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Gazeau–Klauder quasi-coherent states for the Morse oscillator

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Abstract

In the Letter, we have constructed and investigated some properties of the Gazeau–Klauder quasi-coherent states for the Morse potential, previously deduced by Roy and Roy. We have focused our attention on the thermal states and we have found the analytical form for the diagonal P-representation of the density operator.
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1. Introduction

The Morse potential is one of the most simple and "realistic" three-parameter anharmonic potential model, which has proven to be very useful for solving various problems from diverse fields of physics (e.g., spectroscopy, diatomic and polyatomic molecule vibration and scattering). The one-dimensional non-rotational Morse Hamiltonian has the form [1]:

$$H_M(r) = -\frac{\hbar^2}{2m_r}\frac{d^2}{dr^2} + D\left[1 - e^{-\alpha(r-r_e)}\right]^2 \tag{1}$$

where r represents the internuclear distance, r_e is the equilibrium internuclear separation of the system of two nuclei in the diatomic molecule, m_r is the reduced mass, α is the Morse constant of anharmonicity, and D is the dissociation energy of the diatomic molecule (i.e., the depth of the potential energy well).

Based on the recent work of Gazeau and Klauder [2], who have determined a set of criteria which a new coherent state $|J,\gamma\rangle$ (later called "Gazeau–Klauder coherent state") should satisfy, last year, Roy and Roy [3] have constructed and examined the coherent states for the Morse potential, using the formalism of Gazeau and Klauder.

In the present Letter we shall verify explicitly the conditions from the paper [2] for the case of Morse potential and examine other interesting properties of these states.

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2. The basic properties—revisited

In order to associate the usual coherent states with the Hamiltonian problems, Gazeau and Klauder have made some important modifications in the definition of coherent states [2,4]: the parametrization of the state $|z\rangle$ in terms of a single complex number z is extended by replacing z by two independent real numbers J and γ, so that $J \geqslant 0$ and $-\infty < \gamma < \infty$, namely $z = \sqrt{J}\exp(-\mathrm{i}\gamma)$. In this way, the new obtained state is $|J, \gamma\rangle$.

Let us review the concrete construction of the states $|J, \gamma\rangle$ for the Morse oscillator potential, following the path of Roy and Roy [3] and correcting an *omission* in their paper.

The eigenequation and the eigenvalues E_n for the Morse Hamiltonian H_M are

$$H_M|[N], n\rangle = E_n|[N], n\rangle, \tag{2}$$

$$E_n = 4\frac{D}{K}\left(n+\frac{1}{2}\right) - 4\frac{D}{K^2}\left(n+\frac{1}{2}\right)^2 = \hbar\omega\left(n+\frac{1}{2}\right) - \frac{\hbar\omega}{K}\left(n+\frac{1}{2}\right)^2 = E_0 + \hbar\omega\left(1-\frac{1}{K}\right)n - \frac{\hbar\omega}{K}n^2, \tag{3}$$

where we have used the following notations and also the angular frequency ω for the Morse oscillator

$$K = 2\frac{\sqrt{2m_r D}}{\alpha\hbar}, \qquad E_0 = \frac{\hbar\omega}{2}\left(1-\frac{1}{2K}\right), \quad \omega = \alpha\sqrt{\frac{2D}{m_r}}. \tag{4}$$

The eigenequation (2) can be rewritten in the following dimensionless manner:

$$H|[N], n\rangle = e_n|[N], n\rangle, \tag{5}$$

where $n = 0, 1, \ldots, [N/2]$ ($[x]$ represent the integer part of the real number x) and

$$H = \frac{H_M - E_0}{\hbar\omega}, \qquad e_n = \frac{1}{K}n(K-1-n) = \frac{1}{N+1}n(N-n). \tag{6}$$

To make the writing simpler, as in the last equality, in the remaining part of the Letter, instead of the Child's parameter K [5], we also prefer to use the dimensionless parameter N

$$N = K - 1, \tag{7}$$

and thus, the maximal number of the bound states for the Morse oscillator is $n_{\max} = [N/2]$.

With these considerations (we make the specification that some of our notations are different from those of Roy and Roy [3]), the states $|J, \gamma\rangle$ become:

$$|J, \gamma\rangle = \mathcal{N}(J)\sum_{n=0}^{[N/2]}\frac{J^{\frac{n}{2}}e^{-\mathrm{i}\gamma e_n}}{\sqrt{\rho(n)}}|[N], n\rangle. \tag{8}$$

The quantity $\rho(n)$ is defined as a unique function of e_n's, namely,

$$\rho(n) = \prod_{k=1}^{n} e_k = \Gamma(N)\frac{\Gamma(n+1)}{(N+1)^n\Gamma(N-n)}, \qquad \rho(0) = 1. \tag{9}$$

According to [2,3] the Gazeau–Klauder coherent state (GK-CS) (8) must be: (a) normalizable; (b) continuous in two labels J and γ and must satisfy: (c) the resolution of unity, with a necessarily positive associated measure; (d) the temporal stability condition and (e) the action identity.

Then, the matrix elements of an operator A which characterize the Morse oscillator, in a $|J, \gamma\rangle$-representation, are

$$\langle J', \gamma'|A|J, \gamma\rangle = \mathcal{N}(J')\mathcal{N}(J)\sum_{v,n=0}^{[N/2]}\frac{J'^{\frac{v}{2}}J^{\frac{n}{2}}}{\sqrt{\rho(v)\rho(n)}}e^{\mathrm{i}(\gamma' e_v - \gamma e_n)}\langle [N], v|A|[N], n\rangle. \tag{10}$$

By particularizing the operator A and the labels J and γ, we get to a series of interesting properties. So, if $A = I$ (unity operator), due to the orthonormality of the eigenvectors $|[N], n\rangle$, we obtain the overlap

$$\langle J', \gamma' | J, \gamma\rangle = \mathcal{N}(J')\mathcal{N}(J) \sum_{n=0}^{[N/2]} \frac{(J'J)^{\frac{n}{2}}}{\rho(n)} e^{\mathrm{i}(\gamma'-\gamma)e_n}, \tag{11}$$

which becomes simpler if $\gamma' = \gamma$.

If $A = I$, $\gamma' = \gamma$ and $J' = J$, we obtain the normalization to unity

$$\langle J, \gamma | J, \gamma\rangle = [\mathcal{N}(J)]^2 \sum_{n=0}^{[N/2]} \frac{J^n}{\rho(n)} = 1, \tag{12}$$

from which the *normalization* constant is

$$[\mathcal{N}(J)]^{-2} = \sum_{n=0}^{[N/2]} \frac{J^n}{\rho(n)} \equiv \mathcal{F}(J), \qquad \mathcal{N}(J) = \frac{1}{\sqrt{\mathcal{F}(J)}}. \tag{13}$$

We note that the series (13) determining the normalization constant $\mathcal{N}(J)$ is a finite series and thus it exists for all values of J [6]. Consequently, the states $|J, \gamma\rangle$ for the Morse potential (8) are normalizable and the normalization constant (13) is a continuous function in label J.

The *continuity* in two labels J and γ follows from the continuity of the overlap $\langle J', \gamma' | J, \gamma\rangle$ because

$$\big\| |J, \gamma\rangle - |J', \gamma'\rangle \big\|^2 = 2\big(1 - \mathrm{Re}\langle J', \gamma' | J, \gamma\rangle\big) \to 0, \tag{14}$$

when $(J', \gamma') \to (J, \gamma)$.

If the operator A is diagonal in the $|[N], n\rangle$-basis, i.e.,

$$\langle [N], n | A | [N], n\rangle = a_n \delta_{vn} \tag{15}$$

it follows that the diagonal elements in the $|J, \gamma\rangle$-representation are

$$\langle J, \gamma | A | J, \gamma\rangle \equiv \langle A\rangle_J = \frac{1}{\mathcal{F}(J)} \sum_{n=0}^{[N/2]} \frac{J^n}{\rho(n)} a_n. \tag{16}$$

As an example, if $A = \hat{v}^s$, where $\hat{v}$ is the number operator $\hat{v}|[N], n\rangle = n|[N], n\rangle$ and $s = 1, 2, \ldots$ it results

$$\big\langle \hat{v}^s \big\rangle_J = \frac{1}{\mathcal{F}(J)} \sum_{n=0}^{[N/2]} \frac{J^n}{\rho(n)} n^s = \frac{1}{\mathcal{F}(J)} \left(J \frac{d}{dJ}\right)^s \mathcal{F}(J). \tag{17}$$

The expectations of the two first powers of $\hat{v}$ are

$$\langle \hat{v}\rangle_J = J \frac{d}{dJ} \ln \mathcal{F}(J), \tag{18}$$

$$\big\langle \hat{v}^2 \big\rangle_J = J \frac{d}{dJ} \ln \mathcal{F}(J) + \left(J \frac{d}{dJ} \ln \mathcal{F}(J)\right)^2 + J^2 \left(\frac{d}{dJ}\right)^2 \ln \mathcal{F}(J). \tag{19}$$

These expectations are useful in order to calculate the variance of the number operator

$$(\sigma_{\hat{v}})_J \equiv \big\langle \hat{v}^2 \big\rangle_J - \big(\langle \hat{v}\rangle_J\big)^2 = \left(J \frac{d}{dJ} \ln \mathcal{F}(J)\right)^2 + J^2 \left(\frac{d}{dJ}\right)^2 \ln \mathcal{F}(J), \tag{20}$$

as well as the second-order correlation function [7,8] for the Morse oscillator

$$\left(g^2\right)_J = \frac{\langle \hat{v}^2\rangle_J - \langle \hat{v}\rangle_J}{(\langle \hat{v}\rangle_J)^2} = 1 + \frac{(\frac{d}{dJ})^2 \ln \mathcal{F}(J)}{(\frac{d}{dJ} \ln \mathcal{F}(J))^2}. \tag{21}$$

Moreover, the Mandel Q-parameter [9,10] is

$$Q_J = \frac{(\sigma_{\hat{v}})_J}{\langle \hat{v}\rangle_J} - 1 = \langle \hat{v}\rangle_J\left[\left(g^2\right)_J - 1\right] = J\frac{(\frac{d}{dJ})^2 \ln \mathcal{F}(J)}{\frac{d}{dJ} \ln \mathcal{F}(J)}. \tag{22}$$

The last two quantities provide information about the inherent statistical properties of the states $|J,\gamma\rangle$. These properties depend on the analytical expressions of the functions (21) and (22) as depending on the variable J. Because of the structure of these functions, $(g^2)_J$ and Q_J are difficult to be evaluated analytically, so they must be calculated numerically. Generally speaking, the states $|J,\gamma\rangle$ exhibit sub-Poissonian statistics for those values of J for which $Q_J < 0$, Poisson statistics for values for which $Q_J = 0$ and supra-Poissonian statistics for values of J for which $Q_J > 0$.

The *resolution of the unity* in terms of a certain set of states is a very important property because it allows the practical use of these states as a basis in the Hilbert space [7]. Let $\mathcal{H}_{[N/2]}$ be a finite-dimensional subspace of the Hilbert space $\mathcal{H}$, which is spanned by the complete orthonormal set of $[N/2]+1$ states $|[N],n\rangle$ $(n = 0,1,2,\ldots,[N/2])$. Then, $\hat{I}_{[N/2]}$ is the projection operator on the subspace $\mathcal{H}_{[N/2]}$ [11] and the resolution of the unity in terms of the states $|J,\gamma\rangle$ can be performed in the following manner:

$$\int d\mu_N(J,\gamma)\,|J,\gamma\rangle\langle J,\gamma| = \hat{I}_{[N/2]} = \sum_{n=0}^{[N/2]} |[N],n\rangle\langle[N],n|. \tag{23}$$

The states $|J,\gamma\rangle$ exist only if the radius of convergence R is non-zero [4], and this fact is easy to demonstrate for the case of Morse oscillator:

$$R = \lim_{n\to\infty}[\rho(n)]^{\frac{1}{n}} \to \infty, \tag{24}$$

by using the Stirling's formula for $\Gamma(n+1)$ and the following limit [13]:

$$\lim_{N\to\infty}\frac{\Gamma(N+k)}{\Gamma(N)N^k} = 1, \tag{25}$$

valid for any k and N.

If we assume the integration measure $d\mu_N(J,\gamma)$ so that [4]

$$\int(\ldots)\,d\mu_N(J,\gamma) = \frac{1}{\pi}\int_{-\pi}^{\pi} d\gamma \int_0^\infty (\ldots)k(J)\,dJ \tag{26}$$

we obtain

$$\int d\mu_N(J,\gamma)\,|J,\gamma\rangle\langle J,\gamma| = \sum_{n=0}^{[N/2]} \frac{|[N],n\rangle\langle[N],n|}{\rho(n)} \int_0^\infty J^n[\mathcal{N}(J)]^2 k(J)\,dJ = 1. \tag{27}$$

After the function change

$$k(J) = \frac{1}{[\mathcal{N}(J)]^2}h(J), \tag{28}$$

the above integral leads to the following Stieltjes moment problem:

$$\int_0^\infty J^n h(J)\,dJ = \rho(n) = \Gamma(N)\frac{\Gamma(n+1)}{(N+1)^n\Gamma(N-n)}, \tag{29}$$

i.e., the positive constants $\rho(n)$ arise as moments of a probability distribution $h(J)$.

Following the standard method [4] and using the definition of Meijer's G-function and the Mellin inversion theorem, from which it follows that [12,13]

$$\int_0^\infty dx\, x^{s-1} G^{m,n}_{p,q}\left(\alpha x \,\middle|\, \begin{matrix} a_1, \ldots, a_n, a_{n+1}, \ldots, a_p \\ b_1, \ldots, b_m, b_{m+1}, \ldots, b_q \end{matrix}\right) = \frac{1}{\alpha^s}\frac{\prod_{j=1}^m \Gamma(b_j+s)\prod_{j=1}^n \Gamma(1-a_j-s)}{\prod_{j=m+1}^q \Gamma(1-b_j-s)\prod_{j=n+1}^p \Gamma(a_j+s)}, \tag{30}$$

we can express the function $h(J)$ in terms of the Meijer's G-function

$$h(J) = (N+1)\Gamma(N)G^{10}_{02}\big((N+1)J\,\big|\,0, -N\big) = (N+1)^{-\frac{N}{2}+1}\Gamma(N)J^{-\frac{N}{2}}J_N\big(2\sqrt{(N+1)J}\big), \tag{31}$$

where $J_N(\ldots)$ is the Bessel function of the first kind.

In essence, this result is the same as that obtained by Roy and Roy for the probability distribution (see, Eq. (11) of Ref. [3]), taking into account that our notations are rather different: $M+1=N$, so that $n_{\max} = M+1 = [N/2]$. On the other hand, the factor $N+1$ (which is very important in calculations concerning the harmonic limit, as we will see in the last section) is *omitted* in the Ref. [3].

Finally, the correct integration measure becomes

$$d\mu_N(J,\gamma) = (N+1)^{-\frac{N}{2}+1}\Gamma(N)\,d\gamma\,dJ\,\mathcal{F}(J)J^{-\frac{N}{2}}J_N\big(2\sqrt{(N+1)J}\big). \tag{32}$$

In order to verify the *temporal stability condition* of the states $|J,\gamma\rangle$, we apply the operator $\exp(-\mathrm{i}\omega t H)$ and, using the eigenvalue equation (5), we immediately obtain

$$\exp(-\mathrm{i}\omega t H)|J,\gamma\rangle = \mathcal{N}(J)\sum_{n=0}^{[N/2]}\frac{J^{\frac{n}{2}}e^{-\mathrm{i}(\gamma+\omega t)e_n}}{\sqrt{\rho(n)}}\big|[N], n\big\rangle = |J, \gamma+\omega t\rangle. \tag{33}$$

The temporal stability means that, under the chosen dynamics, the temporal evolution of the state $|J,\gamma\rangle$ proceeds to $|J,\gamma+\omega t\rangle$, for an arbitrary fixed positive parameter ω.

The *action identity*, written for the dimensionless Hamiltonian H can be obtained from the Eq. (16), i.e.,

$$\langle J,\gamma|H|J,\gamma\rangle = \frac{1}{\mathcal{F}(J)}\sum_{n=0}^{[N/2]}\frac{J^n}{\rho(n)}e_n = \frac{N}{N+1}\langle\hat{v}\rangle_J - \frac{1}{N+1}\big\langle\hat{v}^2\big\rangle_J \tag{34}$$

and, after the straightforward calculations, becomes

$$\langle J,\gamma|H|J,\gamma\rangle = \frac{N-1}{N+1}J\frac{d}{dJ}\ln\mathcal{F}(J) - \frac{1}{N+1}\left[\left(J\frac{d}{dJ}\ln\mathcal{F}(J)\right)^2 + J^2\left(\frac{d}{dJ}\right)^2\ln\mathcal{F}(J)\right] \equiv f(J). \tag{35}$$

We see that this is a certain function of the label J and this fact characterizes all the coherent states corresponding to systems with a finite-dimensional energy spectrum, as it was mentioned earlier [3].

Therefore, the states $|J,\gamma\rangle$, constructed for the Morse potential, satisfy all criteria (a)–(e) for the coherent states, as it was underlined in [3]. However, a problem comes out in connection to the weight function $k(J)$ in the integration measure $d\mu_N(J,\gamma)$ (26).

According to the general requirements for the coherent states [2,4], the weight function $k(J)$ must be a positive function. Thanks to the Bessel function $J_N(2\sqrt{(N+1)J})$, the results expressed in (32) have both positive and negative components. This kind of measure does not lead to coherent states which require a positive (or at least non-negative) measure for the projection operators. For this reason we consider that the above constructed states $|J,\gamma\rangle$ are not "pure" or "classical" Gazeau–Klauder coherent states, as it was pointed out in [3] and, maybe, it is better to call these states the *Gazeau–Klauder quasi-coherent states for the Morse potential*. Consequently, in the remaining part of this Letter we will call the states $|J,\gamma\rangle$ (8) the Gazeau–Klauder quasi-coherent states (GK-qCSs).

Although these quasi-coherent states do not have a positive weight function, they have a series of interesting properties (some of them were presented in Ref. [3]) which, as we will see, all lead to the corresponding properties of the harmonic oscillator at the harmonic limit.

In the next section, we shall examine other interesting properties of the Gazeau–Klauder quasi-coherent states for the Morse potential, especially those connected with the mixed quantum states, i.e., the thermal states.

3. Thermal states for the Morse potential

Now, we will carry out a detailed discussion on the statistical properties of the previously deduced quasi-coherent states for the Morse oscillator $|J,\gamma\rangle$. We consider a quantum system which consists of a gas of one-dimensional non-rotational Morse oscillators in thermodynamic equilibrium with the thermostat at temperature $T=(k_B\beta)^{-1}$ (where k_B is Boltzmann's constant and β the corresponding temperature constant), which obeys the quantum canonical distribution. The corresponding normalized density operator is then

$$\rho_N=\frac{1}{Z_N}\sum_{n=0}^{[N/2]}e^{-\beta E_n}|[N],n\rangle\langle[N],n|, \tag{36}$$

where Z_N is the normalization constant, i.e., the partition function for a fixed parameter N, which characterizes the maximum number of bound vibrational states for a certain diatomic molecule.

Their matrix elements in the $\{|J,\gamma\rangle\}$-representation are

$$\langle J',\gamma'|\rho_N|J,\gamma\rangle=\frac{1}{Z_N}\frac{1}{\sqrt{\mathcal{F}(J')\mathcal{F}(J)}}\sum_{n=0}^{[N/2]}e^{-\beta E_n}\frac{1}{\rho(n)}(J'J)^{\frac{n}{2}}e^{-\mathrm{i}(\gamma-\gamma')e_n}. \tag{37}$$

Using the integral [13]

$$\int_0^\infty x^\mu J_\nu(ax)\,dx=\frac{1}{a}\left(\frac{2}{a}\right)^\mu\frac{\Gamma(\frac{1}{2}+\frac{\nu}{2}+\frac{\mu}{2})}{\Gamma(\frac{1}{2}+\frac{\nu}{2}-\frac{\mu}{2})},\quad -\operatorname{Re}\nu-1<\operatorname{Re}\mu<\frac{1}{2}, \tag{38}$$

from the normalization condition

$$\operatorname{Tr}\rho_N=\int d\mu_N(J,\gamma)\,\langle J,\gamma|\rho_N|J,\gamma\rangle=1, \tag{39}$$

we recover the correct expression of the vibrational partition function

$$Z_N=\sum_{n=0}^{[N/2]}e^{-\beta E_n}. \tag{40}$$

This suggests that the resolution of unity (23) with the integration measure (32), as well as the expression of the density matrix elements (37) are correct.

Because the GK-qCSs $|J,\gamma\rangle$ form an overcomplete set of states, they may be used as a basis set despite the fact that they are non-orthogonal.

In order to find the quasi-probability distribution function $P_N(z)$ from the diagonal expansion of the density operator ρ_N in the GK-qCSs,

$$\rho_N = \frac{1}{Z_N} \int d\mu_N(J,\gamma)\, |J,\gamma\rangle P_N(J) \langle J,\gamma|, \tag{41}$$

we observe that the equation

$$\langle f|\rho_N|g\rangle = \frac{1}{Z_N} \int d\mu_N(J,\gamma)\, \langle f|J,\gamma\rangle P_N(J) \langle J,\gamma|g\rangle \tag{42}$$

must be fulfilled for any arbitrary vectors $\langle f|$ and $|g\rangle$ from the Hilbert space (or, for any vectors from the basis $|J,\gamma\rangle$ or $|[N],n\rangle$). What is more, from the trace-condition (39) and the scalar product or overlap (11), it follows that the P-function satisfies the normalization condition

$$\int d\mu_N(J,\gamma)\, P_N(J) = 1. \tag{43}$$

The left-hand side of Eq. (42) is

$$\mathrm{LHS} = \frac{1}{Z_N} \sum_{n=0}^{[N/2]} e^{-\beta E_n} \langle f|[N],n\rangle \langle [N],n|g\rangle, \tag{44}$$

while, after the angular integration

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} d\gamma\, e^{-\mathrm{i}(e_n - e_v)\gamma} = \delta_{nv}, \tag{45}$$

the right-hand side becomes

$$\mathrm{RHS} = (N+1)^{-\frac{N}{2}+1} \Gamma(N) \sum_{n=0}^{[N/2]} \frac{\langle f|[N],n\rangle \langle [N],n|g\rangle}{\rho(n)} \int_0^\infty J^{n-\frac{N}{2}} J_N\big(2\sqrt{(N+1)J}\big) P_N(J)\, dJ. \tag{46}$$

Comparing LHS and RHS we obtain that the integral must be

$$\int_0^\infty J^{n-\frac{N}{2}} J_N\big(2\sqrt{(N+1)J}\big) P_N(J)\, dJ = \frac{1}{Z_N} e^{-\beta E_n} \frac{\Gamma(n+1)}{(N+1)^{n-\frac{N}{2}+1} \Gamma(N-n)}, \tag{47}$$

where $P_N(J)$ is an unknown function. In order to determine it, we adopt the following strategy.

The energy eigenvalues of the Morse oscillator (see, Eq. (3)) depend on the square of the vibrational quantum number n and, as a result, the energy exponential $\exp(-\beta E_n)$ is not suitable to be written as a product of a constant quantity and a natural n-power of an exponential (as well as in the case of the harmonic oscillator) and to be used in solving the integral (47) in the standard manner, i.e., as the Stieltjes moment problem [12,13]. So, to avoid this inconvenience, it is necessary to elaborate a special method as indicated below.

First of all, we can write the energy exponential as follows:

$$\beta E_n \equiv \beta E_0 + \mathcal{A} n - \mathcal{B} n^2, \tag{48}$$

where the used notations are:

$$\mathcal{A} \equiv \beta\hbar\omega\left(1 - \frac{1}{K}\right) = \hbar\omega\left(1 - \frac{1}{N+1}\right), \qquad \mathcal{B} \equiv \beta\frac{\hbar\omega}{K} = \beta\frac{\hbar\omega}{N+1}. \tag{49}$$

For most of the diatomic molecules $\mathcal{B} \ll \mathcal{A}$. So, the limits of the parameter $K = N + 1$ (see, Eq. (7)) are very large, e.g., $K = 37.1586$ for H_2 molecule, i.e., for a "light" molecule and $K = 348.78$ for I_2, a "heavy" molecule [14]. As a consequence, the quantity $\mathcal{B}$ can be regarded as a perturbation constant and the energy exponential can be expanded in the power series as follows:

$$e^{-\beta E_n} = e^{-\beta E_0} e^{-\mathcal{A} n} e^{\mathcal{B} n^2} = e^{-\beta E_0} e^{-\mathcal{A} n} \sum_{k=0}^{\infty} \frac{\mathcal{B}^k}{k!} n^{2k}. \tag{50}$$

By writing

$$e^{-\mathcal{A} n} n^{2k} = \left(\frac{d}{d\mathcal{A}}\right)^{2k} e^{-\mathcal{A} n} \tag{51}$$

we finally have

$$e^{-\beta E_n} = e^{-\beta E_0} \sum_{k=0}^{\infty} \frac{\mathcal{B}^k}{k!} \left(\frac{d}{d\mathcal{A}}\right)^{2k} \left[e^{-\mathcal{A}}\right]^n. \tag{52}$$

It is obvious that the P-function also depends on the quantities $\mathcal{A}$ and $\mathcal{B}$, besides the variable J. This leads to the idea that $P_N(J) \equiv P_N(J, \mathcal{A}, \mathcal{B})$ can also be expanded in a power series similarly to the energy exponential (52) in the following manner:

$$\begin{aligned} P_N(J) &= \frac{1}{Z_N} e^{-\beta E_0} \sum_{k=0}^{\infty} \frac{\mathcal{B}^k}{k!} \left[\left(\frac{d}{d\mathcal{A}}\right)^k P_N(J, \mathcal{A}, \mathcal{B})\right]_{\mathcal{B}=0} \\ &\equiv \frac{1}{Z_N} e^{-\beta E_0} (N+1)^{\frac{N}{2}-1} \sum_{k=0}^{\infty} \frac{\mathcal{B}^k}{k!} \left(\frac{d}{d\mathcal{A}}\right)^{2k} X_N(J, \mathcal{A}), \end{aligned} \tag{53}$$

where the function $X_N(J, \mathcal{A})$ is to be determined.

By inserting Eqs. (52) and (53) into Eq. (47), we obtain:

$$\int_0^{\infty} J^{n-\frac{N}{2}} J_N\left(2\sqrt{(N+1)J}\right) X_N(J, \mathcal{A})\, dJ = \frac{1}{[e^{\mathcal{A}}(N+1)]^n} \frac{\Gamma(n+1)}{\Gamma(N-n)}. \tag{54}$$

With the help of a new function

$$X_N(J, \mathcal{A}) = \frac{1}{J_N(2\sqrt{(N+1)J})} h_N(J, \mathcal{A}) \tag{55}$$

and extending the natural values of n to complex s such that $n - \frac{N}{2} = s - 1$, we get to the following Stieltjes moment problem:

$$\int_0^{\infty} J^{s-1} h_N(J, \mathcal{A})\, dJ = \frac{1}{[e^{\mathcal{A}}(N+1)]^{\frac{N}{2}-1}} \frac{1}{[e^{\mathcal{A}}(N+1)]^s} \frac{\Gamma(\frac{N}{2}+s)}{\Gamma(\frac{N}{2}+1-s)}. \tag{56}$$

The solution of such a problem is [12]

$$h_N(J, \mathcal{A}) = \frac{1}{[e^{\mathcal{A}}(N+1)]^{\frac{N}{2}-1}} G_{02}^{10}\left(e^{\mathcal{A}}(N+1)J \,\middle|\, \tfrac{N}{2}, -\tfrac{N}{2}\right) = \frac{1}{[e^{\mathcal{A}}(N+1)]^{\frac{N}{2}-1}} J_N\left(2\sqrt{e^{\mathcal{A}}(N+1)J}\right). \tag{57}$$

Finally, the P-function is

$$P_N(J)=\frac{1}{Z_N}e^{-\beta E_0}\sum_{k=0}^{\infty}\frac{\mathcal{B}^k}{k!}\left(\frac{d}{d\mathcal{A}}\right)^{2k}\left[\left(e^{\mathcal{A}}\right)^{1-\frac{N}{2}}\frac{J_N(2\sqrt{e^{\mathcal{A}}(N+1)J}\,)}{J_N(2\sqrt{(N+1)J}\,)}\right]. \tag{58}$$

We can also use the following operator identity:

$$\sum_{k=0}^{\infty}\frac{\mathcal{B}^k}{k!}\left(\frac{d}{d\mathcal{A}}\right)^{2k}\equiv\exp\left[\mathcal{B}\left(\frac{d}{d\mathcal{A}}\right)^2\right] \tag{59}$$

and so, the P-function becomes

$$P_N(J)=\frac{1}{Z_N}e^{-\beta E_0}\exp\left[\mathcal{B}\left(\frac{d}{d\mathcal{A}}\right)^2\right]\left[\left(e^{\mathcal{A}}\right)^{1-\frac{N}{2}}\frac{J_N(2\sqrt{e^{\mathcal{A}}(N+1)J}\,)}{J_N(2\sqrt{(N+1)J}\,)}\right]. \tag{60}$$

In order to verify the correctness of the above obtained expression, we shall mention an important property of the P-distribution function, i.e.,

$$\int d\mu_N(J,\gamma)\,P_N(J)=1. \tag{61}$$

By using the integral (38) and Eq. (52), after the straightforward calculations, the property (61) can be easily verified.

As it is shown in [8,9], the P-function is analogous to a probability distribution for the values of J. However, it is a quasi-probability distribution function because $P_N(J)$ can take negative values or become highly singular, especially when the density operator corresponds to a classical state with sub-Poissonian statistics. In addition to this, the diagonal representation of the density operator (or the P-representation) is convenient for evaluating expectations of the different operators concerning the Morse oscillator system.

The thermal expectation value for the observable A is

$$\langle A\rangle_N=\mathrm{Tr}(\rho_N A)=\int d\mu_N(J,\gamma)\,P_N(J)\langle J,\gamma|A|J,\gamma\rangle\equiv\langle A\rangle_{J,\gamma}. \tag{62}$$

If the operator A is diagonal in the $|J,\gamma\rangle$-basis, e.g., if it is an integer power s of the number operator $\hat{v}$, then, using Eqs. (17), (38) and (47), we obtain successively:

$$\left\langle\hat{v}^s\right\rangle_N=(N+1)^{1-\frac{N}{2}}\Gamma(N)\sum_{n=0}^{[N/2]}\frac{1}{\rho(n)}n^s\int_0^{\infty}J^{n-\frac{N}{2}}J_N\left(2\sqrt{(N+1)J}\right)P_N(J)\,dJ=\frac{1}{Z_N}\sum_{n=0}^{[N/2]}e^{-\beta E_n}n^s. \tag{63}$$

In order to evaluate the last sum for different values of s, we rewrite the energy exponential (see, Eq. (3)) as follows:

$$e^{-\beta E_n}=e^{-\beta\hbar\omega(n+\frac{1}{2})+\beta\frac{\hbar\omega}{N+1}(n+\frac{1}{2})^2}=e^{-a(n+\frac{1}{2})+\mathcal{B}(n+\frac{1}{2})^2}, \tag{64}$$

where $a=\beta\hbar\omega$ and, consequently,

$$\left\langle\hat{v}^s\right\rangle_N=\frac{1}{Z_N}\sum_{n=0}^{[N/2]}n^s e^{-a(n+\frac{1}{2})+\mathcal{B}(n+\frac{1}{2})^2}. \tag{65}$$

Because the quantity $\mathcal{B}$ is small, it can be considered as a perturbation constant to a harmonic behaviour and it is advantageous to write n^s as a linear combination of the powers of $(n+\frac{1}{2})^l$:

$$n^s=\left(n+\frac{1}{2}-\frac{1}{2}\right)^s=\sum_{l=0}^{s}\binom{s}{l}\left(-\frac{1}{2}\right)^{s-l}\left(n+\frac{1}{2}\right)^l. \tag{66}$$

Therefore, it is possible to express the thermal expectations $\langle \hat{v}^s \rangle_N$ through the derivatives of the $\ln Z_N$:

$$\langle \hat{v}^s \rangle_N = \frac{1}{Z_N} \sum_{l=0}^{s} \binom{s}{l} \left(-\frac{1}{2}\right)^{s-l} (-1)^l \left(\frac{\partial}{\partial a}\right)^l Z_N. \tag{67}$$

In this manner the thermal expectations for the first two powers are

$$\langle \hat{v} \rangle_N = -\frac{\partial}{\partial a} \ln Z_N - \frac{1}{2}, \tag{68}$$

$$\langle \hat{v}^2 \rangle_N = \left(\frac{\partial}{\partial a} \ln Z_N + \frac{1}{2}\right)^2 + \left(\frac{\partial}{\partial a}\right)^2 \ln Z_N. \tag{69}$$

With these expectations we can define and calculate the thermal second-order correlation function $g_N^{(2)}$ and the thermal Mandel parameter Q_N, i.e., the thermal analogue of the corresponding functions for the GK-qCS $|J, \gamma\rangle$ (see, Eqs. (21) and (22)):

$$\left(g^2\right)_N = \frac{\langle \hat{v}^2 \rangle_N - \langle \hat{v} \rangle_N}{(\langle \hat{v} \rangle_N)^2} = 1 + \frac{1}{\frac{\partial}{\partial a} \ln Z_N + \frac{1}{2}} + \frac{(\frac{\partial}{\partial a})^2 \ln Z_N}{(\frac{\partial}{\partial a} \ln Z_N + \frac{1}{2})^2}, \tag{70}$$

$$Q_N = \frac{(\sigma_{\hat{v}})_N}{\langle \hat{v} \rangle_N} - 1 = \langle \hat{v} \rangle_N \left[\left(g^2\right)_N - 1\right] = -1 - \frac{(\frac{\partial}{\partial a})^2 \ln Z_N}{\frac{\partial}{\partial a} \ln Z_N + \frac{1}{2}}. \tag{71}$$

In a similar way, it is possible to express, as functions of the $\ln Z_N$, all thermodynamical and statistical characteristics of a quantum gas of non-rotational Morse oscillators which is in thermodynamical equilibrium with a thermostat (e.g., free energy, internal energy, entropy, heat capacity at the constant volume and so on).

4. The harmonic limit of the obtained results

In the last section let us examine the exact formulation of the harmonic limit of the Morse oscillator. We have proven that this requires the simultaneous (or correlated) prosecution of the following limiting operations [14]:

$$\lim_{\mathrm{HO}} \equiv \begin{cases} D \to \infty, \\ K \to \infty, \\ \alpha \to 0, \\ \frac{4D}{K} = \hbar\omega, \\ D\alpha^2 = \frac{m\omega^2}{2}, \\ K\alpha^2 = 2\frac{m\omega}{\hbar}. \end{cases} \tag{72}$$

At the harmonic limit, all obtained formulae and equations for the one-dimensional Morse oscillator must lead to the corresponding one for the one-dimensional harmonic oscillator.

We begin with the dimensionless Morse eigenvalues (6)

$$\lim_{N\to\infty} e_n = \lim_{N\to\infty} \frac{1}{N+1} n(N-n) = n, \tag{73}$$

so that the quantity $\rho(n)$ (9) has the limit

$$\lim_{N\to\infty} \rho(n) = \lim_{N\to\infty} \Gamma(n+1) \frac{\Gamma(N)}{(N+1)^n \Gamma(N-n)} = n! \equiv \rho_{\mathrm{HO}}(n). \tag{74}$$

Here we have used Eq. (25) and, because of the fact that N is a great number, we can put $N \approx N+1$. Similarly,

$$\lim_{N\to\infty}[\mathcal{N}(J)]^{-2} = \lim_{N\to\infty}\mathcal{F}(J) = \sum_{n=0}^{[N/2]}\frac{J^n}{\lim_{N\to\infty}\rho(n)} = \sum_{n=0}^{\infty}\frac{J^n}{n!} = e^J. \tag{75}$$

With these limits we can easily show that, at the harmonic limit, the GK-qCS for the Morse potential (8) passes to the GK-CS for the one-dimensional harmonic oscillator (HO), which is identical to the usual (Glauber) coherent states (CS) if we consider $z = \sqrt{J}\exp(-\mathrm{i}\gamma)$:

$$\lim_{N\to\infty}|J,\gamma\rangle = e^{-\frac{J}{2}}\sum_{n=0}^{\infty}\frac{J^{\frac{n}{2}}e^{-\mathrm{i}\gamma e_n}}{\sqrt{n!}}|n\rangle = |z\rangle, \tag{76}$$

where $|[N],n\rangle \equiv |n\rangle$.

At the harmonic limit (72), the integration measure (32) becomes

$$\lim_{N\to\infty} d\mu_N(J,\gamma) = d\gamma\, dJ \lim_{N\to\infty}\mathcal{F}\lim_{N\to\infty}\left[(N+1)^{-\frac{N}{2}+1}\Gamma(N)(J)J^{-\frac{N}{2}}\right]\lim_{N\to\infty}J_N\left(2\sqrt{(N+1)J}\right). \tag{77}$$

We calculate the last limit by using the Bessel function power series [13]

$$J_N\left(2\sqrt{b(N+1)J}\right) = \left[\sqrt{b(N+1)J}\right]^N\sum_{k=0}^{\infty}\frac{(-1)^k[\sqrt{b(N+1)J}]^{2k}}{k!\Gamma(N+1+k)}, \tag{78}$$

so that, due to $\Gamma(N+1) = N\Gamma(N)$, we have

$$\begin{aligned}\lim_{N\to\infty}J_N\left(2\sqrt{b(N+1)J}\right) &= \lim_{N\to\infty}\left[\sqrt{b(N+1)J}\right]^N\lim_{N\to\infty}\frac{1}{N}\lim_{N\to\infty}\sum_{k=0}^{\infty}\frac{(-bJ)^k}{k!}\frac{1}{\frac{\Gamma(N+1+k)}{(N+1)^k\Gamma(N+1)}}\\ &= e^{-bJ}\lim_{N\to\infty}\frac{1}{N}\left[\sqrt{b(N+1)J}\right]^N.\end{aligned} \tag{79}$$

Taking $b=1$, the product of the two last limits from Eq. (77) is $\exp(-J)$, and so, using Eq. (75), we finally obtain

$$\lim_{N\to\infty}d\mu_N(J,\gamma) = d\gamma\, dJ = 2\,d\gamma\,|z|\,d|z| = d^2z, \tag{80}$$

i.e., the integration measure for the CS-HO.

The limit of the action identity (35) is

$$\lim_{N\to\infty}\langle J,\gamma|H|J,\gamma\rangle = \lim_{N\to\infty}\frac{N-1}{N+1}J\frac{d}{dJ}\ln\mathcal{F} = J = |z|^2, \tag{81}$$

i.e., the same as for the HO.

In our opinion, one of the main results of our Letter is the expression of the P-distribution function (58). Therefore, it is compulsory to examine their harmonic limit:

$$\lim_{N\to\infty}P_N(J) = \lim_{N\to\infty}\frac{1}{Z_N}e^{-\beta E_0}\lim_{N\to\infty}\exp\left[\mathcal{B}\left(\frac{d}{d\mathcal{A}}\right)^2\right]\lim_{N\to\infty}\left[\left(e^{\mathcal{A}}\right)^{1-\frac{N}{2}}\frac{J_N(2\sqrt{e^{\mathcal{A}}(N+1)J})}{J_N(2\sqrt{(N+1)J})}\right]. \tag{82}$$

The first limit from the right-hand side, taking into account the limit of the quantity $\mathcal{A}$ (49), leads to the expression $1-\exp(-\beta\hbar\omega)$, the second limit is equal to unity, while for the third we use Eq. (79) and we obtain $\exp(\beta\hbar\omega)\exp[-J(e^{\beta\hbar\omega}-1)]$. All in all, the result is the P-distribution function for the harmonic oscillator:

$$\lim_{N\to\infty}P_N(J) = \left(e^{\beta\hbar\omega}-1\right)e^{-|z|^2(e^{\beta\hbar\omega}-1)} = P(|z|). \tag{83}$$

If $N \to \infty$, then $\mathcal{A} \to \beta\hbar\omega$ and $\mathcal{B} \to 0$ and this fact provides that the E_n (Morse oscillator) $\to E_n$ (harmonic oscillator) and Z_N (Morse oscillator) $\to Z$ (harmonic oscillator). As a result, all the thermal expectations (67) for the Morse oscillator lead to the corresponding thermal expectations for the harmonic oscillator.

The same situation is, of course, available for all thermodynamical and statistical characteristics of a quantum canonical gas of non-rotational Morse oscillators. The fact that, at the harmonic limit, all these expectation values lead to the corresponding results for the one-dimensional harmonic oscillator, suggests that our obtained Gazeau–Klauder quasi-coherent states for the Morse potential are correct, as well as our obtained formulae for the diagonal representation of the density operator (41), respectively, for the P-function (58).

5. Concluding remarks

The $|J, \gamma\rangle$ states for the Morse potential were constructed by Roy and Roy [3], using the standard method proposed in the original paper of Gazeau and Klauder [2]. In Ref. [3] some properties of these states were also examined, by underlining the conditions which these states must satisfy.

In the present Letter we have examined some properties of the $|J, \gamma\rangle$ states for the Morse potential, following the basic ideas from the two papers above [2,3].

Despite the fact that the calculations are correct in essence, in Ref. [3], the factor $K^{-1} = (N+1)^{-1}$ in the expression of e_n is omitted. This factor leads to the apparition of the factor $(N+1)^n$ in the denominator of $\rho(n)$ (see, Eq. (9)) and, as a consequence, it will assure that, at the harmonic limit (72), all formulae and equations in our Letter for the Morse oscillator guide us to the corresponding one for the harmonic oscillator.

The obtained states $|J, \gamma\rangle$ (8) fulfill all requirements for the Gazeau–Klauder coherent states [2], i.e.: normalization, continuity in the labels J and γ, resolution of unity, temporal stability and action identity, *excepting the condition of the positivity of the weight function* $k(J)$ in the integration measure $d\mu_N(J, \gamma)$ (32). In spite of this disadvantage, in our opinion, these states are in fact “Gazeau–Klauder *quasi*-coherent states” (GK-qCSs), instead of the “pure” or “classical” Gazeau–Klauder coherent states.

Moreover, despite this drawback, the states $|J, \gamma\rangle$ possess a series of interesting properties, some of them which have been evinced in the present Letter, especially those connected with the mixed (thermal) states. The main reason in favor of the $|J, \gamma\rangle$ states for the Morse potential is the existence of the harmonic limit [14], so that $\lim_{\mathrm{HO}} |J, \gamma\rangle = |z\rangle$. Due to this limit we recover all the results concerning the usual (Glauber) coherent states for the one-dimensional harmonic oscillator.

Also, in the Letter we have constructed the GK-qCSs representation of the density operator for the one-dimensional Morse oscillators quantum canonical gas, as well as their diagonal representation. By applying to an original ansatz to write the Morse energy exponential $\exp(-\beta E_n)$, we have deduced the corresponding P-function. This allows us to calculate the thermal expectation values (thermal averages) for some specific operators (the powers of the number-particle operator $\hat{v}^s$, with $s = 1$ and 2), as well as the thermal analogue of the second-order correlation function and the Mandel parameter.

If we pass from the $|J, \gamma\rangle$-representation (37) to the y-representation (where $y = K \exp[-\alpha(r - r_e)]$ is the dimensionless Morse variable), we recover the following expression for the normalized Morse density operator [15]

$$\langle y|\rho_N|y'\rangle = \frac{1}{Z_N} \sum_{n=0}^{[N/2]} \frac{\alpha(N-2n)}{\Gamma(N+1-n)} e^{-\beta E_n} e^{-\frac{1}{2}(y+y')} (yy')^{\frac{1}{2}(N-2n)} L_n^{N-2n}(y) L_n^{N-2n}(y'). \tag{84}$$

In order to calculate the thermal averages, by comparing these two representations of the density operator, we observe that the $|J, \gamma\rangle$-representation (37) is much simpler than the corresponding y-representation (84). This may be an additional argument in favor of the GK-qCSs.

Besides the correction in the moments formula $\rho(n)$ (9) (in comparison with Eq. (9) from Ref. [3]), by adding the factor $(N+1)^{-n}$ and the consequences of this correction, we consider that the main results of this Letter are:

(a) the ansatz for writing the energy exponential; (b) the expression of P-function; (c) the expression of the density matrix in the GK-qCSs representation (41). In our opinion the above obtained results seem to be entirely new, because, to our knowledge, these have not yet been published in specific literature.

The Morse oscillator is one of the most realistic models for describing the vibrations of a diatomic molecule, being interesting not only from the experimental, but also from the theoretical point of view. Besides the construction of other kinds of coherent states for the Morse potential [16–19], we consider that the present Letter can also contribute to the quantum characterization of the Morse potential systems.

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