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Coherent states and a path integral for the Morse oscillator

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Coherent states for the Morse oscillator are constructed using generalized coherent states associated with the SO(2,1) noninvariance group for this potential. By using the path integral over these states, it is shown that the Morse oscillator may be viewed as a harmonic oscillator evolving in a fictitious time. To show that this picture is mathematically consistent, we compute the path integral for the Green's function and recover the bound-state spectrum.

I. INTRODUCTION

Recently there has been much interest in the construction of coherent states for systems other than the harmonic oscillator. One approach is that taken by Nieto and collaborators[1–4] which is to adopt the requirement that generalized coherent states are minimum uncertainty states. However, the observables in the uncertainty relation are not necessarily the usual x and p but rather a new set of variables, say X and P, which need not be related to the old by a canonical transformation. X and P are chosen so that the transformed Hamiltonian looks like a harmonic oscillator. The coherent states are then obtained by finding the set of states that minimizes the uncertainty relation in the new variables. Another way to produce generalized coherent states is associated with irreducible representations of Lie groups,[5] in particular, those groups which are noninvariance or spectrum generating groups. The noncompact group $SO(2,1) \sim SU(1,1)$ is well known to be a noninvariance group for a number of systems such as the Coulomb problem,[6] the isotropic harmonic oscillator,[7] some many-body problems,[8,9] and the Morse oscillator (s states only).[10]

In this paper we consider the problem of constructing SO(2,1) coherent states (CS) for the Morse oscillator and also the related problem of writing the Green's function as a path integral over the SO(2,1) CS. In doing this latter problem we find it convenient to introduce a fictitious time variable. The introduction of a fictitious time parameter is not new. It was done some time ago by Kustaanheimo and Stiefel[11] for regularizing the Kepler problem in celestial mechanics. It was introduced into quantum mechanics by Duru and Kleinert[12] in their path integral calculation of the Coulomb Green's function, a calculation which was much improved by Ho and Inomata.[13] The present author has also used the fictitious time parameter in a SO(2,1) CS path integral calculation of the Coulomb Green's function.[14] Now upon introducing the fictitious time parameter we find that the classical mechanics is such that the Morse oscillator appears as a harmonic oscillator evolving in the new time on a curved phase space. In order to demonstrate the consistency of this picture we follow through the path integral calculation of the Green's function and recover the bound-state spectrum. Previously the Green's function for the Morse oscillator has been calculated by path integral techniques[15,16] where changing local coordinate variables as well as the time parameter is used to obtain a harmonic-oscillator—type short-time action which yields the Green's function in terms of Gaussian quadratures. In the present calculation, only the time parameter is modified.

The plan of the paper is as follows: In Sec. II we review the SO(2,1) formulation of the one-dimensional analog of the Morse oscillator; in Sec. III we give the SO(2,1) coherent states, a functional form of the Green's function in terms of these states, and the equivalent classical mechanics; in Sec. IV we carry out the path integration and calculate the resolvent; and in Sec. V we conclude the paper with some brief remarks.

II. SO(2,1) AND THE MORSE OSCILLATOR

In 1929, Morse[17] proposed the potential

$$V(r)=D(e^{-2a(r-r_0)}-2e^{-a(r-r_0)}) \tag{2.1}$$

to model the short-range forces of diatomic atoms. For the s states or equivalently, the one-dimensional analog, the Schrödinger equation is exactly solvable. Here we present an algebraic solution, in terms of the SO(2,1) Lie algebra, as given by Cordero and Hojman.[10]

We write the Schrödinger equation as

$$(H-E)|\psi\rangle=0\ , \tag{2.2}$$

where

$$H=\frac{1}{2m}p^2-D(e^{-2ax}-2e^{-ax})\ . \tag{2.3}$$

Here we have set $x=r-r_0$. Now we define a set of operators

$$K_0=\frac{1}{a^2h(x)}(p^2-2E)+h(x)\ , \tag{2.4a}$$

$$K_1=\frac{1}{a^2h(x)}(p^2-2E)-h(x)\ , \tag{2.4b}$$

$$K_2=\frac{i}{ax}(ixp)-\frac{i}{2}\ , \tag{2.4c}$$

where

$$h(x)=\frac{(8mD)^{1/2}}{a}e^{-ax}\ . \tag{2.5}$$

The above operators provide a realization of the SO(2,1) Lie algebra

$$[K_1,K_2]=-iK_0\ , \tag{2.6a}$$

$$[K_2,K_0]=iK_1\ , \tag{2.6b}$$

$$[K_0,K_1]=iK_2\ . \tag{2.6c}$$

The Hamiltonian of Eq. (2.3) may be written in terms of K_0 as

$$H=\frac{a^2h(x)}{2m}\left[K_0-\frac{(2mD)^{1/2}}{a}\right]+E \tag{2.7}$$

so that the Eq. (2.1) becomes

$$\frac{a^2h(x)}{2m}\left[K_0-\frac{(2mD)^{1/2}}{a}\right]|\psi\rangle=0\ . \tag{2.8}$$

The operator K_0, which generates a compact subgroup of SO(2,1) has a discrete spectrum in a $\mathscr{D}^+(k)$ representation such that

$$K_0|n,k\rangle=(n+k)|n,k\rangle\ , \tag{2.9}$$

where $n=0,1,2,\ldots$, and k is the so-called Bargmann index, $k>0$. With $C=K_0^2-K_1^2-K_2^2$ as the Casimir operator, one has

$$C|n,k\rangle=k(k-1)|n,k\rangle\ . \tag{2.10}$$

For the operators of Eqs. (2.4) one has

$$C=\frac{-2mE}{a^2}-\tfrac{1}{4} \tag{2.11}$$

so that

$$k=\tfrac{1}{2}+\sqrt{C+1/4}=\tfrac{1}{2}+\left[-\frac{2mE}{a^2}\right]^{1/2}. \tag{2.12}$$

Thus from Eqs. (2.8), (2.9), and (2.12) we determine the energy levels as

$$E_n=-\frac{a^2}{2m}\left[\frac{(2mD)^{1/2}}{a}-(n+\tfrac{1}{2})\right]^2, \tag{2.13}$$

where $n=0,1,2,\ldots,n_{\max}$, where $n_{\max}$ is the value for which E_n is maximum, $n_{\max}+\frac{1}{2}<(2mD)^{1/2}/a$. The cutoff excludes unbound states. This agrees with the spectrum given by Morse.[17]

Before closing this section a remark is in order. We note that through Eq. (2.12) k depends explicitly on E and thus through Eq. (2.13) on n. Thus we see that each level of the Morse oscillator corresponds to one state out of different $\mathscr{D}^+(k)$ representations of SO(2,1), one representation for each value of E_n. Apparently the number of representations needed to cover the states is $n_{\max}+1$.

III. COHERENT STATES AND PATH INTEGRAL FOR THE GREEN'S FUNCTION

The coherent states associated with SO(2,1) [or SU(1,1)] and the associated formulation of the path integral with them have been developed elsewhere[18–20] so will not be presented here in great detail. We give below only essential definitions and results.

We adopt the definition of Perelomov's[5] of generalized coherent states which gives states generated by a displacement-type operator acting on the ground state $|0,k\rangle$ of the irreducible representation of the group. With $K_\pm=K_1\pm iK_2$ then we have

$$|\xi,k\rangle=\exp(\alpha K_+-\alpha^*K_-)|0,k\rangle$$
$$=(1-|\xi|^2)^k\sum_{n=0}^{\infty}\left[\frac{\Gamma(n+2k)}{n!\Gamma(2k)}\right]^{1/2}\xi^n|n,k\rangle\ , \tag{3.1}$$

where $\alpha=-\frac{1}{2}\tau e^{-i\varphi}$ and $\xi=-\tanh(\tau/2)e^{-i\varphi}$. τ and φ are group parameters similar to the Euler angles, but τ has the range $-\infty<\tau<\infty$. Important properties possessed by these states are that (a) they satisfy a completeness relation

$$I=\int d\mu_k(\xi)\,|\xi,k\rangle\langle\xi,k|\ , \tag{3.2}$$

where

$$d\mu_k(\xi)=\frac{2k-1}{\pi}\frac{d^2\xi}{(1-|\xi|^2)}\ , \tag{3.3}$$

and (b) there exists the reproducing kernel

$$\mathscr{K}_k(\xi',\xi)=\langle\xi'k|\xi k\rangle$$
$$=(1-|\xi'|^2)^k(1-|\xi|^2)^k(1-\xi'^*\xi)^{-2k} \tag{3.4}$$

such that

$$\mathscr{K}_k(\xi',\xi)=\int d\mu_k(\xi'')\mathscr{K}_k(\xi',\xi'')\mathscr{K}_k(\xi'',\xi)\ . \tag{3.5}$$

We now consider the resolvent operator

$$G(E)=(E-H)^{-1}$$
$$=-i\int_0^\infty e^{-iT(H-E)}dT\ . \tag{3.6}$$

Then the Green's function in terms of SO(2,1) CS is given by

$$G_k(\xi'',\xi';E)=\langle\xi^\mu,k|G(E)|\xi',k\rangle$$
$$=-i\int_0^\infty P_E(\xi'',\xi';T)dT\ , \tag{3.7}$$

where

$$P_E(\xi'',\xi';T)=\langle \xi'',k\mid \exp[-iT(H-E)]\mid \xi',k\rangle$$
$$=\langle \xi'',k\mid \exp\left[-\frac{iTa^2h(x)}{2m}(K_0-\lambda)\right]\mid \xi',k\rangle \tag{3.8}$$

We have set $\lambda=(2mD)^{1/2}/a$. We may consider Eq. (3.8) as a propagator for the modified evolution operator $U(T)=\exp[-iT(H-E)]$. This propagator will subsequently be written in path integral form.

Before proceeding any further, however, we must discuss the role of the Bargmann index k. Note that Eq. (3.8) does not contain the energy E explicitly but rather is contained in k via Eq. (2.12). We stress at this point that E is not taken to be one of the energy eigenvalues of Eq. (2.13) but as simply a parameter. Later we recover the bound-state spectrum from the poles in $G(E)$.

Now we write Eq. (3.8) in the usual fashion[18] as

$$P_E(\xi'',\xi';T)=\lim_{N\to\infty}\int\cdots\int\left[\prod_{j=1}^{N-1}d\mu_k(\xi_j)\right]\prod_{j=1}^{N}\langle \xi_j,k\mid \exp\left[-i\,\Delta t_j\,h[x(t_j)]\frac{a^2}{2m}(K_0-\lambda)\right]\mid \xi_{j-1},k\rangle\ , \tag{3.9}$$

where $T=\sum_{j=1}^{N}\Delta t_j$, $\xi''=\xi_N$, and $\xi'=\xi_0$. At this point we introduce a new local time variable σ as

$$\Delta\sigma_j=\Delta t_j e^{-ax(t_j)}\ . \tag{3.10}$$

Thus we have

$$\tilde{P}_E(\xi'',\xi';\sigma)=P_E(\xi'',\xi';T)\ , \tag{3.11}$$

where

$$\sigma=\int_0^T dt\,e^{-ax(t)}\ . \tag{3.12}$$

Then we have

$$G_k(\xi'',\xi';E)=-\frac{i}{\hbar}\int_0^\infty P_E(\xi'',\xi';T)dT$$
$$=-\frac{i}{\hbar}\int_0^\infty \tilde{P}_E(\xi'',\xi';\sigma)\left[\frac{dT}{d\sigma}\right]d\sigma$$
$$=-\frac{i}{\hbar}\left[\frac{dT}{d\sigma}\right]\int_0^\infty e^{i2\omega\lambda\sigma}\tilde{K}(\xi'',\xi';\sigma)d\sigma\ , \tag{3.13}$$

where

$$\tilde{K}(\xi'',\xi';\sigma)=\lim_{N\to\infty}\int\cdots\int\left[\prod_{j=1}^{N-1}d\mu_k(\xi_j)\right]\prod_{j=1}^{N}\langle \xi_j,k\mid \exp(-i\Delta\sigma_j 2\omega K_0)\mid \xi_{j-1},k\rangle\ , \tag{3.14}$$

and where for later purposes we have set $\omega=a^2/4m$. The factor $dT/d\sigma$ is just $\exp[ax(t'')]$ where t'' is the time at the endpoint.

$\tilde{K}(\xi'',\xi';\sigma)$ may be interpreted as a propagator in the new time parameter. It may be written, following the usual procedures[18] in the path integral form

$$\tilde{K}(\xi'',\xi';\sigma)=\lim_{N\to\infty}\int\cdots\int\left[\prod_{j=1}^{N-1}d\mu_k(\xi_j)\right]\prod_{j=1}^{N}\exp\left\{i\left[\frac{ik\Delta\sigma_j}{(1-|\xi_j|^2)}\left[\xi_j^*\frac{\Delta\xi_j}{\Delta\sigma_j}-\xi_j\frac{\Delta\xi_j^*}{\Delta\sigma_j}\right]-\Delta\sigma_j\mathscr{H}_k(\xi_j,\xi_{j-1})\right]\right\}, \tag{3.15}$$

where

$$\mathscr{H}_k(\xi_j,\xi_{j-1})=\frac{\langle \xi_j,k\mid H\mid \xi_{j-1},k\rangle}{\langle \xi_j,k\mid \xi_{j-1},k\rangle}\ , \tag{3.16}$$

and where

$$H=2\omega K_0 \tag{3.17}$$

is the effective Hamiltonian. In the continuum limit the propagator becomes

$$\tilde{K}(\xi'',\xi';\sigma)=\int \mathscr{D}\mu_k(\xi)\exp\left[i\int_0^\sigma d\sigma\,\mathscr{L}_k(\xi,\xi')\right]\ , \tag{3.18}$$

where

$$\mathscr{L}_k=\frac{ik}{(1-|\xi|^2)}(\xi^*\xi'-\xi\xi'^*)-\mathscr{H}_k(\xi,\xi^*)\ , \tag{3.19}$$

and where the prime denotes differentiation with respect to σ. The Euler-Lagrange equations can be shown to yield[18] the equations of motion

$$\xi'=\{\xi,\mathscr{H}_k\}\ , \tag{3.20}$$

where $\{,\}$ is a Poisson bracket defined by

$$\{A,B\}=\frac{(1-|\xi|^2)^2}{2ik}\left[\frac{\partial A}{\partial \xi}\frac{\partial \beta}{\partial \xi^*}-\frac{\partial A}{\partial \xi^*}\frac{\partial B}{\partial \xi}\right]. \tag{3.21}$$

This indicates that the classical phase space spanned by ξ and ξ^* is curved—in fact the Lobachevski plane.[21]

At this point the Morse oscillator may be depicted as a harmonic oscillator evolving in the new time parameter σ. As we have discussed elsewhere,[18,19,22] the Hamiltonian for a harmonic oscillator may be written in the SO(2,1) generators simply as $H_0=2\omega_0 K_0$ where an additive constant has been dropped. The motion on the curved phase space then proceeds in real time as

$$\xi(t)=\xi_0 e^{-2i\omega_0 t}, \tag{3.22}$$

where ξ_0 is constant. As we have already shown above, the effective Hamiltonian for the Morse oscillator evolving in the fictitious time has the same form as for the harmonic oscillator evolving in real time. Thus the solution of Eq. (3.20) is, by analogy to Eq. (3.22),

$$\xi(\sigma)=\xi_0 e^{-2i\omega\sigma}. \tag{3.23}$$

IV. CALCULATION OF THE PATH INTEGRAL

To complete the calculations of the path integral of Eq. (3.15) we write it as

$$\tilde{K}(\xi'',\xi';\sigma)=\lim_{N\to\infty}\int\cdots\int\left[\prod_{j=1}^{N-1}d\mu_k(\xi_j)\right]\prod_{j=1}^{N}\langle\xi_j,k\,|\exp(-i\Delta\sigma_j 2\omega K_0)|\,\xi_{j-1},k\rangle . \tag{4.1}$$

From Eq. (3.1) we have

$$\langle\xi_j,k\,|\exp(-i\Delta\sigma_j 2\omega K_0)|\,\xi_{j-1},k\rangle=\exp(-i\Delta\sigma_j 2\omega k)\langle\xi_j,k\,|\,(\xi_{j-1}e^{-i\Delta\sigma_j 2\omega}),k\rangle . \tag{4.2}$$

Then with repeated use of Eqs. (3.4) and (3.5) we obtain

$$\tilde{K}(\xi'',\xi';\sigma)=\exp(-i\sigma 2\omega k)\times(1-|\xi''|^2)^k(1-|\xi'|^2)^k\times(1-\xi''^*\xi' e^{-i\sigma 2\omega})^{-2k} \tag{4.3}$$

where $\sigma=\lim_{N\to\infty}\sum_{j=1}^{N}\Delta\sigma_j$. Thus the Green's function in integral form is

$$G_k(\xi'',\xi';E)=-\frac{i}{\hbar}\int_0^\infty e^{i\sigma 2\omega(\lambda-k)}(1-|\xi''|^2)^k(1-|\xi'|^2)^k\times(1-\xi''^*\xi' e^{-i\sigma 2\omega})^{-2k}d\sigma . \tag{4.4}$$

To recover the spectrum we take the trace of the resolvent operator as

$$\begin{aligned}\mathrm{Tr}G(E)&=\int d\mu_k(\xi)\,G_k(\xi,\xi;E)\\&=-\frac{i}{2}\left[\frac{dT}{d\sigma}\right]\int_0^\infty d\sigma\exp[i\sigma 2\omega(\lambda-k+\tfrac{1}{2})]\times[\sin(\omega\sigma)]^{-1} .\end{aligned} \tag{4.5}$$

Upon expanding the last factor in (4.5) as

$$\frac{1}{2i}[\sin(\omega\sigma)]^{-1}=e^{-i\omega\sigma}\sum_{q=0}^{\infty}e^{-iq2\omega\sigma}, \tag{4.6}$$

we obtain

$$\begin{aligned}\mathrm{Tr}G(E)&=\left[\frac{dT}{d\sigma}\right]\sum_{q=0}^{\infty}\int_0^\infty d\sigma\exp[i\sigma 2\omega(\lambda-k-q)]\\&=2i\omega\left[\frac{dT}{d\sigma}\right]\sum_{q=0}^{\infty}(\lambda-k-q)^{-1}\\&=2i\omega\left[\frac{dT}{d\sigma}\right]\sum_{q=0}^{\infty}\left[\lambda-q-\frac{1}{2}-\left[-\frac{2mE}{a^2}\right]^{1/2}\right]^{-1} .\end{aligned} \tag{4.7}$$

Obviously poles occur whenever

$$E=E_q=-\frac{a^2}{2m}\left[\frac{(2mD)^{1/2}}{a}-(q+\tfrac{1}{2})\right]^2 \tag{4.8}$$

in agreement with Eq. (2.13).

V. CONCLUSION

In this paper we have given a coherent state picture of the Morse oscillator wherein the motion takes place on a curved phase space and with the time parameter being a fictitious time related to real time by Eq. (3.12). This may be contrasted with the works of Nieto and Simmons[1] where the Morse oscillator is made to look like a harmonic oscillator by using noncanonical variables.

The group theoretical formulation we have used however is not the only one possible. Alhassid *et al.*[23] have recently shown that U(2) may be used to describe the bound states while U(1,1) describes the scattering states. This picture is attractive since the Morse oscillator has a finite number of bound states so that one representation of U(2) should contain all those states. However this formulation appears to require that the well depth D be quantized. This requirement need not be satisfied with the SO(2,1) formulation.

Elsewhere[19,24] we have considered coherent states for the Coulomb problem. Again using the SO(2,1) spectrum generating group, the radial motion appears oscillatorlike in fictitious time.[19] Using the Kustaanheimo-Stiefel transformation[11] the Coulomb problem can be rendered into a constrained four-dimensional harmonic oscillator.[25] Ordinary coherent states may be written for this oscillator, again evolving in a new time parameter. When projected back into physical space, these states are seen to follow the classical Kepler orbits in real time.[24] Thus it appears that the introduction of a new time parameter is of great utility in formulating generalized coherent states.

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