

Considerations Concerning the Pseudoharmonic Oscillator Model

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Abstract

Even if the harmonic oscillator potential has its advantages, it is unrealistic in several aspects, when compared to the real interaction potentials involved in the many branches of physics. As an intermediate potential between the harmonic (an "ideal" potential) and the anharmonic potentials, in the present article we deal with the so-called "pseudoharmonic potential". We have calculated the expected values of some thermodynamical functions, which characterize the quantum ideal gas of pseudoharmonical oscillators and some thermal moments of the internuclear distance, generally and for two approximations related to the internuclear distance r_0 .

Key words: pseudoharmonic oscillator, thermal average, Hellmann-Feynman

1. Introduction

In many branches of physics, even if the harmonic oscillator (HO) potential certainly has its advantages and applications, it is unrealistic in several aspects. First, the HO potential is used for its mathematical solvability, i.e. it allows the exact mathematical solution of the Schrödinger equation. When compared to the real interaction potentials involved e.g. in diatomic molecule physics, then these disadvantages become more evident. The HO potential is a good theoretical model, but comparison with the experimental spectroscopic data shows that this model is often unsatisfactory, because many properties of real physical systems are not harmonical but anharmonical. So, it is necessary to use one of the anharmonic potentials.

As an intermediate potential between the HO potential (an "ideal" potential) and the anharmonic potentials (such as the Morse potential, the more "realistic" potential), in the present article we deal with the so-called *pseudoharmonic oscillator* (PHO) potential.

We consider that the physical system is a quantum ideal gas of the diatomic molecules, which fulfil the conditions of the quantum canonical distribution. The PHO potential, which describes the molecular vibrations, is a spherically symmetric potential, with the effective potential defined as in Ref.[1]:

$$V_J^{(p)}(r) = \frac{m\omega^2}{8} r_0^2 \left(\frac{r}{r_0} - \frac{r_0}{r} \right)^2 + \frac{\hbar^2}{2m} \frac{J(J+1)}{r^2}, \quad (1)$$

where r_0 is the equilibrium distance between the nuclei of the diatomic molecule.

This potential admits, also, the exact analytical solution for the Schrödinger equation and this is one of the reasons we deal with it. The radial eigenfunctions and eigenvalues have been calculated in Ref.[1] and the final expressions are:

$$R_{vJ}^{(p)}(r) \equiv \frac{1}{r} u_v^\alpha(r) = \left[\frac{B^3 v!}{2^\alpha \Gamma(\alpha + v + 1)} \right]^{\frac{1}{2}} (Br)^{\alpha - \frac{1}{2}} \exp\left(-\frac{B^2}{4} r^2\right) L_v^\alpha\left(\frac{B^2}{2} r^2\right), \quad (2)$$

$$E_{vJ}^{(p)} = \hbar\omega \left(v + \frac{1}{2}\right) + \frac{\hbar\omega}{2} \alpha - \frac{m\omega^2}{4} r_0^2 \equiv \hbar\omega v + E_0, \quad (3)$$

where v and J are the vibrational and the rotational quantum numbers. We observe that the vibrational and the rotational degrees of freedom are uncoupled, which offers some mathematical advantages in the calculations related to the PHO potential. This will become more evident in the next sections. Also, we have used the notations:

$$B = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}}; \quad \alpha = \left[\left(J + \frac{1}{2}\right)^2 + \left(\frac{m\omega}{2\hbar} r_0^2\right)^2 \right]^{\frac{1}{2}}. \quad (4)$$

2. Density matrix

In Ref.[2] we have deduced the expression for the whole (total) density matrix for PHO in the position representation:

$$\rho^{(p)}(\vec{r}, \vec{r}'; \beta) = \frac{1}{4\pi} \sum_{J=0}^{\infty} (2J+1) P_J(\cos \gamma) \rho_J^{(p)}(r, r'; \beta), \quad (5)$$

where $P_J(\cos \gamma)$ is the Legendre polynomial and γ - the angle between the vectors \vec{r} and \vec{r}' .

The radial density matrix in the position representation $\rho_J^{(p)}(r, r'; \beta)$ was deduced as the solution of the Bloch equation and it is [2]:

$$\begin{aligned} \rho_J^{(p)}(r, r'; \beta) &= \exp\left(\beta \frac{m\omega^2}{4} r_0^2\right) \frac{m\omega}{2\hbar} \frac{1}{\sinh \beta \frac{\hbar\omega}{2}} \times \\ &\times \frac{1}{(rr')^{\frac{1}{2}}} \exp\left[-\frac{m\omega}{4\hbar} (r^2 + r'^2) \coth \beta \frac{\hbar\omega}{2}\right] I_\alpha\left(\frac{m\omega}{2\hbar} \frac{1}{\sinh \beta \frac{\hbar\omega}{2}} rr'\right), \end{aligned} \quad (6)$$

where $I_\alpha(x)$ is the modified Bessel function.

The trace of the whole density matrix is the whole partition function:

$$Z^{(p)}(\beta) = \int d\vec{r} \rho^{(p)}(\vec{r}, \vec{r}; \beta) = \sum_{J=0}^{\infty} (2J+1) Z_J^{(p)}(\beta), \quad (7)$$

while the trace of the radial density matrix is the rotational partition function:

$$Z_J^{(p)}(\beta) = \int_0^\infty dr r^2 \rho_J^{(p)}(r, r; \beta) = \frac{1}{2 \sinh y} e^{\beta \frac{m\omega}{4} r_0^2} e^{-\beta \frac{\hbar\omega}{2} \alpha}. \quad (8)$$

Finally, we obtain:

$$Z^{(p)}(\beta) = \frac{1}{2 \sinh y} e^{\beta \frac{m\omega}{4} r_0^2} T_\alpha(y), \quad (9)$$

where we have used the following notations:

$$y = \beta \frac{\hbar\omega}{2}; \quad T_\alpha(y) = \sum_{J=0}^{\infty} (2J+1) e^{-y\alpha}. \quad (10)$$

The partition function $Z^{(p)}(\beta)$ is a quantity of maximal informational importance because, by means of the partition function, it is possible to express all the characteristic observables of the PHO quantum gas.

So, the internal energy of the system of quantum PHO gas is:

$$U_{syst}^{(p)} = NU^{(p)} = -N \frac{\partial}{\partial \beta} \ln Z^{(p)} = -N \frac{m\omega^2}{4} r_0^2 + N \frac{\hbar\omega}{2} \left[\coth y - \frac{\partial}{\partial y} (\ln T_\alpha) \right], \quad (11)$$

where N is the whole number of the PHO in the quantum gas.

Using the expression of the internal energy, the specific heat for one mole (i.e. the molar heat capacity) of the PHO-s quantum ideal gas is:

$$C_V^{(p)} = \frac{1}{\nu} \frac{\partial U_{syst}^{(p)}}{\partial T} = N_A \frac{\partial U^{(p)}}{\partial T} = -R\beta^2 \frac{\partial U^{(p)}}{\partial \beta}. \quad (12)$$

For the PHO-s system, it is useful to write this expression with respect to the variable y and, then, it becomes:

$$\frac{C_V^{(p)}}{R} = \left(\frac{y}{\sinh y} \right)^2 + \frac{\hbar\omega}{2} \beta^2 \frac{\partial^2}{\partial \beta \partial y} (\ln T_\alpha) = \left(\frac{y}{\sinh y} \right)^2 + y^2 \frac{\partial^2}{\partial y^2} (\ln T_\alpha). \quad (13)$$

On the other hand, the free energy of the PHO quantum gas, which corresponds to one molecule (one PHO) is:

$$F^{(p)} = -\frac{1}{\beta} \ln Z^{(p)} = -\frac{1}{\beta} \ln \frac{1}{2 \sinh y} - \frac{m\omega^2}{4} r_0^2 - \frac{1}{\beta} \ln T_\alpha. \quad (14)$$

In the previous equations we have used the superscript (p) for the observables concerning the PHO, while the superscript (0) will be used for similar observables concerning the HO.

3. Quantum-statistical averages

The quantum-statistical average or the thermal average for an observable A , which characterize the quantum gas of pseudoharmonical oscillators obeying the quantum canonical distribution can be calculate as follows:

$$\begin{aligned} \langle A \rangle^{(p)} &= \frac{Tr A \rho^{(p)}}{Tr \rho^{(p)}} = \frac{1}{Z^{(p)}} \sum_{J=0}^{\infty} (2J+1) Z_J^{(p)} \langle A \rangle_J^{(p)} = \\ &= \frac{1}{T_\alpha} \sum_{J=0}^{\infty} (2J+1) e^{-y\alpha} \langle A \rangle_J^{(p)}, \end{aligned} \quad (15)$$

where we have used the corresponding expressions for the whole density matrix in the position representation and the whole partition function.

The free energy is connected with the position thermal moments, that is, with the quantum-statistical averages of the powers of displacement from the equilibrium position operator. The formalism of the moments of the spectral density distribution has already been applied in the case of spectra of oscillators coupled by kinetic terms (see, Ref.[3] and references therein), though we use here not the spectral but the thermal moments. For this reason, we consider that the free energy of the PHO-s gas is a function of some parameters \hbar, m, ω and r_0 , generically denoted by λ_i , so that:

$$dF^{(p)} = \sum_i \frac{\partial F^{(p)}}{\partial \lambda_i} d\lambda_i. \quad (16)$$

On the other hand, in Ref.[4], we have extended the quantum virial and Hellmann-Feynman theorems to the quantum-statistical averages in the case of the central field potentials. As a consequence, we have obtained the following equation involving the quantum-statistical averages:

$$\frac{\partial F^{(p)}}{\partial \lambda_i} = \left\langle \frac{\partial H^{(p)}}{\partial \lambda_i} \right\rangle = \frac{1}{2} \left(\frac{\partial}{\partial \lambda_i} \ln \frac{\hbar^2}{2m} \right) \left\langle r \frac{\partial V^{(p)}}{\partial r} \right\rangle + \left\langle \frac{\partial V^{(p)}}{\partial \lambda_i} \right\rangle. \quad (17)$$

By using Eq.(4), the effective potential of the PHO (1) can be written in the following manner:

$$V_J^{(p)}(r) = \frac{m\omega^2}{8} r^2 - \frac{m\omega^2}{4} r_0^2 + \frac{\hbar^2}{2m} \left(\alpha^2 - \frac{1}{4} \right) \frac{1}{r^2}. \quad (18)$$

After straightforward calculations, by performing the partial derivatives of the free energy expression (14) on the one hand and by applying Eq.(17) to the effective potential (18) on the other hand, we obtain successively:

$$\frac{\partial F^{(p)}}{\partial \hbar} = \frac{\omega}{2} \coth y - \frac{\omega}{2} \frac{\partial}{\partial y} T_\alpha - \frac{\omega}{2} T_\alpha^{(-1)} = \frac{m\omega^2}{4\hbar} \langle r^2 \rangle - \frac{\hbar}{m} \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2 \left\langle \frac{1}{r^2} \right\rangle, \quad (19)$$

$$\frac{\partial F^{(p)}}{\partial m} = -\frac{\omega^2}{4} r_0^2 + \frac{\hbar\omega}{2m} \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2 T_\alpha^{(-1)} = -\frac{\omega^2}{4} r_0^2 + \frac{\hbar^2}{m^2} \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2 \left\langle \frac{1}{r^2} \right\rangle, \quad (20)$$

$$\begin{aligned} \frac{\partial F^{(p)}}{\partial \omega} &= \frac{\hbar}{2} \coth y - \frac{m\omega}{2} r_0^2 - \frac{\hbar}{2} \frac{\partial}{\partial y} T_\alpha + \frac{\hbar}{2} \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2 T_\alpha^{(-1)} = \\ &= \frac{m\omega}{4} \langle r^2 \rangle - \frac{m\omega}{2} r_0^2 + \frac{\hbar^2}{m\omega} \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2 \left\langle \frac{1}{r^2} \right\rangle, \end{aligned} \quad (21)$$

$$\frac{\partial F^{(p)}}{\partial r_0} = -\frac{m\omega^2}{2} r_0 + \frac{\hbar\omega}{r_0} \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2 T_\alpha^{(-1)} = -\frac{m\omega^2}{2} r_0 + 2 \frac{\hbar^2}{mr_0} \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2 \left\langle \frac{1}{r^2} \right\rangle, \quad (22)$$

where we have used the following notation:

$$T_\alpha^{(-1)} = \frac{1}{T_\alpha} \sum_{J=0}^{\infty} (2J+1) \frac{1}{\alpha} e^{-y\alpha}. \quad (23)$$

By combining these relations, we obtain the following quantum-statistical or thermal averages for the position variable:

$$\langle r^2 \rangle = \frac{2\hbar}{m\omega} \left(\coth y - \frac{\partial}{\partial y} \ln T_\alpha \right), \quad (24)$$

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{m\omega}{2\hbar} T_\alpha^{(-1)}. \quad (25)$$

In order to verify the above obtained relations concerning the PHO we must apply the harmonic limit defined as [2]:

$$\begin{aligned} \lim_{\substack{\omega \rightarrow 2\omega_0 \\ r_0 \rightarrow 0 \\ \alpha \rightarrow J + \frac{1}{2}}} A &\equiv \lim_{HO} A = A^0, \end{aligned} \quad (26)$$

i.e. when we apply the harmonic limit to a certain observable $A^{(p)}$ concerning the PHO, if the relation is proper, we must obtain the corresponding observable $A^{(0)}$ concerning the HO-3D (the 3-dimensional isotropic harmonic oscillator) which has the frequency ω_0 .

Before performing this limiting operation, it is useful to point out the harmonic limit for the following expressions, which are obtained after straightforward calculations:

$$\lim_{HO} T_\alpha = T_{J+\frac{1}{2}} = \frac{1}{2} \frac{1}{\sinh^2 \beta \frac{\hbar\omega_0}{2}} \cosh \beta \frac{\hbar\omega_0}{2}, \quad (27)$$

$$\lim_{HO} \frac{\partial}{\partial y} T_\alpha = -\coth \beta \frac{\hbar\omega_0}{2} + \frac{1}{2} \frac{1}{\coth \beta \frac{\hbar\omega_0}{2}}, \quad (28)$$

$$\lim_{HO} T_\alpha^{(-1)} = 2 \tanh \beta \frac{\hbar\omega_0}{2}. \quad (29)$$

Therefore we obtain [2]:

$$\lim_{HO} Z^{(p)} = \left(\frac{1}{2 \sinh \beta \frac{\hbar\omega_0}{2}} \right)^3 = Z^{(0)}, \quad (30)$$

$$\lim_{HO} U^{(p)} = 3N \frac{\hbar\omega_0}{2} \coth \beta \frac{\hbar\omega_0}{2} = U^{(0)}, \quad (31)$$

$$\lim_{HO} F^{(p)} = \frac{1}{\beta} \ln 2 \sinh \beta \frac{\hbar\omega_0}{2} = F^{(0)}, \quad (32)$$

$$\lim_{HO} \frac{C_V^{(p)}}{R} = 3 \left(\frac{\beta \frac{\hbar\omega_0}{2}}{\sinh \beta \frac{\hbar\omega_0}{2}} \right)^3 = \frac{C_V^{(0)}}{R}. \quad (33)$$

$$\lim_{HO} \langle r^2 \rangle = 3 \frac{\hbar}{2m\omega_0} \coth \beta \frac{\hbar\omega_0}{2} = \langle r^2 \rangle^{(0)}, \quad (34)$$

$$\lim_{HO} \left\langle \frac{1}{r^2} \right\rangle = \frac{2m\omega_0}{\hbar} \tanh \beta \frac{\hbar\omega_0}{2} = \left\langle \frac{1}{r^2} \right\rangle^{(0)}. \quad (35)$$

4. Two approximations

It is easy to observe that the sum T_α^{-1} can be written in the following manner:

$$T_\alpha^{-1} = \frac{1}{T_\alpha} \sum_{J=0}^{\infty} (2J+1) \frac{1}{\alpha} e^{-y\alpha} = \frac{1}{T_\alpha} \int_y^{\infty} T_\alpha(y) dy. \quad (36)$$

Because of the presence of an infinite series (like T_α and their derivatives), the above obtained quantum-statistical averages for the PHO can be calculated only numerically, i. e. with limited precision. So, it is useful to simplify the expression of the sum denoted by T_α , taking into account the possible values of the equilibrium distance r_0 .

We examine two approximations concerning these values: the approximation of small values of r_0 (called *m-approximation*) and the approximation of large values of r_0 (called *M-approximation*). The corresponding observables and thermal moments will be denoted by the m , respectively M -index.

In the *m-approximation*, i. e. if r_0 is small, by performing the power series development of the expression of α up to the power two, we obtain:

$$\alpha_m = \left[\left(J + \frac{1}{2} \right)^2 + C \right]^{\frac{1}{2}} \approx J + \frac{1}{2} + \frac{C}{2} \frac{1}{J + \frac{1}{2}}, \quad (37)$$

where we have denoted:

$$C = \left(\frac{m\omega}{2\hbar} r_0^2 \right)^2. \quad (38)$$

For such values of temperature T for which the variable y is small, the sum T_α can be written as the following integral:

$$T_m = 2 \sum_{J=0}^{\infty} \left(J + \frac{1}{2} \right) e^{-y\alpha_m} = 2 \int_0^{\infty} dx x e^{-yx - \frac{1}{2}yC\frac{1}{x}}, \quad (39)$$

where we have denoted $x = J + \frac{1}{2}$.

This integral is of the following kind [7]:

$$\int_0^{\infty} dx x^{\nu-1} e^{-\gamma x - \frac{\beta}{x}} = 2 \left(\frac{\beta}{\gamma} \right)^{\frac{\nu}{2}} K_\nu(2\sqrt{\beta\gamma}), \quad [\operatorname{Re}\beta > 0, \operatorname{Re}\gamma > 0], \quad (40)$$

where $K_\nu(z)$ is the Bessel function of the second kind. This function becomes, for $\nu > 0$ fixed and $z \rightarrow 0$ [6]:

$$K_\nu(z) \approx \frac{1}{2} \Gamma(\nu) \left(\frac{2}{z} \right)^\nu, \quad (41)$$

where $\Gamma(\nu)$ is the Euler's gamma function.

In this manner we obtain:

$$T_m = \frac{2}{y^2} \quad (42)$$

and, consequently:

$$T_m^{-1} = y. \quad (43)$$

By using these last two equations and also Eqs.(9), (11)-(14), (24) and (25), after straightforward calculations, we obtain successively:

$$Z_m = \frac{1}{y^2} \frac{1}{\sinh y} e^{y \frac{m\omega}{2\hbar} r_0^2}, \quad (44)$$

$$F_m = -\frac{m\omega^2}{4} r_0^2 + \frac{\hbar\omega}{2} \frac{1}{y} \ln \sinh y + \hbar\omega \frac{1}{y} \ln y, \quad (45)$$

$$U_m = -\frac{m\omega^2}{4} r_0^2 + \frac{\hbar\omega}{2} \left(\coth y + 2 \frac{1}{y} \right), \quad (46)$$

$$\frac{C_{V;m}}{R} = \left(\frac{y}{\sinh y} \right)^2 + 2, \quad (47)$$

$$\langle r^2 \rangle_m = \frac{2\hbar}{m\omega} \left(\coth y + 2 \frac{1}{y} \right), \quad (48)$$

$$\left\langle \frac{1}{r^2} \right\rangle_m = \frac{m\omega}{2\hbar} y. \quad (49)$$

The M -approximation, i.e. the case of large values of r_0 is more interesting. We can transform the expression for α from Eq.(4) and perform the power series development of the square root up to the power of order two:

$$\alpha_M = \frac{m\omega}{2\hbar} r_0^2 \left[1 + \left(\frac{J + \frac{1}{2}}{\frac{m\omega}{2\hbar} r_0^2} \right)^2 \right]^{\frac{1}{2}} \approx \frac{m\omega}{2\hbar} r_0^2 + \frac{1}{2} \frac{\left(J + \frac{1}{2} \right)^2}{\frac{m\omega}{2\hbar} r_0^2}. \quad (50)$$

In this approximation, the sum T_α becomes:

$$T_M = 2 \exp \left(-\beta \frac{m\omega^2}{4} r_0^2 \right) \sum_{J=0}^{\infty} \left(J + \frac{1}{2} \right) \exp \left[-\beta \frac{\hbar^2}{2mr_0^2} \left(J + \frac{1}{2} \right)^2 \right]. \quad (51)$$

As it is usual (see, e.g. Refs.[7], [8]), the last sum may be replaced by an integral. The motivation is simple: if we again denote $J + \frac{1}{2} = x$, then the quantity before x into the exponential (i.e. $-\beta \frac{\hbar^2}{2mr_0^2} \equiv \frac{\Theta_{rot}}{T}$, where Θ_{rot} is the rotational constant) is very small for more gases and for all temperatures for which these gases are not in the liquid state. In other words, the separation between the rotational energy levels is so small that this replacement is wholly possible. So, the last equation becomes:

$$\begin{aligned} T_M &= 2 \exp \left(-\beta \frac{m\omega^2}{4} r_0^2 \right) \int_0^{\infty} dx x \exp \left(-\beta \frac{\hbar^2}{2mr_0^2} x^2 \right) = \\ &= \frac{m\omega}{\hbar} r_0^2 \frac{1}{y} \exp \left(-y \frac{m\omega}{2\hbar} r_0^2 \right). \end{aligned} \quad (52)$$

Consequently, the sum T_M^{-1} is:

$$T_M^{-1} = \frac{1}{T_M} \int_y^{\infty} T_M(y) dy = y e^{y \frac{m\omega}{2\hbar} r_0^2} \int_y^{\infty} dy \frac{1}{y} e^{-y \frac{m\omega}{2\hbar} r_0^2}. \quad (53)$$

This integral leads to the integral exponential function ($\text{Ei}(z)$)[5]:

$$\int_x^\infty dx \frac{1}{x} e^{-ax} = -\text{Ei}(-ax), \quad (54)$$

which has the following series development [5]:

$$\begin{aligned} \text{Ei}(-z) &= e^{-z} \sum_{k=1}^n (-1)^k \frac{(k-1)!}{z^k} + R_n, \\ |R_n| &< \frac{n!}{|z|^{n+1} \cos \frac{\varphi}{2}}, \quad z = |z|e^{i\varphi}, \quad \varphi^2 < \pi^2. \end{aligned} \quad (55)$$

For the M -approximation are relevant the first two terms of the series development and so, we obtain:

$$T_M^{-1} = \frac{2\hbar}{m\omega} \left[\frac{1}{r_0^2} - \frac{1}{y} \frac{2\hbar}{m\omega} \left(\frac{1}{r_0^4} \right) + \dots \right]. \quad (56)$$

By using the above obtained expressions for T_M and T_M^{-1} , after straightforward calculations, Eqs.(9), (11)-(14), (24) and (25) lead to the following relations:

$$Z_M = \frac{m\omega}{2\hbar} r_0^2 \frac{1}{y} \frac{1}{\sinh y}, \quad (57)$$

$$F_M = \frac{\hbar\omega}{2} \frac{1}{y} \ln 2 \sinh y + \frac{\hbar\omega}{2} \frac{1}{y} \ln y + \frac{\hbar\omega}{2} \frac{1}{y} \ln \frac{\hbar}{m\omega} \frac{1}{r_0^2}, \quad (58)$$

$$U_M = \frac{\hbar\omega}{2} \left(\coth y + \frac{1}{y} \right), \quad (59)$$

$$\frac{C_{V;M}}{R} = \left(\frac{y}{\sinh y} \right)^2 + 1, \quad (60)$$

$$\langle r^2 \rangle_M = r_0^2 + \frac{2\hbar}{m\omega} \left(\coth y + \frac{1}{y} \right), \quad (61)$$

$$\left\langle \frac{1}{r^2} \right\rangle_M = \frac{1}{r_0^2} - \frac{1}{y} \frac{2\hbar}{m\omega} \frac{1}{r_0^4}. \quad (62)$$

The expression of the potential practically is the same in both representations, i.e.:

$$V_{J;m}^{(p)}(r) \approx V_{J;M}^{(p)}(r) \approx V_J^{(p)}(r), \quad (63)$$

since:

$$\alpha_m^2 \approx \alpha_M^2 \approx \alpha^2, \quad (64)$$

if we neglect the term containing $(r_0^2)^4$, respectively $(r_0^2)^{-4}$. As a consequence, the quantum-statistical averages for r^2 and r^{-2} in both approximations can be obtained also by the moment methods, i.e. by the method based on the application of hypervirial and Hellmann-Feynman theorems, in the same manner as in Section 3. This fact shows that both approximations are suitable.

This method allows the possibility also to obtain the quantum-statistical averages of the other observables which characterize the quantum system (the PHO-s quantum ideal gas). It is well known that, in these calculations, the partition function (i.e. the trace

of the density matrix) is a very important quantity because this function contains all statistical-thermodynamical information about the quantum system.

5. Conclusion

In the present article we try to present an alternative anharmonic potential confronted by the harmonic oscillator (HO) potential. This potential is the so-called pseudoharmonic oscillator (PHO) potential, which is a central field potential and a more realistic potential in comparison with the HO potential. It becomes infinite at the origin of the internuclear coordinate r and it extends only in the physical region ($0 < r < \infty$). Due to the mathematical facilities in the approach of the PHO (it admits an exact solution of the Schrödinger equation and the exact expression of the expected values), the PHO is useful, for instance, for the examination of molecular vibrations.

In the article we have calculated some thermodynamical functions, which characterize the PHO-s quantum ideal gas (i.e. partition function, free energy, internal energy, specific heat) and some thermal moments of the internuclear distance. Due to the fact that these expressions contain the infinite sum (T_α and T_α^{-1}), we have tried to obtain the corresponding expressions for two approximations: m -approximation (for small internuclear equilibrium distance r_0) and M -approximation (for large r_0). In these expressions the contribution of the anharmonicity is evinced in an analytical manner.

All these results (Eqs.(9), (11)-(14), (24) and (25)) can be obtained also if we use the density matrix in coherent states representation. It is easy to demonstrate that the PHO agrees with the Barut-Girardello coherent states. This question is the subject matter of our other article [9]. Moreover, the connection between PHO and the Barut-Girardello coherent states leads to the idea that the pseudoharmonical oscillator may have some applications in quantum optics.

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