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Algebraic construction of the coherent states of the Morse potential based on supersymmetric quantum mechanics

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By introducing the shape-invariant Lie algebra spanned by the supersymmetric ladder operators plus the identity operator, we generate a discrete complete orthonormal basis for the quantum treatment of the one-dimensional Morse potential. In this basis, which we call the pseudo-number-states, the Morse Hamiltonian is tridiagonal. Then we construct algebraically the continuous overcomplete set of coherent states for the Morse potential in close analogy with the harmonic oscillator. These states coincide with a class of states constructed earlier by Nieto and Simmons [Phys. Rev. D **20**, 1342 (1979)] by using the coordinate representation. We also give the unitary displacement operator creating these coherent states from the ground state. [S1050-2947(99)50109-1]

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I. INTRODUCTION

Coherent states [1] for systems other than the harmonic oscillator (HO) have attracted much attention for the past several years [2–8]. There are a number of different approaches to this problem and the one presented here is based on the methods of supersymmetric quantum mechanics (SUSY QM) [9–12]. Since the SUSY description combined with the concept of shape invariance is a generalization of the ladder operator method of the harmonic oscillator, it seems straightforward to use the SUSY ladder operators to construct coherent states for other, nonharmonic potentials, too. Based on this idea, an algebraic construction of coherent states was proposed by Fukui and Aizawa [3] for the class of shape-invariant potentials having an infinite number of bound-energy eigenstates. Their definition, however, does not work for potentials, where the number of normalizable energy eigenstates is finite. Among these latter problems the Morse potential deserves particular attention, because it plays an important role in treating molecular vibrations and in laser chemistry.

In this paper we present an alternative algebraic method by using the SUSY ladder operators to obtain coherent states for the one-dimensional Morse potential. Using the shape-invariant Lie algebra spanned by the SUSY ladder operators and the identity, we will introduce an orthonormal basis in the state space called pseudo-number-states. In contrast to the set of energy eigenstates, this basis is a complete discrete set of normalizable states that tridiagonalizes the Morse Hamiltonian. With the help of the pseudo-number-states we introduce the coherent states, in analogy with those of the harmonic oscillator. They are labeled with a complex number β, and they satisfy the minimal requirements established by Klauder (see in Ref. [4]) to be termed as coherent: they are continuous functions of the label β, and form an (over) complete set in Hilbert space. We also show that a unitary displacement operator exists in a quite similar form, as in the case of the harmonic oscillator, so that the coherent states are generated by this operator from the ground state as $|\beta\rangle = D(\beta)|0\rangle$. We note that the coordinate representation wave functions corresponding to our coherent states have been obtained earlier by Nieto and Simmons [2] in an entirely different way.

II. PSEUDO-NUMBER-STATES

In this work we consider the Morse Hamiltonian

$$\hat{H}(s) = \hat{P}^2/2m + V_0\Big[s + \tfrac{1}{2} - \exp(-\gamma\hat{X})\Big]^2, \qquad (1)$$

where s, V_0, and γ are real parameters determining the shape of the potential. Using dimensionless operators $X=\gamma\hat{X}$ and $P=1/\sqrt{2mV_0}\hat{P}$, and choosing the units so that $\gamma\hbar/\sqrt{2mV_0}=1$, we have $[X,P]=i$ and $\hat{H}(s)=V_0H(s)$ with

$$H(s)=P^2+\Big[s+\tfrac{1}{2}-\exp(-X)\Big]^2. \tag{2}$$

From now on we consider this latter $H(s)$ as the Hamiltonian. If $s>0$, there then exists a normalizable ground state $|\Psi_0(s)\rangle$ with energy $E_0(s)$. According to the theory of SUSY QM, one can introduce the ladder operators $A(s)$, $A^\dagger(s)$, so that $A(s)$ annihilates the ground state, and the Hamiltonian can be factorized:

$$A(s)|\Psi_0(s)\rangle=0,\quad H(s)=A^\dagger(s)A(s)+E_0(s). \tag{3}$$

In the case of the Morse potential the ladder operators $A(s)$ and $A^\dagger(s)$ can be written as [10]

$$\begin{aligned} A(s)&=s-\exp(-X)+iP,\\ A^\dagger(s)&=s-\exp(-X)-iP. \end{aligned} \tag{4}$$

Considering the partner Hamilton operator, $H^p(s)=A(s)A^\dagger(s)+E_0(s)$, one finds that the Morse potential is shape invariant [9,10], which means that

$$H^p(s)=H(f(s))+R(f(s)), \tag{5}$$

with $f(s)=s-1$ and $R(s)=2(s+1)$. Due to this property one can determine the energy eigenstates, as well as the eigenvalues in the following way:

$$\begin{aligned} |\Psi_n(s)\rangle&\propto A^\dagger(s)\cdots A^\dagger(s-n+1)|\Psi_0(s-n)\rangle,\\ E_n(s)&=E_0(s)+\sum_{k=1}^{n}R(s-k). \end{aligned} \tag{6}$$

The Morse potential has only a finite number of bound states (the integer part of $s+1$), which cannot form a complete set of states in the Hilbert space. Hence the full quantum description of the Morse potential is impossible when restricting oneself to only these bound states. One can of course use the continuous part of the spectrum of H, but instead we consider here the following infinite series of states:

$$\begin{aligned} |0\rangle&\equiv|\Psi_0(s)\rangle\\ |1\rangle&\equiv C_1^{-1}A^\dagger(s)|0\rangle\\ &\vdots\\ |n\rangle&\equiv C_n^{-1}A^\dagger(s+n-1)|n-1\rangle\\ &\vdots \end{aligned} \tag{7}$$

where n is a positive integer ($n\in N^+$) and $C_n=\sqrt{n(2s+n-1)}$ is a normalization coefficient. Note the difference between the parameter shifts in Eqs. (6) and (7).

A key observation from our point of view is that the SUSY ladder operators $A(s)$, $A^\dagger(s)$ and the identity I span a Lie algebra. Since for any number n we have

$$A(s+n)=A(s)+nI, \tag{8}$$

the Lie algebra is invariant with respect to a shift of the shape parameter s, and an easy calculation shows that the parameter-dependent SUSY ladder operators satisfy the following commutation relations:

$$\begin{aligned} [A(s+m),A(s+n)]&=0,\\ [A^\dagger(s+m),A^\dagger(s+n)]&=0,\\ [A(s+m),A^\dagger(s+n)]&=2sI-[A(s)+A^\dagger(s)]. \end{aligned} \tag{9}$$

Equations (8) and (9) are valid for any complex n, but we shall exploit this property only for real integer n.

Using the commutation relations (9) and the fact that $A(s)$ annihilates the ground state $A(s)|\Psi_0(s)\rangle=0$, one can verify that the states defined in Eq. (7) are mutually orthogonal:

$$\langle m|n\rangle=\delta_{m,n}. \tag{10}$$

We are going to call these states the pseudo-number-states of the Morse potential, and we give here the corresponding wave functions in terms of the variable $y=2\exp(-x)$. With the help of Eqs. (3) and (7) we find that the wave functions in question obey the following recursion relation:

$$\begin{aligned} \varphi_0(y)&:=\langle y|0\rangle=\frac{1}{\sqrt{\Gamma(2s)}}y^s\exp(-y/2),\\ \varphi_n(y)&:=\langle y|n\rangle=C_n^{-1}\left(y\frac{\partial}{\partial y}+(s+n-1)-\frac{y}{2}\right)\varphi_{n-1}(y). \end{aligned} \tag{11}$$

Comparing Eq. (11) with the Rodrigues's formula for the generalized Laguerre polynomials $L_n^\alpha(y)$ [13], one finds that the normalized wave functions of the pseudo-number-states are

$$\varphi_n(y)=\left[\Gamma(2s)\binom{n+2s-1}{n}\right]^{-1/2}y^s\exp(-y/2)L_n^{2s-1}(y). \tag{12}$$

Due to the completeness of the Laguerre polynomials with respect to the weight function $\exp(-y)y^{2s-1}$ [13], the functions (12) form a complete orthonormal set in the space $L^2[(0,\infty),dy/y]$ [the square integrable functions on the $(0,\infty)$ interval, with respect of the measure dy/y], and therefore the set of pseudo-number-states is a complete, orthonormal basis in Hilbert space.

Calculating the matrices of the SUSY ladder operators shifted by an arbitrary integer k, one finds the following matrix elements:

$$\begin{aligned} \langle m|A(s+k)|n\rangle&=\sqrt{n(2s+m)}\,\delta_{m+1,n}-(m-k)\,\delta_{m,n},\\ \langle m|A^\dagger(s+k)|n\rangle&=\sqrt{m(2s+n)}\,\delta_{m,n+1}-(n-k)\,\delta_{m,n},\\ \langle m|H(s)|n\rangle&=\left[2n\left(n+s-\frac{1}{2}\right)+E_0(s)\right]\delta_{m,n}\\ &\quad-(n-1)\sqrt{n(2s+n-1)}\,\delta_{m+1,n}\\ &\quad-(m-1)\sqrt{n(2s+n-1)}\,\delta_{m,n+1}. \end{aligned} \tag{13}$$

We see that the Hamiltonian is not diagonal; it has, however, nonvanishing elements only in, above, and below the main diagonal.

III. COHERENT STATES

We use now the SUSY operator analogy with the HO, and define the coherent states of the Morse potential as

$$|\beta\rangle = g(\beta)\left\{ I + \sum_{n=1}^{\infty} \frac{\beta^n}{n!} A^\dagger(s+n-1)\cdots A^\dagger(s) \right\}|0\rangle, \tag{14}$$

where β is a c number and $g(\beta)$ is a normalization function to be determined below. The expression of C_n implies the introduction of a generalized factorial $\{n\}!$ with the definition

$$\{0\}! = 1, \quad \{n\}! = \frac{n!}{2s\cdots(2s+n-1)} = \binom{n+2s-1}{n}^{-1} \quad (n>0). \tag{15}$$

Then the coherent states in Eq. (14) can be written by the help of Eq. (7) as

$$|\beta\rangle = g(\beta)\sum_{n=0}^{\infty} \frac{\beta^n}{\sqrt{\{n\}!}}|n\rangle. \tag{16}$$

To obtain the explicit form of $g(\beta)$ (chosen to be real), and to find the label space (the set of allowed β's) we set

$$1 = \langle\beta|\beta\rangle = g^2(\beta)\sum_{n=0}^{\infty}\frac{|\beta|^{2n}}{\{n\}!} = g^2(\beta)\left\{ 1 + \sum_{n=1}^{\infty}\frac{2s\cdots(2s+n-1)}{n!}|\beta|^{2n}\right\}. \tag{17}$$

The sum in the above expression is convergent if and only if $|\beta|<1$, i.e., the label space is the complex open unit disk, and then the sum in the braces in Eq. (17) yields $(1-|\beta|^2)^{-2s}$. So we finally have for the coherent states of the Morse potential,

$$|\beta\rangle = (1-|\beta|^2)^s \sum_{n=0}^{\infty}\sqrt{\binom{n+2s-1}{n}}\beta^n|n\rangle \quad (\beta\in\mathbf{C}, |\beta|<1). \tag{18}$$

The various sets of coherent states that have been introduced in the past for an arbitrary system have two fundamental common properties established in Ref. [4]: strong continuity in the label space and completeness in the sense that there exists a positive measure on the label space such that the identity operator admits the resolution of unity. The first property follows from the definition: if $\beta\to\beta'$, $(|\beta|,|\beta'|<1)$, then $\||\beta\rangle-|\beta'\rangle\|^2\to 0$. To verify the second property, valid for $s>1/2$, we consider the measure $\delta\beta = (2s-1)/(1-|\beta|^2)^2 d\,\mathrm{Re}\,\beta d\,\mathrm{Im}\,\beta (|\beta|<1)$ and find

$$\int_{|\beta|<1}|\beta\rangle\langle\beta|\,\delta\beta = (2s-1)\sum_{n,m=0}^{\infty}\frac{|n\rangle\langle m|}{\sqrt{\{n\}!\{m\}!}}\int_{|\beta|<1}(\beta^*)^m \times\beta^n(1-|\beta|^2)^{2s-2}d\,\mathrm{Re}\,\beta d\,\mathrm{Im}\,\beta. \tag{19}$$

Introducing polar coordinates in the label space, the integral above can be calculated easily, and we find the resolution of unity as

$$\int_{|\beta|<1}|\beta\rangle\langle\beta|\,\delta\beta = \pi\sum_{n=0}^{\infty}|n\rangle\langle n| = \pi I. \tag{20}$$

We also present here the wave functions corresponding to the states $|\beta\rangle$. From Eqs. (12) and (16) we have

$$\varphi_\beta(y) := \langle y|\beta\rangle = (1-|\beta|^2)^s\sum_{n=0}^{\infty}\frac{\beta^n}{\sqrt{\{n\}!}}\langle y|n\rangle = \frac{(1-|\beta|^2)^s}{\sqrt{\Gamma(2s)}}y^s\exp(-y/2)\sum_{n=0}^{\infty}\beta^n L_n^{2s-1}(y). \tag{21}$$

Using the generating function formula for the Laguerre polynomials [13], one obtains that the corresponding wave functions in the y coordinate are

$$\varphi_\beta(y) = \frac{(1-|\beta|^2)^s}{\sqrt{\Gamma(2s)}(1-\beta)^{2s}}y^s\exp\left(-\frac{y}{2}\frac{1+\beta}{1-\beta}\right). \tag{22}$$

These wave functions are essentially the same as those discovered in another way by Nieto and Simmons [2], who called them generalized minimal uncertainty coherent states (MUCS) of the Morse potential. They introduced certain special coordinates in the classical phase space, transforming the trajectories of the bound motions into ellipses. According to [2], the MUCS-type coherent states are those that minimize the uncertainty relation of the quantum operators corresponding to these new classical coordinates called ''natural classical variables'' in Ref. [2]. It is interesting that our algebraic approach has led to the same states. Often the eigenvalue equation that defines the MUCS amounts to the ladder operator coherent states, if the ground state is a member of the minimum-uncertainty set. Here we have found that to be the case. Otherwise, the minimum-uncertainty defining equation often yields the defining equation for lowering operator squeezed states [14].

IV. DISPLACEMENT OPERATOR GENERATING $|\beta\rangle$

In this section we present another interpretation of the state $|\beta\rangle$ by giving the physical meaning of its parameter. We recast the wave function (22) into the original coordinate variable x. Substituting $y=2\exp(-x)$, one has

$$\varphi_\beta(x) := \langle x|\beta\rangle = \frac{e^{-i\varphi}2^s}{\Gamma^{1/2}(2s)}e^{-s(x-\tilde{x})} \times\exp\{-e^{-(x-\tilde{x})}\}\exp\left\{\frac{-i}{s}\tilde{p}e^{-(x-\tilde{x})}\right\}, \tag{23}$$

where $e^{-i\varphi} = [(|1-\beta|)/1-\beta]^{2s}$ is a phase term and $\tilde{x}$ and $\tilde{p}$ are real numbers depending on β:

$$\tilde{x} := \ln\left(\mathrm{Re}\frac{1+\beta}{1-\beta}\right), \quad \tilde{p} := s\frac{\mathrm{Im}\,(1+\beta)/(1-\beta)}{\mathrm{Re}\,(1+\beta)/(1-\beta)}. \tag{24}$$

Calculating the expectation values of the operators X and P in the state $|\beta\rangle$ one obtains

$$\langle\beta|X|\beta\rangle = \tilde{x} + \langle 0|X|0\rangle, \quad \langle\beta|P|\beta\rangle = \tilde{p}. \tag{25}$$

We see that, apart from an additive constant (the expectation value of the position in the ground state), $\tilde{x}$ and $\tilde{p}$ are just the position and momentum operator expectation values, respectively. Hence we can introduce a new labeling for the coherent states with the help of the real numbers $\tilde{x}$ and $\tilde{p}$ instead of the original complex β. In these coordinates, $|\beta\rangle$ can be written as $|\tilde{x},\tilde{p}\rangle$, and the appropriate label space is $\mathbf{R}^2$ with the measure $d\tilde{x}\,d\tilde{p}$ on it. Then the resolution of unity (20) has a form similar to that in the case of the HO:

$$\frac{2s-1}{4\pi s}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\tilde{x},\tilde{p}\rangle\langle\tilde{x},\tilde{p}|d\tilde{x}d\tilde{p}=I. \tag{26}$$

It is not hard to see that the square of the modulus of the wave function in Eq. (23) is equal to that of the ground-state function shifted along the x axis. Equation (23) also implies that our coherent states can be written as

$$\begin{aligned}|\tilde{x},\tilde{p}\rangle&=e^{-i\varphi}\exp(-i\tilde{x}P)\exp\left(-\frac{i}{s}\tilde{p}e^{-X}\right)|0\rangle\\&=e^{-i\varphi}\exp\left(-\frac{i}{s}\tilde{p}e^{\tilde{x}I}\right)\exp\left(-\frac{i}{s}\tilde{p}e^{-X}\right)\exp(-i\tilde{x}P)|0\rangle\\&=D(\tilde{x},\tilde{p})|0\rangle,\end{aligned} \tag{27}$$

where $|0\rangle:=|\beta=0\rangle=|\tilde{x}=0,\ \tilde{p}=0\rangle$ is identical to the ground state, itself being a coherent state, and $D(\tilde{x},\tilde{p})$ is a displacement operator. Using Eq. (4) for $A(s)$ and $A^{\dagger}(s)$, the latter can be rewritten as

$$\begin{aligned}D(\tilde{x},\tilde{p})=e^{-i\varphi}\exp(-i\tilde{p}I)\exp\left(\frac{\tilde{x}}{2}[A^{\dagger}(s)-A(s)]\right)\\\times\exp\left(\frac{i}{2s}\tilde{p}[A(s)+A^{\dagger}(s)]\right).\end{aligned} \tag{28}$$

We see that $D(\tilde{x},\tilde{p})$ is unitary for arbitrary $\tilde{x}$ and $\tilde{p}$, and it also proves that our states belong to the category of displacement operator coherent states according to [2].

V. CONCLUSIONS AND FINAL REMARKS

By using the set of generalized creation and annihilation operators we have introduced the complete orthonormal set of pseudo-number-states and the set of the coherent states for the Morse potential. We have shown how the parameter of $|\beta\rangle$ is connected with the expectation values of the coordinate and the momentum, and have determined the unitary displacement operator generating this state from the ground state.

In our construction of the states $|\beta\rangle$, the fundamental role has been played by the shape-invariant Lie algebra (9) spanned by the SUSY ladder operators plus the identity. The pseudo-number-states have been generated by their elements $A^{\dagger}(s+n)$, while the displacement operator $D(\tilde{x},\tilde{p})$ that yields the coherent states is the element of the corresponding Lie group obtained by exponentiating the SUSY ladder algebra. This indicates that the states $|\beta\rangle$ are coherent also in the Perelomov sense [5]. The algebra defined by Eq. (9) is solvable, but not nilpotent, and it is not isomorphic to the Heisenberg-Weyl algebra of the harmonic oscillator. Moreover, this ladder algebra is not isomorphic either to the class of so(2,1)≅su(1,1)≅sp(1,**R**), which has been applied to the various recent treatments of the Morse potential [7,15]. Therefore the SUSY ladder operator algebra and the coherent states presented here can be regarded as an alternative algebraic viewpoint for the description of the one-dimensional Morse potential. We also think that our construction will be useful in describing molecular interactions with the electromagnetic field.

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