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Harmonic Oscillator in External Fields: Applications to Trapped Bosons and Fermions

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Properties of harmonic oscillator in external fields are studied. The formalism developed is applied to a harmonic oscillator in a nonhomogeneous gravitational field. Partition functions and thermodynamic potentials for trapped Bose and Fermi gases are found. Thermodynamics of trapped Bosons and Fermions in external fields is discussed.

KEY WORDS: harmonic oscillator; gravitational field; trapped atoms.

1. INTRODUCTION

The model of the harmonic oscillator plays a very important part and has numerous applications in quantum physics. Harmonic oscillators describe such processes as oscillations of molecules and atoms in solids, vibration of the surface of the spherical atomic nuclei. Properties of light and theory of radiation are also described by infinite collection of oscillators. These results are presented in a number of publications. The theory of the harmonic oscillator is effectively used for the study of the properties of confined alkali atoms in harmonic traps (Butts and Rokhsar, 1997; Dalfovo *et al.*, 1999; Grossmann and Holthaus, 1995). In this work the model of harmonic oscillator in formalism of creation and annihilation operators in external fields is developed. The behavior of the oscillator in constant (homogeneous) and variable (nonhomogeneous) fields is studied. As an application, a model of harmonic oscillator in external gravitational field is considered. The developed formalism is applied for the study of thermal properties of noninteracting Bose and Fermi gases in harmonic traps. The paper is organized in the following way. In Section 2 the general formalism of harmonic oscillator is considered. Section 3 is devoted to the properties of a harmonic oscillator in a homogeneous and nonhomogeneous electric field. These results allow us to formulate clearly the harmonic oscillator problem in three-dimensional nonhomogeneous

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gravitational field in Newtonian approximation. In Section 4 the partition functions and grand thermodynamic potentials of trapped Bose and Fermi ensembles are calculated. Thermodynamical properties of trapped Bosons and Fermions are discussed in Section 5.

2. GENERAL FORMALISM

Let us consider quantum mechanics of simple one-dimensional harmonic oscillator. One-dimensional Hamiltonian of the harmonic oscillator has the form

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}, \tag{1}$$

where m is the mass, and ω is the angular frequency of the oscillator. The relation between the angular frequency ω and the spring constant k of the oscillator is written as $\omega^2 = k/m$. The purpose of this section is to proceed along with the usual steps to quantize the classical harmonic oscillator with creation and annihilation operator formalism. Introducing the well-known two dimensionless annihilation and creation operators

$$\begin{aligned} a &= \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x + \frac{ip}{m\omega}\right), \\ a^+ &= \left(\frac{m\omega}{2\hbar}\right)^{1/2}\left(x - \frac{ip}{m\omega}\right), \end{aligned} \tag{2}$$

with commutation properties

$$[a, a^+] = 1, \qquad [a, a] = [a^+, a^+] = 0, \tag{3}$$

one can write the equation for the Hamiltonian (1) (Landay and Lifshitz, 1975) as

$$H = \frac{\hbar\omega}{2}[aa^+ + a^+a] = \hbar\omega\left[a^+a + \frac{1}{2}\right]. \tag{4}$$

The Hamiltonian (4) with three commutators (3) completely describes the harmonic oscillator in terms of creation and annihilation operators. Creation and annihilation operators act on eigenvectors $|n\rangle$ of the Hamiltonian (4) according to the following rules $a^+|n\rangle = \sqrt{n+1}|n+1\rangle$, $a|n\rangle = \sqrt{n}|n-1\rangle$, and matrix elements of these operators are

$$\begin{aligned} \langle n'|a^+|n\rangle &= (n+1)^{1/2}\delta_{n',n+1}, \\ \langle n'|a|n\rangle &= n^{1/2}\delta_{n',n-1}. \end{aligned} \tag{5}$$

The eigenvalues n of the operator a^+a are the positive integers and zero, that means that the Hamiltonian (4) is diagonal in the representation of occupation numbers and $H_n = \hbar\omega(n + 1/2)$. The product a^+a is treated as a number operator for excitations of the oscillator. The position and momentum operators can be expressed from the Eq. (2) as

$$x = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (a^+ + a),$$
$$p = i\left(\frac{\hbar m\omega}{2}\right)^{1/2} (a^+ - a). \tag{6}$$

Matrix elements for these operators are written as

$$\langle n'|x|n\rangle = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left[(n+1)^{1/2}\delta_{n',n+1} + n^{1/2}\delta_{n',n-1}\right],$$
$$\langle n'|p|n\rangle = i\left(\frac{\hbar m\omega}{2}\right)^{1/2} \left[(n+1)^{1/2}\delta_{n',n+1} - n^{1/2}\delta_{n',n-1}\right], \tag{7}$$

and have no diagonal elements. Time dependence of annihilation and creation operators is found with the Heisenberg equation. For an operator $O(t) = e^{iHt/\hbar} O\, e^{-iHt/\hbar}$ time development of $O(t)$ can be written as

$$\frac{\partial O(t)}{\partial t} = \frac{i}{\hbar}[H, O(t)]. \tag{8}$$

In the case of annihilation and creation operators the Eq. (8) gives

$$\frac{\partial a(t)}{\partial t} = -i\omega a(t),$$
$$\frac{\partial a^+(t)}{\partial t} = i\omega a^+(t). \tag{9}$$

The solutions of (9) are written as

$$a(t) = e^{-i\omega t} a,$$
$$a^+(t) = e^{i\omega t} a^+, \tag{10}$$

where $a = a(0)$, $a^+ = a^+(0)$ are given at the moment $t = 0$. Then the position and the momentum operators (6) in time dependent form will be

$$x(t) = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (e^{i\omega t} a^+ + e^{-i\omega t} a),$$
$$p(t) = i\left(\frac{\hbar m\omega}{2}\right)^{1/2} (e^{i\omega t} a^+ - e^{-i\omega t} a). \tag{11}$$

3. HARMONIC OSCILLATOR IN EXTERNAL FIELDS

3.1. Electric Field

Let us consider the harmonic oscillator in external fields. For the simplicity we will consider the constant electric field E. The Hamiltonian of the harmonic oscillator in external field of a constant intensity may be written in the form

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} + eEx = \hbar\omega\left[a^+a + \frac{1}{2}\right] + eE\left(\frac{\hbar}{2m\omega}\right)^{1/2}(a^+ + a), \quad (12)$$

where e is the charge of the harmonic oscillator. Denoting $\zeta = eE(\hbar/2m\omega)^{1/2}$, we obtain

$$H = \hbar\omega\left[a^+a + \frac{1}{2}\right] + \zeta(a^+ + a). \quad (13)$$

Time evolution for operators a, a^+ is found from (8) and (13):

$$\begin{aligned} \frac{\partial a(t)}{\partial t} &= -i\omega\left(a + \frac{\zeta}{\hbar\omega}\right), \\ \frac{\partial a^+(t)}{\partial t} &= i\omega\left(a^+ + \frac{\zeta}{\hbar\omega}\right). \end{aligned} \quad (14)$$

One can define a new set of operators $\tilde{a} = a + \zeta/\hbar\omega$, $\tilde{a}^+ = a^+ + \zeta/\hbar\omega$ and rewrite Eq. (14) in the form

$$\begin{aligned} \frac{\partial \tilde{a}(t)}{\partial t} &= -i\omega\tilde{a}, \\ \frac{\partial \tilde{a}^+(t)}{\partial t} &= i\omega\tilde{a}^+. \end{aligned} \quad (15)$$

Time evolution of these operators will be

$$\begin{aligned} \tilde{a}(t) &= e^{-i\omega t}\tilde{a}, \\ \tilde{a}^+(t) &= e^{i\omega t}\tilde{a}^+. \end{aligned} \quad (16)$$

The operators $\tilde{a}$, $\tilde{a}^+$ have the same commutation relations as a, a^+:

$$[\tilde{a}, \tilde{a}^+] = 1, \qquad [\tilde{a}, \tilde{a}] = [\tilde{a}^+, \tilde{a}^+] = 0, \quad (17)$$

and Hamiltonian (13) will be written in the form

$$H = \hbar\omega\left[\tilde{a}^+\tilde{a} + \frac{1}{2}\right] - \frac{\zeta^2}{\hbar\omega}. \quad (18)$$

The last term of the Hamiltonian (18) indicates the energy shift due to the interaction of the oscillator with the electric field. The position operator is easily found from (11) and (16):

$$x(t) = \left(\frac{\hbar}{2m\omega}\right)^{1/2} \left(e^{i\omega t}\tilde{a}^{+} + e^{-i\omega t}\tilde{a} - \frac{2\zeta}{\hbar\omega}\right). \tag{19}$$

From the Eq. (19) we obtain the expression for the equilibrium point

$$x_0 = -\frac{2\zeta}{\hbar\omega}\left(\frac{\hbar}{2m\omega}\right)^{1/2} = -\frac{eE}{m\omega^2}. \tag{20}$$

As follows from this analysis, the oscillator oscillates with the same frequency ω but the point of equilibrium is shifted in respect with (20). Thus the Hamiltonian (18) describes a simple harmonic motion. If the electric field E has gradient in x-direction, then

$$E(x_0 + x) = E(x_0) + \frac{dE(x_0)}{dx}x. \tag{21}$$

The equation for Hamiltonian (12) will be

$$H = \frac{p^2}{2m} + \frac{m\Omega_x^2 x^2}{2} + eEx, \tag{22}$$

where the angular frequency Ω_x is expressed as

$$\Omega_x^2 = \omega^2\left(1 + \frac{2e}{m\omega^2}\frac{dE(x_0)}{dx}\right). \tag{23}$$

One can introduce creation and annihilation operators $\tilde{A} = A + \zeta/\hbar\Omega_x$ and $\tilde{A}^{+} = A^{+} + \zeta/\hbar\Omega_x$, where $\tilde{A}$, $\tilde{A}^{+}$ are written as

$$\begin{aligned} A &= \left(\frac{m\Omega_x}{2\hbar}\right)^{1/2}\left(x + \frac{ip}{m\Omega_x}\right), \\ A^{+} &= \left(\frac{m\Omega_x}{2\hbar}\right)^{1/2}\left(x - \frac{ip}{m\Omega_x}\right). \end{aligned} \tag{24}$$

The commutation relations for these operators are

$$[\tilde{A}, \tilde{A}^{+}] = 1, \qquad [\tilde{A}, \tilde{A}] = [\tilde{A}^{+}, \tilde{A}^{+}] = 0, \tag{25}$$

and the time evolution is described by the equations

$$\begin{aligned} \tilde{A}(t) &= e^{-i\Omega_x t}\tilde{A}, \\ \tilde{A}^{+}(t) &= e^{i\Omega_x t}\tilde{A}^{+}. \end{aligned} \tag{26}$$

The Hamiltonian of the harmonic oscillator in a nonhomogeneous electric field will be

$$H = \hbar\Omega_x \left(\tilde{A}^+ \tilde{A} + \frac{1}{2} \right) - \frac{\zeta^2}{\hbar\Omega_x}. \tag{27}$$

The position operator is written as

$$x(t) = \left(\frac{\hbar}{2m\Omega_x} \right)^{1/2} \left(e^{i\Omega_x t} \tilde{A}^+ + e^{-i\Omega_x t} \tilde{A} - \frac{2\zeta}{\hbar\Omega_x} \right). \tag{28}$$

The Eq. (28) defines the displacement of the equilibrium point $x_0 = -eE/m\Omega_x^2$. This result shows that displacement depends not only on the intensity of the field but also on its gradient.

3.2. Gravitational Field

The considered example with the harmonic oscillator in electric field gives us the direct way to extend the formalism of second quantization for the case of a three-dimensional harmonic oscillator in an external gravitational field. Let us assume that the harmonic oscillator interacts with a nonhomogeneous gravitational field. The potential of this field can be written in the following form

$$\Phi_{\vec{X}_0}(\vec{x}) = \Phi_0 - g_i x^i + \frac{1}{2}\Gamma_{ij} x^i x^j, \tag{29}$$

where we use Einstein summation rule and assume $x^i = \{x, y, z\}$. In the Eq. (29) the first right hand term Φ_0 is the potential of gravitational field at the equilibrium point $\vec{X}_0$ (the fixed parameter in our case) of the harmonic oscillator, $g_i = -\partial\Phi(\vec{X}_0)/\partial x^i$ is ith projection of gravitational acceleration, and $\Gamma_{ij} = \partial^2\Phi(\vec{X}_0)/\partial x^i \partial x^j$ is (i, j)-component of gravity gradient tensor. Let us select the coordinate axes of the harmonic oscillator in such a way as to get the components of the vector of gravitational acceleration in the form

$$g_x = 0, \qquad g_y = 0, \qquad g_z = -|\vec{g}|. \tag{30}$$

In this approximation the leading components of the gravity gradient tensor are $\{\Gamma_{ii}\}$, and 3D Hamiltonian of the harmonic oscillator will be the sum of three commute operators $H = H_x + H_y + H_z$ with

$$\begin{aligned} H_x &= \frac{p_x^2}{2m} + \frac{m}{2}\Omega_x^2 x^2, \\ H_y &= \frac{p_y^2}{2m} + \frac{m}{2}\Omega_y^2 y^2, \\ H_z &= \frac{p_z^2}{2m} + \frac{m}{2}\Omega_z^2 z^2 + mgz + m\Phi_0, \end{aligned} \tag{31}$$

where the angular frequencies are given by the equations

$$\begin{aligned}\Omega_x^2(\Gamma) &= \omega_x^2\left(1+\frac{\Gamma_{xx}}{\omega_x^2}\right),\\ \Omega_y^2(\Gamma) &= \omega_y^2\left(1+\frac{\Gamma_{yy}}{\omega_y^2}\right),\\ \Omega_z^2(\Gamma) &= \omega_z^2\left(1+\frac{\Gamma_{zz}}{\omega_z^2}\right).\end{aligned} \tag{32}$$

Based on the previous results one can obtain

$$\begin{aligned}H_x &= \hbar\Omega_x\left(\tilde{A}_x^+\tilde{A}_x+\frac{1}{2}\right),\\ H_y &= \hbar\Omega_y\left(\tilde{A}_y^+\tilde{A}_y+\frac{1}{2}\right),\\ H_z &= \hbar\Omega_z\left(\tilde{A}_z^+\tilde{A}_z+\frac{1}{2}\right)-\frac{mg^2}{2\Omega_z^2}+m\Phi_0.\end{aligned} \tag{33}$$

The Hamiltonian for the 3D harmonic oscillator in nonhomogeneous gravitational field can be rewritten as the sum of two contributions $H = H_e + H_0$:

$$\begin{aligned}H_e &= \hbar\sum_{i=x,y,z}\Omega_i\tilde{A}_i^+\tilde{A}_i,\\ H_0 &= \frac{\hbar}{2}\sum_{i=x,y,z}\Omega_i-\frac{mg^2}{2\Omega_z^2}+m\Phi_0,\end{aligned} \tag{34}$$

where the contribution H_e is written as the product of creation and annihilation operators, and H_0 does not include operators and describes only the energy shift.

4. APPLICATION TO THE THERMODYNAMICS OF TRAPPED ATOMS

The developed formalism can be applied for the computation of partition function (sum over states) of the trapped quantum gas in nonhomogeneous gravitational field. The grand canonical partition function is given by the equation (Huang, 1987)

$$Z = \mathrm{Tr}\,\exp[-\beta(H_\mathrm{t}-\mu N)], \tag{35}$$

where H_t is the total Hamiltonian of the system, N is the particle number operator, μ is chemical potential, and $\beta = T^{-1}$ is inverse temperature. As the matrix of total Hamiltonian is diagonal, the result of computation of (35) is quite simple.

For noninteracting Bose and Fermi gases we will have

$$Z_{\rm B} = \prod_{n_x,n_y,n_z} \left[1 - z\, e^{-\beta E_{n_x,n_y,n_z}(\Gamma)}\right]^{-1},$$
$$Z_{\rm F} = \prod_{n_x,n_y,n_z} \left[1 + z\, e^{-\beta E_{n_x,n_y,n_z}(\Gamma)}\right], \tag{36}$$

where $z = \exp(\beta\mu')$ is fugacity, and energy $E_{n_x,n_y,n_z}(\Gamma) = \hbar(\Omega_x n_x + \Omega_y n_y + \Omega_z n_z)$ with $n_x, n_y, n_z = 0, 1, 2, \ldots$ is the function of the components of gravity gradient tensor. The chemical potential in the Eq. (36) $\mu' = \mu - E_0$ absorbs the energy shift (34). From the equations for partition functions (36) follow the equations for the grand thermodynamic potentials of trapped Bose and Fermi gases in external gravitational field:

$$G_{\rm B} = \beta^{-1} \sum_{n_x,n_y,n_z} \ln\left[1 - z\, e^{-\beta E_{n_x,n_y,n_z}(\Gamma)}\right],$$
$$G_{\rm F} = -\beta^{-1} \sum_{n_x,n_y,n_z} \ln\left[1 + z\, e^{-\beta E_{n_x,n_y,n_z}(\Gamma)}\right]. \tag{37}$$

The number of particles and the internal energy for trapped Bose and Fermi gases are obtained from (37):

$$N_{\rm B} = \sum_{n_x,n_y,n_z} \left[z^{-1}\, e^{\beta E_{n_x,n_y,n_z}(\Gamma)} - 1\right]^{-1},$$
$$E_{\rm B} = \sum_{n_x,n_y,n_z} \frac{E_{n_x,n_y,n_z}(\Gamma)}{z^{-1}\, e^{\beta E_{n_x,n_y,n_z}(\Gamma)} - 1}, \tag{38}$$

and

$$N_{\rm F} = \sum_{n_x,n_y,n_z} \left[z^{-1}\, e^{\beta E_{n_x,n_y,n_z}(\Gamma)} + 1\right]^{-1},$$
$$E_{\rm F} = \sum_{n_x,n_y,n_z} \frac{E_{n_x,n_y,n_z}(\Gamma)}{z^{-1}\, e^{\beta E_{n_x,n_y,n_z}(\Gamma)} + 1}. \tag{39}$$

Thermodynamical properties of trapped Bosons and Fermions are found as the solutions of the system of the Eqs. (38) and (39). The variants of this formalism in application to noninteracting trapped Fermi gas is given in (Butts and Rokhsar, 1997; Schneider and Wallis, 1998) and the study of thermodynamics of trapped Fermions in external gravitational field is given in (Kulikov, in press).

5. FINAL REMARKS

This paper presents the formalism of quantization of the harmonic oscillator in terms of creation and annihilation operators. The aim of the paper is to extend this formalism on the interaction of oscillator with external fields. We considered the influence of homogeneous and nonhomogeneous electric and gravitational fields on the properties of harmonic oscillator. Another aim of the paper is to apply this technique for the study of thermodynamics of Bosonic and Fermionic ensembles in gravitational and harmonic trapping potentials. Using the developed formalism we constructed the partition functions and the equations for grand thermodynamic potentials of noninteracting Bosons and Fermions and obtained the equations for the number of particles and the internal energy of trapped Bosons and Fermions. It is easy to see that the Eqs. (38) and (39) are written as the systems of two equations $N = N(z, T, \Gamma)$ and $E = E(z, T, \Gamma)$. The solutions of these equations allow us to obtain interesting properties of trapped quantum gases at ultralow temperatures in external gravitational field including microgravity applications. The elimination of the parameter z from the system of equations $N = N(z, T, \Gamma)$ and $E = E(z, T, \Gamma)$ can give the dependence of the internal energy on the density of particles, temperature, and components of gravity gradient: $E = E(N/V, T, \Gamma)$. As a consequence, it allows us to obtain the equation for the specific heat of trapped Bosons. The first equation in (38) leads to the dependence of critical temperature of condensation on the gravitational contributions. As follows from (39), the equations for chemical potential, the Fermi energy and the specific heat will also depend on the diagonal components of gravity gradient tensor. These results could yield substantial and new information about thermal properties of trapped quantum ensembles in external gravitational field.

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