Photon-added coherent states for the Morse oscillator

DUŠAN POPOV *), IOAN ZAHARIE

Department of Physics, University "Politehnica" of Timişoara, Piaţa Regina Maria No.1, Of. Postal 5, 300004 Timişoara, Romania

SHI-HAI DONG

Programa de Ingeniería Molecular, Instituto Mexicano del Petróleo, Lázaro Cárdenas 152, 07730 México, D.F., México

Received 17 July 2005;
final version 5 September 2005

In the paper we have constructed and investigated some properties of the Perelomov's "generalized coherent states" and photon-added coherent states for the Morse one-dimensional Hamiltonian (MO-PACSs), using the $SU(2)$ group generators. We have found the integration measure in the resolution of unity and we have calculated some expectation values in the MO-PACSs representation. Using these states, the diagonal P-representation of the density operator is constructed as a new result for Morse potential. In addition, we have calculated some thermal expectation values for the quantum canonical diatomic gas of the Morse oscillators.

PACS: 03.65.Ca, 03.65.–w, 05.30.–d, 31.15.Hz, 42.50.–p
Key words: coherent states, Morse oscillator, density matrix, thermal expectations

1 Introduction

Among many models for the internuclear potential of the diatomic molecule, a particular role is given to the one-dimensional non-rotational Morse Hamiltonian proposed by Morse [1]:

$$H_{\mathrm{M}}(r) = -\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + D_{\mathrm{e}}\left[1 - \mathrm{e}^{-\alpha(r-r_{\mathrm{e}})}\right]^2 , \tag{1}$$

where r represents the internuclear distance, r_{e} is the equilibrium internuclear separation of the system of two nuclei in the diatomic molecule, μ the reduced mass, α the Morse constant of anharmonicity, and D_{e} the dissociation energy of the diatomic molecule (i.e. the depth of the potential energy well). The Morse potential is one of the most simple and "realistic" three-parameter anharmonic potential models, particularly used in specific calculations in spectroscopy [2], in diatomic molecule vibration and scattering [3–5], and in other fields (e.g. in the description of vibrations of polyatomic molecules by representing each bond in the molecule by a Morse potential [6]). So, the Morse potential [1] has proven to be very useful for solving various problems from diverse fields of physics and chemistry.

*) Corresponding author; e-mail: dusan_popov@yahoo.co.uk

This potential has been the subject matter of several algebraic investigations. The $SU(1,1)$ symmetry has been used by several authors [7,8], also the raising and lowering operator formalism [9–14] or supersymmetric quantum mechanics (SUSYQM) technique [15,16]. The $SU(2)$ model has also been used for the problem of the coupling Morse oscillators [17]. The Green's function for the Morse oscillator was calculated in the noncompact group $SO(2,1) \sim SU(1,1)$ algebraic approach [18], based on the application of the Fourier transformation of the corresponding density matrix [19].

The coherent states of the Morse potential have also been examined by several authors, beginning from Nieto and Simmons Jr. [10,20] into the general context of the construction of analytic coherent states for generalized potentials. Gerry [21] has constructed the $SO(2,1)$ coherent states for the Morse oscillator and has written the Green's function as a path integral over the $SO(2,1)$. Also, the coherent states of the Morse oscillator, using a new analytical method for the calculation of creation and annihilation operators, were established in [22, 23]. Recently, the Gazeau–Klauder coherent states for the Morse potential and the Barut–Girardello coherent states for this potential based on the Lie algebra $U(1,1)$ have been carried out [24, 25]. Statistical properties of the Gazeau–Klauder quasi-coherent states, or the Klauder–Perelomov coherent states for the Morse potential were the subject matter of two recent works [26,27].

The arguments for such an increasing interest for the Morse potential generally, and for the construction of the coherent states of the Morse oscillator especially, in our opinion, are the following: (a) the Morse potential allows an analytical solution of the Schrödinger equation and is characterized by a finite number (denoted here by $[N/2]$, where N is a constant which characterizes the potential shape of the Morse oscillator, as we can see below) of bound states (where $[x]$ represents the integer part of x); (b) theoretical spectroscopic results obtained by using the Morse potential in the case of vibrational motion of diatomic [28] (as well as polyatomic [6,29]) molecules, and also in the case of molecular interactions, agree well with experimental spectrum [30]; (c) the systematic analysis of transition intensities and Franck–Condon factors are also possible [31,32].

Our aim is to construct the Perelomov's "generalized coherent states" for the Morse potential beginning from the connection between the $SU(2)$ model and the one-dimensional Morse system [17,33], and also the photon-added coherent states and to show that, at the harmonic limit of the Morse oscillator ($N \to \infty$), all obtained results lead to the corresponding results for the harmonic oscillator.

2 Morse−Hamiltonian factorizability versus the $SU(2)$ model

The factorization method was first proposed by Schrödinger [34], and then generalized by Infeld and Hull [35] and others [36]. This algebraic technique consists in replacing a certain second-order differential operator (as it is, in our case, the Hamilton operator) with two equivalent products of first-order operators. As a consequence, the factorization method leads to raising and lowering operators. On the other hand, this method was a starting point for the introduction of supersymmetric quantum mechanics (SUSYQM) [37], or for the combination of elements of various methods of solving the Schrödinger equation (SUSYQM, algebraic techniques and special-function theory) for exactly solvable one-dimensional potentials of non-relativistic quantum mechanics [38].

The aim of this section is to factorize the Morse Hamiltonian (1) in such a way that it can be compared with the factorization in terms of angular momentum generators [17, 33]. This will allow the construction of new coherent states for the Morse oscillator. If we perform the variable change $x = r - r_\mathrm{e}$, $y = K\mathrm{e}^{-\alpha x}$, and $K \equiv \sqrt{8\mu D_\mathrm{e}}/(\alpha\hbar)$, the Morse Hamiltonian (1) becomes

$$H_\mathrm{M}(y) = -\frac{\hbar^2\alpha^2}{2\mu}\left(y\frac{\mathrm{d}}{\mathrm{d}y}\right)^2 + D_\mathrm{e} - \frac{2D_\mathrm{e}}{K}y + \frac{D_\mathrm{e}}{K^2}y^2. \tag{2}$$

Using the factorization method [9, 37], we factorize the Morse Hamiltonian as

$$H_\mathrm{M} = A_+A_- + A_-A_+\,, \tag{3}$$

where $A_\pm$ are first-order differential operators of the form

$$A_- = a_1 y\frac{\mathrm{d}}{\mathrm{d}y} + b_1 y + c_1\,, \qquad A_+ = a_2 y\frac{\mathrm{d}}{\mathrm{d}y} + b_2 y + c_2\,, \tag{4}$$

which play the role of raising and lowering operators on the vibrational quantum number v. After the straightforward calculations, we obtain

$$A_- = \frac{1}{\sqrt{2}}\frac{\hbar\alpha}{\sqrt{2\mu}}\left(-y\frac{\mathrm{d}}{\mathrm{d}y} - \frac{1}{2}y + \frac{K}{2}\right), \quad A_+ = \frac{1}{\sqrt{2}}\frac{\hbar\alpha}{\sqrt{2\mu}}\left(y\frac{\mathrm{d}}{\mathrm{d}y} - \frac{1}{2}y + \frac{K}{2}\right). \tag{5}$$

Following the Refs. [17, 32, 33], we rewrite the Morse Hamiltonian as follows:

$$H_\mathrm{M} = \tfrac{1}{2}\hbar\omega_0\left(b_+b_- + b_-b_+\right)\,, \tag{6}$$

where we have introduced the new ladder operators

$$b_- = \sqrt{\frac{2}{\hbar\omega_0}}A_- = \frac{1}{\sqrt{2}}\alpha\sqrt{\frac{\hbar}{\mu\omega_0}}\left(-y\frac{\mathrm{d}}{\mathrm{d}y} - \frac{1}{2}y + \frac{K}{2}\right), \tag{7}$$

$$b_+ = \sqrt{\frac{2}{\hbar\omega_0}}A_+ = \frac{1}{\sqrt{2}}\alpha\sqrt{\frac{\hbar}{\mu\omega_0}}\left(y\frac{\mathrm{d}}{\mathrm{d}y} - \frac{1}{2}y + \frac{K}{2}\right) \tag{8}$$

with the fundamental vibration frequency of the Morse oscillator: $\omega_0 = \alpha\sqrt{2D_\mathrm{e}/\mu}$.

The Schrödinger equation for the Morse Hamiltonian (1) can be solved exactly. The eigenfunctions are [1, 3, 39, 40]

$$\mathit{\Psi}_v(y) \equiv \langle y|v\rangle = \left[\frac{\alpha(K-2v-1)v!}{\Gamma(K-v)}\right]^{1/2} \mathrm{e}^{-y/2}y^{(1/2)(K-2v-1)}L_v^{K-2v-1}(y), \tag{9}$$

while the energy levels are given by

$$E_v = \frac{4D_{\rm e}}{K}\left(v+\frac{1}{2}\right) - \frac{4D_{\rm e}}{K^2}\left(v+\frac{1}{2}\right)^2 . \tag{10}$$

We now recall some properties of the $SU(2)$ model, closely related with the Morse potential. It is known from the Refs. [17, 33, 41] that the anharmonicities induced by molecular potentials, such as the Morse and Pöschl–Teller, can be described by $SU(2)$ algebra, which can be constituted by the following raising, lowering and z-component operators

$$[J_z,\, J_\pm] = \pm J_\pm \qquad\qquad [J_+,\, J_-] = 2J_z\,. \tag{11}$$

The Hamiltonian $H_{SU(2)}$ (called "$SU(2)$ model") is given by [17, 33, 41]

$$H_{SU(2)} = \frac{A}{N}(J^2 - J_z^2) = \frac{A}{2N}(J_+J_- + J_-J_+)\,, \tag{12}$$

where A and N are two constants whose physical interpretation will be carried out later. It is diagonal in the $|jm\rangle$ basis, where j and m are the quantum numbers that characterize the eigenvalues of the J^2 and J_z, respectively. The eigenequation of the $H_{SU(2)}$ operator is

$$H_{SU(2)}|jm\rangle = \frac{A}{N}[j(j+1) - m^2]|jm\rangle. \tag{13}$$

The above eigenvalues can be identified, up to an insignificant constant, with the energy eigenvalues (10) of the Morse oscillator potential, if we fix the following values of the quantum numbers: $j = [N/2]$, where $v = j - m = 0, 1, 2, \ldots, [N/2]$ and the newly introduced quantum number v corresponds to the number of vibrational quanta in the Morse oscillator. So, in the new denotation of the basis $|jm\rangle \equiv |[N/2], v\rangle$, the eigenvalues of the $H_{SU(2)}$ Hamiltonian are given by

$$E_v = -\frac{A}{4N} + A\frac{N+1}{N}\left(v+\frac{1}{2}\right) - \frac{A}{N}\left(v+\frac{1}{2}\right)^2 . \tag{14}$$

If we compare this equation with the Morse eigenvalue equation (10), we see that the above eigenvalues are similar, up to an insignificant constant, to the Morse eigenvalues. In other words, the eigenvalues (14) correspond to the displaced Morse potential

$$H_{\rm M}^{(\rm d)} = H_{\rm M} + E^{(\rm d)} \equiv H_{SU(2)} \tag{15}$$

if we perform the following identification:

$$A = \frac{4D_{\rm e}}{K}\frac{1}{1+\frac{1}{N}} = \hbar\omega_0\frac{1}{1+\frac{1}{N}}\,, \quad E^{(d)} = -\frac{D_{\rm e}}{K^2} = -\frac{\hbar^2}{2\mu}\left(\frac{\alpha}{2}\right)^2 . \tag{16}$$

Here we have used Child's parameter K [29] defined by $K = N + 1$.

So, except an unimportant constant term in equation (14), the Morse energy spectrum and the energy spectrum of the $H_{SU(2)}$ Hamiltonian are the same. They are the two sides of the same coin. This leads to the idea that there also is, a connection between the two sets of operators, $b_\pm$ and $J_\pm$. This connection is [17]

$$b_- = \frac{1}{\sqrt{N}} J_+ \,, \quad b_+ = \frac{1}{\sqrt{N}} J_- \,. \tag{17}$$

The operators (J_+, J_-, J_z) of the angular momentum satisfy the well-known equations

$$J_\pm |jm\rangle = \sqrt{j(j+1) - m(m \pm 1)} |jm \pm 1\rangle \,, \quad J_z |jm\rangle = m|jm\rangle \,. \tag{18}$$

Consequently, the operators $b_\pm$ act on the eigenstate $|j = [N/2]\,, v = j - m\rangle \equiv |\,[N/2]\,, v\rangle$ also as the raising and lowering operators of the angular momentum kind, i.e.,

$$b_- |\left[\tfrac{1}{2}N\right], v\rangle = \sqrt{v\left(1 - \frac{v-1}{N}\right)} |\left[\tfrac{1}{2}N\right], v-1\rangle \,, \tag{19}$$

$$b_+ |\left[\tfrac{1}{2}N\right], v\rangle = \sqrt{(v+1)\left(1 - \frac{v}{N}\right)} |\left[\tfrac{1}{2}N\right], v+1\rangle \,. \tag{20}$$

Accordingly, the ground state correspond to $m = j = [N/2]$ and the bounded states of the Morse oscillator correspond to the positive branch of the irreducible representation with $j = [N/2]$, i.e. for $m = 0, 1, \ldots, [N/2]$.

Defining the diagonal operator [17]

$$\hat{v} \equiv \tfrac{1}{2}N - J_z = \tfrac{1}{2}N\left(1 - [b_-, b_+]\right) \,, \tag{21}$$

it is easy to prove that $\hat{v}$ plays the role of number particle (vibrational quanta)-operator:

$$\hat{v} |\left[\tfrac{1}{2}N\right], v\rangle = v |\left[\tfrac{1}{2}N\right], v\rangle \,. \tag{22}$$

Before ending this section let us examine the exact wording of the harmonic limit of the Morse oscillator. We have proved that this requires the simultaneous (or correlated) prosecution of the following limiting operations [42]:

$$\lim_{\mathrm{MO}\to\mathrm{HO}} \equiv \begin{cases} D_\mathrm{e} \to \infty, \\ K \to \infty, \\ \alpha \to 0, \\ \dfrac{D_\mathrm{e}}{K} = \tfrac{1}{4}\hbar\omega_0, \\ D_\mathrm{e}\alpha^2 = \tfrac{1}{2}\mu\omega_0^2, \\ K\alpha^2 = 2\dfrac{\mu\omega_0}{\hbar}. \end{cases} \tag{23}$$

The harmonic limit of the raising and lowering operators of the Morse potential (7) and (8) can be deduced in the manner indicated below. Firstly, we pass to the variable x:

$$\begin{aligned} b_{+} &= \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega_0}}\left[\left(\alpha y\frac{\mathrm{d}}{\mathrm{d}y}\right) - \frac{\alpha}{2}y + \frac{K\alpha}{2}\right] \\ &= \frac{1}{\sqrt{2}}\sqrt{\frac{\hbar}{m\omega_0}}\left(-\frac{\mathrm{d}}{\mathrm{d}x} - \frac{K\alpha}{2}\mathrm{e}^{-\alpha x} + \frac{K\alpha}{2}\right). \end{aligned} \tag{24}$$

Then we perform a series development of the exponential function up to the linear term of the variable x [42]

$$\tfrac{1}{2}K\alpha\mathrm{e}^{-\alpha x} \approx \tfrac{1}{2}K\alpha - \tfrac{1}{2}K\alpha^2 x\,. \tag{25}$$

Performing the limiting operations (23), we obtain

$$\lim_{\mathrm{MO}\to\mathrm{HO}} b_{+} = \frac{1}{\sqrt{2}}\left(-\sqrt{\frac{\hbar}{m\omega_0}}\frac{\mathrm{d}}{\mathrm{d}x} + \sqrt{\frac{m\omega_0}{\hbar}}x\right) \equiv a^{+} \tag{26}$$

and, similarly,

$$\lim_{\mathrm{MO}\to\mathrm{HO}} b_{-} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{\hbar}{m\omega_0}}\frac{\mathrm{d}}{\mathrm{d}x} + \sqrt{\frac{m\omega_0}{\hbar}}x\right) \equiv a\,, \tag{27}$$

i.e., we have obtained the creation and annihilation operators of the one-dimensional HO.

In addition, in terms of Eq. (20), the Morse wave function can be taken as

$$\Psi_v(y) = \sqrt{\frac{N^v(N-v)!}{v!N!}}\;(b_{+})^v\Psi_0(y)\,, \tag{28}$$

where $\Psi_0(y)$ is the ground state of the Morse wave function

$$\Psi_0(y) = \sqrt{\frac{\alpha}{(N-1)!}}\mathrm{e}^{-y/2}y^{N/2}\,. \tag{29}$$

On the other hand, the harmonic limit of the Morse wave function is given by

$$\lim_{N\to\infty}\Psi_v(y) = \frac{1}{\sqrt{v!}}\;(a_{+})^v\;\phi_0(y)\,, \tag{30}$$

where $\phi_0(y)$ is the ground state for the harmonic oscillator.

3 Coherent states for the Morse oscillator

With the previous considerations, let us begin from the definition of the Perelomov's "generalized coherent states" by means of normally ordered displacement operator [43, 44]

$$|\zeta;\left[\tfrac{1}{2}N\right]\rangle = \exp\left[\zeta J_{+} - \zeta^{*}J_{-}\right]|\left[\tfrac{1}{2}N\right],0\rangle. \tag{31}$$

Using a well-known disentangled formula [43, 44]:

$$\exp\left[\zeta J_+ - \zeta^* J_-\right] = \mathrm{e}^{\eta J_+}\, \mathrm{e}^{\ln(1+|\eta|^2) J_z}\, \mathrm{e}^{-\eta^* J_-} \tag{32}$$

and passing to the operator b_+ (see Eq. (17)), we are lead to the following definition of the coherent states for the Morse oscillator (MO-CSs):

$$|z; \left[\tfrac{1}{2}N\right]\rangle = \left[\mathcal{N}(|z|^2)\right]^{-1/2} \exp\left[z b_+\right] |\left[\tfrac{1}{2}N\right], 0\rangle\,, \tag{33}$$

where we have used a new complex variable: $z = -\eta\sqrt{N} = -\sqrt{N}(\zeta/|\zeta|)\tan|\zeta| \equiv |z|\mathrm{e}^{\mathrm{i}\varphi} = r\mathrm{e}^{\mathrm{i}\varphi}$.

Using Eq. (20), it is not difficult to prove that we have

$$|z; \left[\tfrac{1}{2}N\right]\rangle = \left[\mathcal{N}(|z|^2)\right]^{-1/2} \sum_{v=0}^{[N/2]} \frac{z^v}{\sqrt{\rho(v;N)}} |\left[\tfrac{1}{2}N\right], v\rangle\,, \tag{34}$$

where the positive quantities are defined as follows:

$$\rho(v;N) = N^v \frac{\Gamma(v+1)\Gamma(N+1-v)}{\Gamma(N+1)}\,. \tag{35}$$

We point out here that we have written the normalized vacuum and a certain state of the finite-dimensional Fock space $\mathcal{F}^{[N/2]}$ as $|[N/2], 0\rangle$ and $|[N/2], v\rangle$, respectively, instead of $|0\rangle$ and $|v\rangle$ in order to emphasize the representation $[N/2]$ of the $SU(2)$ group. We shall also extend this manner of notation to the coherent states (CSs).

From the normalization to unity of the CSs we obtain that the normalization constant is

$$\mathcal{N}(|z|^2) = \sum_{v=0}^{[N/2]} \frac{(|z|^2)^v}{\rho(v;N)}\,, \tag{36}$$

which is a polynomial of degree $[N/2]$ with the positive coefficients.

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 $|[N/2], v\rangle$ ($v = 0, 1, 2, \ldots, [N/2]$) [3]. Then, the projection operator on the subspace $\mathcal{H}_{[N/2]}$ is

$$\sum_{v=0}^{[N/2]} |\left[\tfrac{1}{2}N\right], v\rangle\langle\left[\tfrac{1}{2}N\right], v| = \hat{I}_{[N/2]}\,. \tag{37}$$

Resolution of the identity in terms of a certain set of states is very important property, because it allows the practical use of these states as a basis in the Hilbert space [45]. The resolution of the unity in terms of the MO-CSs can be performed in the following manner:

$$\int \mathrm{d}\mu_N(z) |z; \left[\tfrac{1}{2}N\right]\rangle\langle z; \left[\tfrac{1}{2}N\right]| = \hat{I}_{[N/2]}, \tag{38}$$

where $\hat{I}_{[N/2]}$ is the projection operator (see Eq. (37)).

In order to determine the unknown integration measure $\mathrm{d}\mu_N(z)$, we must remember that, at the harmonic limit of the Morse oscillator $N \to \infty$, this measure must lead to the well-known integration measure of the usual one-dimensional harmonic-oscillator coherent states (HO-CSs):

$$\lim_{N\to\infty} \mathrm{d}\mu_N(z) = \frac{\mathrm{d}^2 z}{\pi} = \frac{\mathrm{d}\varphi}{\pi}\,\mathrm{d}r\, r\,. \tag{39}$$

This fact, as well as the proper structure of the MO-CSs, leads to the following expression of the integration measure $\mathrm{d}\mu_N(z)$,

$$\mathrm{d}\mu_N(z) = \frac{\mathrm{d}\varphi}{\pi}\,\mathrm{d}r\, r\, h(r^2)\,\mathcal{N}(|z|^2)\,, \tag{40}$$

where the unknown function $h(r^2)$ must be determined.

By substituting Eq. (40) into Eq. (38) we obtain

$$\sum_{v,n=0}^{[N/2]} \frac{|\left[\frac{1}{2}N\right], v\rangle\langle\left[\frac{1}{2}N\right], n|}{\rho(v;N)\rho(n;N)} \int_0^\infty \mathrm{d}r\, r\, h(r^2) \int_0^{2\pi} \frac{\mathrm{d}\varphi}{\pi}(z^*)^n z^v = \hat{I}_{[N/2]}\,. \tag{41}$$

Here and below, all integrals are performed over the whole complex z-plane, where $z = r\exp(\mathrm{i}\varphi)$, $r \in [0,\infty)$, $\varphi \in [0,\, 2\pi]$, $\mathrm{d}^2 z = \mathrm{d}(\mathrm{Re}\, z)\mathrm{d}(\mathrm{Im}\, z) = \mathrm{d}\varphi\,\mathrm{d}r\, r$.

After performing the angular integration, i.e.,

$$\int_0^{2\pi} \frac{\mathrm{d}\varphi}{\pi}(z^*)^n z^v = r^{n+v}\int_0^{2\pi} \frac{\mathrm{d}\varphi}{\pi}\mathrm{e}^{\mathrm{i}(v-n)\varphi} = 2r^{2v}\delta_{vn}\,, \tag{42}$$

Eq. (41) becomes

$$2\sum_{v=0}^{[N/2]} \left[\frac{1}{\rho(v;N)}\int_0^\infty \mathrm{d}r\, r^{2v+1}\, h(r^2)\right] |\left[\tfrac{1}{2}N\right], v\rangle\langle\left[\tfrac{1}{2}N\right], v| = \hat{I}_{[N/2]}\,. \tag{43}$$

When we perform the variable change $r^2 = x$ and extend the natural values of v to complex s so that $v \to s-1$, the integral from the above equation is called the Mellin transform [46, 47]

$$\int_0^\infty \mathrm{d}x\, x^{s-1} h(x) = \frac{1}{N}\frac{1}{\Gamma(N+1)}\frac{1}{N^{-s}}\Gamma(s)\Gamma(N+2-s)\,. \tag{44}$$

From the definition of Meijer's G-function and Mellin's inversion theorem, we have [46]

$$\int_0^\infty \mathrm{d}x\, x^{s-1} G^{m,n}_{p,q}\left(\alpha x \left| \begin{matrix} a_1,\ \ldots,\ a_n,\ a_{n+1},\ \ldots,\ a_p \\ b_1,\ \ldots,\ b_m,\ b_{m+1},\ \ldots,\ b_q \end{matrix}\right.\right) =$$
$$= \frac{1}{\alpha^s}\frac{\prod_{j=1}^m \Gamma(b_j+s)\prod_{j=1}^n \Gamma(1-a_j-s)}{\prod_{j=m+1}^q \Gamma(1-b_j-s)\prod_{j=n+1}^p \Gamma(a_j+s)}. \tag{45}$$

In the above equation the argument of G-function is αx, where α is a real or complex constant, while a_j ($j = 1, \ldots, p$) and b_h ($h = 1, \ldots, q$) are real or complex numbers such that $a_j - b_h \neq 0, 1, 2, \ldots$ ($j = 1, \ldots, n$; $h = 1, \ldots, m$). The numbers m, n, p, and q are integers with $0 \leq n \leq p$, $0 \leq m \leq q$ [46].

Comparing the last two equations, we obtain that

$$h(r^2) = \frac{1}{N}\frac{1}{\Gamma(N+1)} G_{11}^{11}\left(\frac{r^2}{N}\middle| \begin{matrix} -N-1 \\ 0 \end{matrix}\right) = \frac{N+1}{N}\frac{1}{\left(1+\dfrac{r^2}{N}\right)^{N+2}}\,, \tag{46}$$

where we have used the particular expression of the Meijer's G-function $G_{pq}^{mn}\left(x|\ldots\right)$ [46].

Finally, the searched integration measure becomes

$$\mathrm{d}\mu_N(z) = \frac{N+1}{N}\frac{\mathrm{d}^2 z}{\pi}\frac{1}{\left(1+\dfrac{|z|^2}{N}\right)^{N+2}}\mathcal{N}(|z|^2)\,. \tag{47}$$

Having in mind that [48]

$$\lim_{N\to\infty}\frac{\Gamma(N+1-v)}{\Gamma(N+1)}N^{-v} = 1\,, \tag{48}$$

we can demonstrate that the previously obtained CSs and integration measure for the MO lead, at the harmonic limit $N \to \infty$ (see, also, Eq. (23)), to the corresponding quantities for HO-1D:

$$\lim_{N\to\infty}|z;[N/2]\rangle = |z\rangle = \mathrm{e}^{-(1/2)|z|^2}\sum_{v=0}^{\infty}\frac{z^v}{\sqrt{v!}}|v\rangle\,, \quad \lim_{N\to\infty}\mathrm{d}\mu_N(z) = \frac{\mathrm{d}^2 z}{\pi} \tag{49}$$

which constitute the first step of the validity of our calculation.

The CSs are normalizable but non-orthogonal, so the scalar product of two CSs is

$$\langle z;\left[\tfrac{1}{2}N\right]|z';\left[\tfrac{1}{2}N\right]\rangle = \frac{\mathcal{N}(z^* z')}{\sqrt{\mathcal{N}(|z|^2)\mathcal{N}(|z'|^2)}}\,. \tag{50}$$

The physical utility of the CSs in different applications consists in the calculations of the expectation (mean) values of a certain physical observable A which characterizes, in our case, the Morse oscillator, with respect to the MO-CSs $|z;[N/2]\rangle$.

Generally, the matrix elements in CSs representation are

$$\langle z;\left[\tfrac{1}{2}N\right]|A|z';\left[\tfrac{1}{2}N\right]\rangle = \\ = \left[\mathcal{N}(|z|^2)\mathcal{N}(|z'|^2)\right]^{-1/2}\sum_{n,v=0}^{[N/2]}\frac{(z^*)^n z'^v}{\sqrt{\rho(n;N)\rho(v;N)}}\langle\left[\tfrac{1}{2}N\right],n|A|\left[\tfrac{1}{2}N\right],v\rangle. \tag{51}$$

From a practical point of view, the most important operators are those which are diagonal in the basis $|[N/2], v\rangle$. A typical example is the number (particle) operator $\widehat{v}$,

$$\widehat{v}|[N/2], v\rangle = v|[N/2], v\rangle \,. \tag{52}$$

The matrix elements of their integer powers ($s = 1,\, 2, \ldots$) are

$$\langle z; \left[\tfrac{1}{2}N\right] |\widehat{v}|z'; \left[\tfrac{1}{2}N\right]\rangle = \frac{1}{\sqrt{\mathcal{N}(|z|^2)\mathcal{N}(|z'|^2)}} \left(x\frac{\mathrm{d}}{\mathrm{d}x}\right)^s \mathcal{N}(x)\,, \tag{53}$$

where $x = z^* z'$.

As regards the integration limits, using the Stirling formula [48], we can demonstrate that the convergence radius R of the previously defined MO-CSs is

$$R = \lim_{v\to\infty} \left[\rho(v; N)\right]^{1/v} = \lim_{v\to\infty} \left[N^v \frac{\Gamma(v+1)\Gamma(N+1-v)}{\Gamma(N+1)}\right]^{1/v} = \infty\,, \tag{54}$$

so, the integrations can be performed over entire z-complex plane.

Moreover, the photon-number distribution of the field in the MO-CSs $|z; [N/2]\rangle$, i.e. the probability of finding v photons in the field state $|z; [N/2]\rangle$, is, by definition,

$$p_v\left(z; \left[\tfrac{1}{2}N\right]\right) = |\langle \left[\tfrac{1}{2}N\right], v|z; \left[\tfrac{1}{2}N\right]\rangle|^2 = \frac{(|z|^2)^v}{\rho(v; N)\mathcal{N}(|z|^2)}\,. \tag{55}$$

Accordingly, the k-order moment is

$$n^{(k)}_{z;N} \equiv \langle z; \left[\tfrac{1}{2}N\right] |\widehat{v}(\widehat{v}-1)\ldots(\widehat{v}-k+1)|z; \left[\tfrac{1}{2}N\right]\rangle = \frac{1}{\mathcal{N}(|z|^2)} \left[\frac{\mathrm{d}}{\mathrm{d}(|z|^2)}\right]^k \mathcal{N}(|z|^2)\,. \tag{56}$$

If N becomes greater, i.e., the number of vibrational bound states becomes greater, this fact being realized in the case of "heavy" diatomic molecule, the photon-number distribution function approaches the Poisson distribution:

$$\lim_{N\to\infty} p_v\left(z; [N/2]\right) = \mathrm{e}^{-|z|^2} \frac{(|z|^2)^v}{v!}\,. \tag{57}$$

The Poisson distribution is characteristic for the HO-1D CSs.

Moreover, the inherent statistical properties of the CSs also follow from calculating the Mandel parameter defined as [49, 50]

$$Q_{z;N} = \frac{\sigma_{z;N}}{n^{(1)}_{z;N}} - 1 = \frac{n^{(2)}_{z;N} - \left(n^{(1)}_{z;N}\right)^2}{n^{(1)}_{z;N}}\,, \tag{58}$$

where $\sigma_{z;N}$ is the variance of the number particle operator $\widehat{v}$, calculated in the coherent state $|z; [N/2]\rangle$. If the Mandel parameter $Q_{z;N}$ is > 0, $= 0$ or < 0, then the corresponding CSs and statistics are called super-Poissonian, Poissonian or sub-Poissonian.

4 Photon-added coherent states

Beginning from the previously defined MO-CSs, using Eq. (34), let us construct the photon-added coherent states (PACSs), by the multiple action of operator b_+ on the usual coherent state [51], i.e.,

$$|z; \left[\tfrac{1}{2}N\right]; m\rangle = \left[\mathcal{N}_m(|z|^2)\right]^{-1/2} (b_+)^m |z; \left[\tfrac{1}{2}N\right]\rangle \,. \tag{59}$$

These states depend on extra parameter m, i.e. on the number of added or excited photons, which influences the statistics of photons, as we shall see below.

Using the results of the previous section, we obtain the following expression:

$$|z; \left[\tfrac{1}{2}N\right]; m\rangle = \left[\mathcal{N}_m(|z|^2)\mathcal{N}(|z|^2)\right]^{-1/2} \sum_{v=0}^{[N/2]} \frac{z^v}{\sqrt{\rho_m(v; N)}} | \left[\tfrac{1}{2}N\right], v+m\rangle \,, \tag{60}$$

where we have denoted

$$\begin{aligned} \rho_m(v; N) &= N^{v+m} \frac{\left[\Gamma(v+1)\right]^2 \Gamma(N+1-v-m)}{\Gamma(v+m+1)\Gamma(N+1)} \\ &= N^m \frac{\Gamma(v+1)\Gamma(N+1-v-m)}{\Gamma(v+m+1)\Gamma(N+1-v)} \rho(v; N) \,. \end{aligned} \tag{61}$$

The number of excited photons must fulfill the condition $1 < m < [N/2] - v$. From Eq. (60) we can see that the PACS $|z; [N/2]; m\rangle$ is a linear combination of all number states $|[N/2], v\rangle$ starting with $v = m$. In other words, the first m number states $v = 0, 1, \ldots, m-1$ are absent from the state $|z; [N/2]; m\rangle$. Then, the unity operator in the corresponding Fock subspace $\mathcal{F}_{(m)}^{[N/2]}$ of the finite-dimensional Fock space $\mathcal{F}^{[N/2]}$ is

$$\sum_{v=0}^{[N/2]} | \left[\tfrac{1}{2}N\right], v+m\rangle\langle \left[\tfrac{1}{2}N\right], v+m| = I_{[N/2]}^{(m)} \,. \tag{62}$$

It is not difficult to verify that the MO-PACSs are normalizable but non orthogonal. Despite this fact, they may be used as a basis in the corresponding Hilbert space of the complex z-functions.

The normalization constant $\mathcal{N}_m(|z|^2)$ can be written as

$$\mathcal{N}_m(|z|^2) = \frac{1}{\mathcal{N}(|z|^2)} \sum_{v=0}^{[N/2]} \frac{(|z|^2)^v}{\rho_m(v; N)} \,, \tag{63}$$

with the evident conditions $\rho_0(v; N) \equiv \rho(v; N)$ and $\mathcal{N}_0(|z|^2) = 1$.

Next, let us determine a positive measure $\mathrm{d}\mu_N^{(m)}(z)$ from the resolution of unity:

$$\int \mathrm{d}\mu_N^{(m)}(z) |z; \left[\tfrac{1}{2}N\right]; m\rangle\langle z; \left[\tfrac{1}{2}N\right]; m| = \hat{I}_{[N/2]}^{(m)}. \tag{64}$$

Following the same method as in the previous section, we put that

$$\mathrm{d}\mu_N^{(m)}(z) = \frac{\mathrm{d}^2 z}{\pi}\mathcal{N}_m(|z|^2)\mathcal{N}(|z|^2)h_m(|z|^2)\,. \tag{65}$$

After the angular integration as in Eq. (42), we obtain the following Stieltjes moment problem [47]:

$$2\int_0^\infty \mathrm{d}r\, r^{2v+1} h_m(r^2) = \rho_m(v;N) \tag{66}$$

which, after the substitutions $r^2 = x$ and $v = s-1$ leads to

$$\int_0^\infty \mathrm{d}x\, x^{s-1} h_m(x) = \frac{N^{m-1}}{\Gamma(N+1)}\frac{1}{N^{-s}}\frac{\left[\Gamma(s)\right]^2\Gamma(N+2-m-s)}{\Gamma(m+s)}. \tag{67}$$

By using Eq. (45), we obtain the expression for the function $h_m(x)$ and, finally, the integration measure becomes

$$\mathrm{d}\mu_N^{(m)}(z) = \frac{N^{m-1}}{\Gamma(N+1)}\frac{\mathrm{d}^2 z}{\pi}\mathcal{N}_m(|z|^2)\mathcal{N}(|z|^2)G_{22}^{21}\left(\frac{|z|^2}{N}\middle|\begin{matrix} m-N-1; & m \\ 0, & 0; \end{matrix}\right). \tag{68}$$

The photon-number distribution for the MO-PACSs can be written as follows:

$$\begin{aligned} p_v^{(m)}\left(z;\left[\tfrac{1}{2}N\right]\right) &= |\langle\left[\tfrac{1}{2}N\right],v|z;\left[\tfrac{1}{2}N\right];m\rangle|^2 \\ &= \frac{1}{\mathcal{N}_m(|z|^2)}\left[\frac{\Gamma(v+1)}{\Gamma(v-m+1)}\right]^2\frac{1}{(|z|^2)^m}p_v\left(z;\left[\tfrac{1}{2}N\right]\right), \end{aligned} \tag{69}$$

which is zero for $v < m$. In this sense the number of exciting photons evidently influences the statistics of the photons.

In the manner of the previous section, we can write the matrix elements of a physical observable A in the MO-PACSs-basis $|z;[N/2];m\rangle$ as follows:

$$\begin{aligned} \langle z;\left[\tfrac{1}{2}N\right];m|A|z';\left[\tfrac{1}{2}N\right];m\rangle &= \left[\mathcal{N}_m(|z|^2)\mathcal{N}(|z|^2)\mathcal{N}_m(|z'|^2)\mathcal{N}(|z'|^2)\right]^{-1/2} \\ \times \sum_{n,v=0}^{[N/2]} &\frac{(z^*)^n z'^v}{\sqrt{\rho_m(n;N)\rho_m(v;N)}}\langle\left[\tfrac{1}{2}N\right],n+m|A|\left[\tfrac{1}{2}N\right],v+m\rangle\,, \end{aligned} \tag{70}$$

If $A = \widehat{v}^s$ (where s is an integer), then the expectation value of this operator is

$$\begin{aligned} \langle z;\left[\tfrac{1}{2}N\right];m|\widehat{v}^s|z;\left[\tfrac{1}{2}N\right];m\rangle &\equiv \langle\widehat{v}^s\rangle_{z;[N/2]}^{(m)} = \\ &= \left[\mathcal{N}_m(|z|^2)\mathcal{N}(|z|^2)\right]^{-1}\sum_{v=0}^{s}\binom{s}{k}m^{s-k}\left(x\frac{d}{dx}\right)^k\mathcal{N}_m(x)\,, \end{aligned} \tag{71}$$

where $x = |z|^2$ and where we have used the Newton binomial development.

Consequently, by particularizing the exponent s, the Mandel parameter for MO-PACSs is

$$Q_{z;N}^{(m)} = \frac{\sigma_{z;N;m}}{n_{z;N;m}^{(1)}} - 1 = \frac{x^2 \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 \ln \mathcal{N}_m(x) - m}{x \frac{\mathrm{d}}{\mathrm{d}x} \ln \mathcal{N}_m(x) + m}. \tag{72}$$

The Mandel parameter $Q_{z;N}^{(m)}$ as a function of $|z|^2$ and with the number of excited photons m as an extra discrete parameter, may take positive, zero or negative values. These three situations correspond to the PACSs with super-Poissonian, Poissonian or sub-Poissonian statistics.

5 Mixed states

It is well known that a very large class of systems in quantum optics can be described in terms of a density operator which corresponds to a mixed quantum state of the field. The most usual example of mixed states is the thermal state (TS). In this context we consider a quantum system which consists of a gas of one-dimensional non-rotational ($J = 0$, where J is the rotational quantum number) Morse oscillators in thermodynamic equilibrium with the reservoir (thermostat) at temperature $T = (k_{\mathrm{B}}\beta)^{-1}$ (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

$$\rho_N^{(m)} = \frac{1}{Z_N^{(m)}} \sum_{v=0}^{[N/2]} \mathrm{e}^{-\beta E_{v+m}} | \left[\tfrac{1}{2}N\right], v+m\rangle\langle\left[\tfrac{1}{2}N\right], v+m| \,, \tag{73}$$

where $Z_N^{(m)}$ is the normalization constant, i.e. the partition function for a fixed parameter N (or, equivalently, for a fixed Child's parameter K, which characterizes the maximum number of bound vibrational states for a certain diatomic molecule).

In the next examination of the statistical properties of the mixed (thermal) states of the MO, it will be very useful to follow the observations and the ansatz of our previous paper [26].

The equation (14)) can be written as follows:

$$\beta E_{v+m} = \mathcal{A}\left(v + m + \tfrac{1}{2}\right) - \mathcal{B}(v+m)^2 = \varepsilon_0 + \mathcal{A}(v+m) - \mathcal{B}(v+m)^2 \,, \tag{74}$$

where we have used the notations

$$\varepsilon_0 = \beta \frac{A}{2} \,, \quad \mathcal{A} = \beta A \,, \quad \mathcal{B} = \beta \frac{A}{N} \,. \tag{75}$$

For most of the diatomic molecules $\mathcal{B} \ll \mathcal{A}$. So, the limits of the Child's parameter $K = N+1$ 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 [42]. Consequently, the energy exponential can be expanded in the power series as follows:

$$e^{-\beta E_{v+m}} = e^{-\varepsilon_0} e^{-\mathcal{A}(v+m)} e^{\mathcal{B}(v+m)^2} = e^{-\varepsilon_0} e^{-\mathcal{A}(v+m)} \sum_{k=0}^{\infty} \frac{\mathcal{B}^k}{k!} (v+m)^{2k} \,. \tag{76}$$

Writing

$$e^{-\mathcal{A}(v+m)} (v+m)^{2k} = \left(\frac{d}{d\mathcal{A}}\right)^{2k} e^{-\mathcal{A}(v+m)} \tag{77}$$

we finally have

$$e^{-\beta E_{v+m}} = e^{-\varepsilon_0} \sum_{k=0}^{\infty} \frac{\mathcal{B}^k}{k!} \left(\frac{d}{d\mathcal{A}}\right)^{2k} \left[e^{-\mathcal{A}}\right]^{v+m} \equiv e^{-\varepsilon_0} \exp\left[\mathcal{B}\left(\frac{d}{d\mathcal{A}}\right)^2\right] \left[e^{-\mathcal{A}}\right]^{v+m} , \tag{78}$$

where we have used the last operator identity in order to simplify the writing of such expressions which contain the exponential expansion with respect to the quantity $\mathcal{B}$.

The Q-function (or Q-distribution function or Husimi's function) is defined by the diagonal elements of the density operator in the CSs basis. Using the previously indicated ansatz, the Q-function of the MO-PACSs is

$$\begin{aligned} Q^{(m)}(|z|^2) &\equiv \langle z; \left[\tfrac{1}{2}N\right]; m|\rho_N^{(m)}|z; \left[\tfrac{1}{2}N\right]; m\rangle = \\ &= \frac{e^{-\varepsilon_0}}{Z_N^{(m)}} \exp\left[\mathcal{B}\left(\frac{d}{d\mathcal{A}}\right)^2\right] \left[e^{-\mathcal{A}m} \frac{\mathcal{N}_m(|z|^2 e^{-\mathcal{A}})}{\mathcal{N}_m(|z|^2)}\right] . \end{aligned} \tag{79}$$

By imposing that the density operator has to be normalized to unity (which is equivalent to the assertion that the Q-function is normalized to unity), i.e.,

$$\mathrm{Tr}\rho_N^{(m)} = \int d\mu_N^{(m)} \langle z; \left[\tfrac{1}{2}N\right]; m|\rho_N^{(m)}|z; \left[\tfrac{1}{2}N\right]; m\rangle = 1 \,, \tag{80}$$

and using the explicit expressions for Meijer G-functions, we find that the normalization constant, i.e., the statistical sum is

$$Z_N^{(m)} = \sum_{v=0}^{[N/2]} e^{-\beta E_{v+m}} \,. \tag{81}$$

In addition to this, using the previous ansatz, the partition function of the MO quantum gas can be also written as

$$Z_N^{(m)} = e^{-\varepsilon_0} \exp\left[\mathcal{B}\left(\frac{d}{d\mathcal{A}}\right)^2\right] \left[e^{-\mathcal{A}m} \frac{1-\left(e^{-\mathcal{A}}\right)^{[N/2]+1}}{1-e^{-\mathcal{A}}}\right] . \tag{82}$$

The diagonal expansion of the density operator $\rho_N^{(m)}$ in the MO-PACSs basis is

$$\rho_N^{(m)} = \int d\mu_N^{(m)} |z; \left[\tfrac{1}{2}N\right]; m\rangle P_N^{(m)}(|z|^2) \langle z; \left[\tfrac{1}{2}N\right]; m| \,. \tag{83}$$

The method of finding the quasi-distribution function (or P-function) follows some successive steps:

a) We substitute the expression of MO-PACSs, using Eq. (60) and the integration measure, using Eq. (68).

b) We perform the angular integration and the following function change:

$$P_N^{(m)}(|z|^2) = \left[G_{22}^{21}\left(\frac{|z|^2}{N} \middle| \begin{matrix} m-N-1; & m \\ 0, & 0; \end{matrix} \right) \right]^{-1} R_N^{(m)}(|z|^2)\,. \tag{84}$$

c) We perform the substitution $|z|^2 = x$ and we are lead to the following Stieltjes problem:

$$\int_0^\infty \mathrm{d}x\, x^{s-1} R_N^{(m)}(x) = \frac{1}{Z_N^{(m)}} \frac{\Gamma(N+1)}{N^{m-1}} \mathrm{e}^{-\beta E_{v+m}} \rho_m(v;N)\,. \tag{85}$$

d) By applying the described ansatz for the exponential function in the r.h.s., i.e. $\exp(-\beta \mathrm{E}_{v+m})$, we write also the function $R_N^{(m)}(x)$ in the manner of same ansatz, as follows [26]:

$$R_N^{(m)}(x) = \frac{1}{Z_N^{(m)}} \mathrm{e}^{-\varepsilon_0} \exp\left[\mathcal{B}\left(\frac{\mathrm{d}}{\mathrm{d}\mathcal{A}}\right)^2 \right] \left[\mathrm{e}^{-\mathcal{A}(m-1)} X_N^{(m)}(x;\mathcal{A}) \right]. \tag{86}$$

e) So, the Stieltjes moment problem is transferred to the function $X_N^{(m)}(x;\mathcal{A})$, i.e.,

$$\int_0^\infty \mathrm{d}x\, x^{s-1} X_N^{(m)}(x;\mathcal{A}) = \frac{1}{(\mathrm{e}^{\mathcal{A}} N^{-1})^s} \frac{[\Gamma(s)]^2\, \Gamma(N+2-m-s)}{\Gamma(m+s)}\,. \tag{87}$$

f) The mathematical solution can be found in the Ref. [46] and there is

$$X_N^{(m)}(|z|^2;\mathcal{A}) = G_{22}^{21}\left(\frac{\mathrm{e}^{\mathcal{A}}}{N}|z|^2 \middle| \begin{matrix} m-N-1; & m \\ 0, & 0; \end{matrix} \right). \tag{88}$$

Finally, the P-function for MO in the PACSs representation can be symbolically written in the following manner:

$$P_N^{(m)}(|z|^2) = \frac{1}{Z_N^{(m)}} \mathrm{e}^{-\varepsilon_0} \exp\left[\mathcal{B}\left(\frac{\mathrm{d}}{\mathrm{d}\mathcal{A}}\right)^2 \right] \left[\mathrm{e}^{-\mathcal{A}(m-1)} \frac{G_{22}^{21}\left(\frac{\mathrm{e}^{\mathcal{A}}}{N}|z|^2 \middle| \begin{matrix} m-N-1; & m \\ 0, & 0; \end{matrix} \right)}{G_{22}^{21}\left(\frac{|z|^2}{N} \middle| \begin{matrix} m-N-1; & m \\ 0, & 0; \end{matrix} \right)} \right]. \tag{89}$$

It is not difficult to prove, using Eq. (45), that the P-function is also normalized to unity:

$$\int \mathrm{d}\mu_N^{(m)} P_N^{(m)}(|z|^2) = 1. \tag{90}$$

At the end of this section we point out that, on one hand, all our obtained results and formulae for PACSs of the MO (generically denoted by $\mathcal{F}_{\mathrm{MO}}^{(m)}$) lead to the corresponding results and formulae for ordinary MO-CSs (generically denoted by $\mathcal{F}_{\mathrm{MO}}$), i.e.,

$$\lim_{m\to 0} \mathcal{F}_{\mathrm{MO}}^{(m)} = \mathcal{F}_{\mathrm{MO}}\,. \tag{91}$$

On the other hand, the results and formulae for the ordinary MO-CSs, when $N \to \infty$ (i.e. at the harmonic limit, see Eq. (23)), lead to the corresponding results and formulae for ordinary HO-1D CSs (generically denoted by $\mathcal{F}_{\mathrm{HO}}$):

$$\lim_{\mathrm{MO}\to\mathrm{HO}} \mathcal{F}_{\mathrm{MO}} \equiv \lim_{N\to\infty} \mathcal{F}_{\mathrm{MO}} = \mathcal{F}_{\mathrm{HO}}\,. \tag{92}$$

As an illustration, we only give two examples.

Using the property of Meijer G-functions [46]:

$$G_{22}^{21}\left(\frac{\mathrm{e}^{\mathcal{A}}}{N}|z|^2 \middle| \begin{matrix} -N-1; & 0 \\ 0, & 0; \end{matrix}\right) = G_{11}^{11}\left(\frac{\mathrm{e}^{\mathcal{A}}}{N}|z|^2 \middle| \begin{matrix} -N-1 \\ 0 \end{matrix}\right) = \Gamma(N+2)\frac{1}{\left(1+\frac{\mathrm{e}^{\mathcal{A}}}{N}|z|^2\right)^{N+2}} \tag{93}$$

and Eq. (89), we obtain the P-function for the ordinary MO-CSs:

$$\lim_{m\to 0} P_N^{(m)}(|z|^2) = \frac{1}{Z_N}\mathrm{e}^{-\varepsilon_0}\exp\left[\mathcal{B}\left(\frac{\mathrm{d}}{\mathrm{d}\mathcal{A}}\right)^2\right]\left[\mathrm{e}^{\mathcal{A}}\left(\frac{1+\frac{|z|^2}{N}}{1+\frac{\mathrm{e}^{\mathcal{A}}}{N}|z|^2}\right)^{N+2}\right] \equiv P_N(|z|^2)\,. \tag{94}$$

By calculating the harmonic limit of the P-function for the ordinary MO-CSs, i.e.,

$$\lim_{N\to\infty} P_N(|z|^2) = \lim_{N\to\infty}\frac{1}{Z_N}\mathrm{e}^{-\varepsilon_0}\,\lim_{N\to\infty}\exp\left[\mathcal{B}\left(\frac{\mathrm{d}}{\mathrm{d}\mathcal{A}}\right)^2\right]\lim_{N\to\infty}\mathrm{e}^{\mathcal{A}}\,\lim_{N\to\infty}\left(\frac{1+\frac{|z|^2}{N}}{1+\frac{\mathrm{e}^{\mathcal{A}}}{N}|z|^2}\right)^{N+2} \tag{95}$$

and having in mind the significance of the constants ε_0, $\mathcal{A}$ and $\mathcal{B}$ from Eq. (75), we obtain that the first limit is $(\overline{n}+1)^{-1}$, the second is equal to unity, the third is $\exp(\beta\hbar\omega_0)$ and the fourth one is an exponential function of the type $\exp(a|z|^2)$. So, finally, we obtain

$$\lim_{N\to\infty} P_N(|z|^2) = \frac{1}{\overline{n}}\mathrm{e}^{-|z|^2/\overline{n}} \equiv P_{\mathrm{HO}}(|z|^2)\,, \tag{96}$$

where we have used the Bose–Einstein mean occupancy

$$\overline{n} = \left[\exp(\beta\hbar\omega_0) - 1\right]^{-1}. \tag{97}$$

5.1 Thermal expectation values

Once the expression of the P-function is deduced, we can express the thermal expectation value (thermal average) of an operator (physical observable) A concerning the MO:

$$\langle A\rangle_N^{(m)} = \mathrm{Tr}(\rho_N^{(m)} A) = \int \mathrm{d}\mu_N^{(m)}(z) P_N^{(m)}(|z|) \langle z; \left[\tfrac{1}{2}N\right]; m|A|z; \left[\tfrac{1}{2}N\right]; m\rangle. \tag{98}$$

As an example of useful operators A we indicate the integer powers of the number operator $\hat{v}^s$ (with $s = 1, 2, \ldots$). This is a diagonal operator in the Fock basis $|[N/2]; v\rangle$ and, finally, their thermal expectation value becomes

$$\langle \hat{v}^s\rangle_N^{(m)} = \frac{1}{Z_N^{(m)}} \sum_{v=0}^{[N/2]} \mathrm{e}^{-\beta E_{v+m}} (v+m)^s\,. \tag{99}$$

This expression can be considerably simplified if we use our ansatz referring to the expression $\exp\left(-\beta E_{v+m}\right)$ (see, also, the previous section) and finally, we can express the appearing sums through the derivatives of $\ln Z_N^{(m)}$. So, we obtain, for an arbitrary integer s

$$\langle \hat{v}^s\rangle_N^{(m)} = (-1)^s \frac{1}{Z_N^{(m)}} \left(\frac{\partial}{\partial \mathcal{A}}\right)^s Z_N^{(m)} \tag{100}$$

and for the first two integer powers respectively

$$\langle \hat{v}\rangle_N^{(m)} = -\frac{\partial}{\partial \mathcal{A}} \ln Z_N^{(m)}, \tag{101}$$

$$\langle \hat{v}^2\rangle_N^{(m)} = \left(\frac{\partial}{\partial \mathcal{A}} \ln Z_N^{(m)}\right)^2 + \left(\frac{\partial}{\partial \mathcal{A}}\right)^2 \ln Z_N^{(m)}. \tag{102}$$

With these expectation values we can define and calculate the Mandel parameter $Q_N^{(m)}$ (i.e. the thermal analogue of the corresponding function in the MO-PACSs basis $|z; [N/2]; m\rangle$):

$$Q_N^{(m)} = \frac{(\sigma_{\hat{v}})_N^{(m)}}{\langle \hat{v}\rangle_N^{(m)}} - 1 = -1 - \frac{\left(\dfrac{\partial}{\partial \mathcal{A}}\right)^2 \ln Z_N^{(m)}}{\dfrac{\partial}{\partial \mathcal{A}} \ln Z_N^{(m)}}\,, \tag{103}$$

where $(\sigma_{\hat{v}})_N^{(m)} \equiv \langle \hat{v}^2\rangle_N^{(m)} - (\langle \hat{v}\rangle_N^{(m)})^2$ is the thermal variance of the operator $\hat{v}$.

We observe that the previous results for the case of added photons have the same aspect as those for the ordinary Klauder–Perelomov CSs for the MO [27], the difference due to the added photons being included in the expression of the partition function $Z_N^{(m)}$.

Also, using Eq. (98), it is not difficult to deduce all thermal expectation values, thermodynamical and statistical characteristics of a quantum gas of non-rotational one-dimensional Morse oscillators which is in thermodynamic equilibrium with a reservoir, e.g. the free energy $F_N^{(m)}$, the internal energy $U_N^{(m)}$, the entropy $S_N^{(m)}$, the molar heat capacity at the constant volume $C_{V,N}^{(m)}$ and so on. But, this will be the subject of a forthcomming paper.

6 Conclusions

The Morse oscillator is one of the most realistic and interesting potential models, not only from the experimental, but also from the theoretical point of view. Due to the fact that the Morse potential has a finite number of the bounded states, we cannot construct the Klauder–Perelomov or Gazeau–Klauder coherent states *in stricto senso* for this potential because the positivity of the measure is not everywhere positive [26, 27].

In the present work we have constructed a new set of coherent states (in fact, the Perelomov's "generalized coherent states") for the Morse oscillator (MO-CSs) and, also, the photon-added coherent states (MO-PACSs), based on the connection between the $SU(2)$ group model (this is the appropriate and natural dynamical symmetry group for the finite number of bound states [23, 12]) and the one-dimensional Morse potential. This connection was pointed out earlier by several authors [17, 32, 33], who have deduced the properties of the raising and lowering operators $b_\pm$ connected by the angular momentum operators $J_\pm$ (17). By writing the Morse Hamiltonian as an operator proportional to the anticommutator $[b_+, b_-]_+$, we have deduced the expressions of the operators $b_\pm$ as depending on the dimensionless variable y, which is the first result of our paper.

The MO-PACSs were obtained by multiple action of operator b_+ on the MO-CSs, as usual [51, 52]. The expectation values in the MO-PACSs representation hold out some possibilities to use these states. Also, the obtained expression for the Mandel Q-parameter $Q_{N,z}^{(m)}$ provide information about the inherent properties of the MO-PACSs $|z; [N/2]; m\rangle$, i.e., the values of the variable $|z|$ for which these states exhibit sub-Poissonian, Poissonian or supra-Poissonian statistics.

We have constructed the MO-PACSs representation of the density operator of the one-dimensional Morse oscillators quantum canonical gas, as well as their diagonal representation. By applying an original ansatz to write the Morse energy exponential $\exp(-\beta E_{v+m})$ [26], we have deduced the corresponding P-function, which allowed us to calculate the thermal expectation values (thermal averages) for some specific operators, as well as the thermal analogue of the Mandel parameter. In this manner, other interesting thermal averages, as free and internal energy, entropy and molar heat capacity at the constant volume, can be calculated.

Besides the implicit construction of the photon-added coherent states of the Morse oscillator (Eq. (60)) and examination of their properties, the main results of this paper are: (a) the expressions of the operators $b_\pm$ as functions of the variable y (Eqs. (7) and (8)); (b) the expression of the integration measure $\mathrm{d}\mu_N^{(m)}(z)$; (c) the ansatz for writing the energy exponential (Eqs. (76–78)); (d) the expression of the P-function (Eq. (89)).

Due to a series of their properties and potential applications, these states, like the usual coherent states, are very interesting for examination and for use in quantum optics [43, 53, 54] or in quantum information theory [44]. So, the Morse oscillator remains an interesting subject matter for the future scientific examinations.

Two of the authors (D. P. and I. Z.) wish to thank the Romanian National Council of Scientific Research for financial support by the Grant CNCSIS A647.

References

[1] P.M. Morse: Phys. Rev. **34** (1929) 57.

[2] M.L. Sage: Chem. Phys. **35** (1978) 375.

[3] A. Matsumoto and K. Iwamoto: J. Quant. Spectrosc. Radiat. Transfer **50** (1993) 103.

[4] V.S. Vasan and R.J. Cross: J. Chem. Phys. **78** (1983) 3869.

[5] R.H. Tipping and J.F. Ogilvie: J. Chem. Phys. **79** (1983) 2537.

[6] F. Iachello and S. Oss: Phys. Rev. Lett. **66** (1991) 2946; Chem. Phys. Lett. **187** (1991) 500.

[7] Y. Alhassid, F. Iachello, and F. Gürsey: Chem. Phys. Lett. **99** (1983) 27.

[8] S. Kais and R.D. Levine: Phys. Rev. A **41** (1990) 2301.

[9] J.N. Huffaker and P.H. Dwivedi: J. Math. Phys. **16** (1975) 862.

[10] M.M. Nieto and L.M. Simmons, Jr.: Phys. Rev. A **19** (1979) 438.

[11] R. Montemayor and L. Urrutia: Amer. J. Phys. **51** (1973) 641.

[12] S.H. Dong, R. Lemus, and A. Frank: Int. J. Quant. Chem. **86** (2002) 433.

[13] C.J. Ballhausen: J. Phys. Chem. **99** (1995) 2530.

[14] I.L. Cooper: J. Phys. A: Math. Gen. **26** (1993) 1601.

[15] G. Lévai: J. Phys. A: Math. Gen. **27** (1994) 3809.

[16] M.G. Benedict and B. Molnár: Phys. Rev. A **60** (1999) R1737.

[17] A. Frank, R. Lemus, M. Carvajal, C. Jung, and E. Ziemniak: Chem. Phys. Lett. **308** (1999) 91.
M. Carvajal, R. Lemus, A. Frank, C. Jung, and E. Ziemniak: Chem. Phys. **260** (2000) 105.

[18] L. Chetouani, L. Guechi, and T.F. Hammann: Helv. Phys. Acta **65** (1992) 1069; Czech. J. Phys. **43** (1993) 13.

[19] B.S. Tošić and D. Popov: J. Phys. Chem. Solids **61** (2000) 1561.

[20] M.M. Nieto and L.M. Simmons, Jr.: Phys. Rev. D **20** (1979) 1321 (Part I); 1332 (Part II); 1342 (Part III).

[21] C. Gerry: Phys. Rev. A **33** (1986) 2207.

[22] Gh.E. Drăgănescu and N.M. Avram: Can. J. Phys. **76** (1998) 273.

[23] S.H. Dong: Can. J. Phys. **80** (2002) 129.

[24] H. Fakhri and A. Chenaghlou: Phys.Lett. A **310** (2003) 1.

[25] B. Roy and P. Roy: Phys. Lett. A **296** (2002) 187.

[26] D. Popov: Phys. Lett. A **316** (2003) 369.

[27] M. Daoud and D. Popov: Int. J. Mod. Phys. B **18** (2004) 325.

[28] D. Steele, E.R. Lipincott, and J.K. Vanderslice: Rev. Mod. Phys. **34** (1962) 239.

[29] M.S. Child and L. Halonen: Adv. Chem. Phys. **57** (1984) 1.

[30] F. Iachello, S. Oss, and R. Lemus: J. Mol. Spectrosc. **146** (1991) 56; **149** 132.

[31] N.M. Avram and Gh.E. Drăgănescu: Int. J. Quant. Chem. **64** (1997) 655.

[32] R. Lemus and A. Frank: J. Mol. Spectrosc. **201** (2000) 198.

[33] R. Lemus and A. Frank: Chem. Phys. **242** (1999) 25; Int. J. Quant. Chem. **75** (1999) 465.

[34] E. Schrödinger: Proc. R. Irish Acad. A **46** (1940) 183.

[35] L. Infeld and T.E. Hull: Rev. Mod. Phys. **23** (1951) 21.

[36] G. Haidinger, N. Bessis, and G. Bessis: J. Math. Phys. **15** (1974) 716.

[37] E. Witten: Nucl. Phys. B **188** (1981) 513.

[38] G. Lévai and B.W. Williams: J. Phys. A: Math. Gen **26** (1993) 3301.

[39] L. Pauling and E.B. Wilson, Jr.: *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1935, p. 35.

[40] L.D. Landau and E.M. Lifshitz: *Quantum Mechanics, Non-Relativistic Theory* (3rd ed.), Pergamon, 1977.

[41] Y. Alhassid, F. Gürsey, and F. Iachello: Ann. Phys. **148** (1983) 346.

[42] D. Popov: Physica Scripta **63** (2001) 257.

[43] A.M. Perelomov: *Generalized Coherent States and Their Applications*, Springer-Verlag, Berlin–Heidelberg–New York, 1986.

[44] K. Fujii: *Introduction to Coherent States and Quantum Information Theory*, quant-ph/0112090.

[45] C. Brif, A. Voudras, and A. Mann: J. Phys. A: Math. Gen **29** (1996) 5873.

[46] A.M. Mathai and R.K. Saxena: *Generalized Hypergeometric Functions with Applications in Statistics and Physical Sciences*, Lecture Notes in Mathematics, Vol. 348, Springer-Verlag, Berlin–Heidelberg–New York, 1973.

[47] J.M. Sixdeniers, K.A. Penson, and A.I. Solomon: J. Phys. A: Math. Gen. **32** (1999) 7543.

[48] I.S. Gradshteyn and I.M. Ryshik: *Tables of Integrals, Series and Products* (4th ed.), Fizmatgiz, Moscow, 1962, p. 951 (in Russian).

[49] A.I. Solomon: Phys. Lett. A **196** (1994) 29.

[50] L. Mandel and E. Wolf: *Optical Coherence and Quantum Optics*, Cambridge University Press, Cambridge, 1995.

[51] V.V. Dodonov: J. Opt. B: Quantum Semiclass. Opt. **4** (2002) R1.

[52] D. Popov: J. Phys. A: Math. Gen. **35** (2002) 7205.

[53] C. Brif and Y. Ben-Aryeh: Quantum Opt. **6** (1994) 391.

[54] D.F. Walls and G.J. Milburn: *Quantum Optics*, Springer-Verlag, Berlin–Heidelberg–New York, 1994.