set to be $D = 1$.

Table 3 presents the computational results for the energy eigenvalues obtained using the discretized system-specific coherent states and the harmonic oscillator coherent states with $\Delta x = \Delta y = 0.4$. Compared with the DVR results using 50 grid points in x and in y (for a total of 2500 basis functions), the computational results obtained by the system-specific coherent states achieve higher accuracy than the harmonic oscillator coherent states. In addition, Table 3 presents the computational results obtained from the standard harmonic oscillator

basis of the direct product of the eigenstates of a harmonic oscillator in each dimension with frequency $\omega = 2\sqrt{2}$. These results were obtained by a $(N_x, N_y) = (9,9)$ basis set calculation with 81 basis functions and a $(N_x, N_y) = (15,15)$ basis set calculation with 225 basis functions. Again, compared with the results obtained from the other two basis sets, the computational results from the system-specific coherent states achieve significantly higher accuracy using a small number of basis functions. Furthermore, Figure 4 displays the logarithm of the relative error of the excited state energies for the system-specific coherent states and the harmonic oscillator coherent states with different values for the grid spacing with 225 basis functions. As shown in this figure, the system-specific coherent states yield much more accurate results for the excited state energies than the harmonic oscillator coherent states for different grid spacings, and the relative errors reach around 10^{-6} for a wide range of the grid spacings.

4. Discussion and perspectives

The application of SUSY-QM to non-relativistic quantum systems generalizes the powerful ladder operator approach used in the treatment of the harmonic oscillator. The lowering operator of the harmonic oscillator annihilates the ground state, while the charge operator annihilates the ground state of the corresponding ground state for other quantum systems. The similarity between the lowering operator of the harmonic oscillator and the SUSY charge operator implies that the superpotential can be regarded as a system-specific generalized displacement variable. Analogous to the ground state of the harmonic oscillator which minimizes the Heisenberg uncertainty product, the ground state of any bound quantum system was identified as the minimizer of the SUSY Heisenberg uncertainty product. Then, system-specific coherent states were constructed by applying shift operators to the ground state of the system, which serves as a fiducial function. In addition, we employed the discretized system-specific coherent states as a dynamically-adapted basis set to determine the excited state energies and wave functions for the Morse oscillator, the double well potential, and the two-dimensional anharmonic oscillator system. Variational calculations in terms of the discretized system-specific coherent states demonstrated that these dynamically-adapted coherent states yield significantly more accurate excited state energies and wave functions than were obtained with the same number of the conventional coherent states and the standard harmonic oscillator basis.

As presented in the current study, the ladder operator approach of the harmonic oscillator and the SUSY-QM formulation share strong similarity. This observation suggests that the connection of the SUSY-QM with the Heisenberg minimum uncertainty $(\mu-)$ wavelets should be explored ([13, 14, 21, 22]). The SUSY-displacement with the SUSY Heisenberg uncertainty product can lead to the construction of the SUSY minimum uncertainty wavelets and the SUSY distributed approximating functionals. These new functions and their potential applications in mathematics and physics are currently under investigation. In addition, this study presents a practical computational approach for discretized system-specific coherent states in calculations of excited states. The issue of completeness of discretized system-specific coherent states should be examined. These relevant studies will be reported elsewhere in the future.

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