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Coherent presentation of density operator of the harmonic oscillator in thermostat

R.M. Avakyan [a], A.G. Hayrapetyan [b,*], B.V. Khachatryan [a], R.G. Petrosyan [a]

[a] *Department of Physics, Yerevan State University, 0025 Yerevan, Armenia*
[b] *Institute of Applied Problems of Physics, National Academy of Sciences of Republic of Armenia, 0014 Yerevan, Armenia*

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Abstract

Based on basis of the coherent states the density matrix of harmonic oscillator in thermostat is obtained. This method is mathematically refined and physically transparent for the interpretation of quantum phenomena in classical language. Such an approach gives an opportunity to easily find the density matrix in the multi-dimensional case.

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It is well known that the full description of quantum systems for pure and especially for mixed ensembles is given by means of the density matrix. Naturally the problem of finding the density matrix arises. For a large number of simple model systems the given problem has a simple solution but these systems are hardly of great interest. In case of real systems lots of mathematical difficulties appear in finding density matrix. The coherent states method, which was enthusiastically developed in Glauber's papers [1] and also by Malkin and Manko [2], is extremely fruitfully for these purposes. Integrals in this method are ordinary which makes calculations essentially easier. Furthermore they give us an opportunity to demonstrate the connection between classical and quantum theories.

In present Letter one-dimensional linear oscillator in thermostat is considered. This problem was solved for the first time in [3] in the context of Schrödinger's quantum mechanics where the mathematical apparatus is very cumbersome. The same problem is adduced also in the book [4]. Let us calculate density matrix of oscillator in coordinate and momentum representation based on the coherent states method.

Hamiltonian of the linear harmonic oscillator has the following form

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

where m is the mass, ω is the cyclic frequency, $\hat{p}$ and $\hat{x}$ are Hermitian operators of the momentum and coordinate respectively. Last two operators satisfy the following commutation relation

$$[\hat{x}, \hat{p}] = i\hbar. \tag{2}$$

* Corresponding author.
E-mail address: armen@iapp.sci.am (A.G. Hayrapetyan).

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We introduce the annihilation and creation operators $\hat{a}$ and $\hat{a}^\dagger$ respectively, which are defined by the relations

$$\hat{a} = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} + i\hat{p}), \tag{3}$$

$$\hat{a}^\dagger = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega\hat{x} - i\hat{p}). \tag{4}$$

Formulae (1) and (2) can be transformed in the following form

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right),$$

$$\left[\hat{a}, \hat{a}^\dagger\right] = 1. \tag{5}$$

Coherent states are described by eigenfunctions of non-Hermitian operator $\hat{a}$ and are defined by the following equation

$$\hat{a}|z\rangle = z|z\rangle, \tag{6}$$

where z is the corresponding eigenvalue of $\hat{a}$ and

$$|z\rangle = e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle \tag{7}$$

is the eigenfunction. The vectors $|n\rangle$ are the eigenfunctions of the operator of the number of quanta:

$$\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle, \quad n = 0, 1, 2, \ldots. \tag{8}$$

Let us now calculate the density matrix taking into account that in quantum mechanics the state of a system in a thermostat is described by the following statistical operator

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Z(\beta)}, \tag{9}$$

where $\hat{H}$ is the Hamiltonian of the system,

$$\beta = \frac{1}{kT}, \tag{10}$$

and

$$Z(\beta) = \mathrm{Tr}\, e^{-\beta\hat{H}} \tag{11}$$

is the so called statistical sum. It has the following form for the linear harmonic oscillator:

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})} = \frac{e^{-\frac{1}{2}\beta\hbar\omega}}{1 - e^{-\beta\hbar\omega}}.$$

A matrix element of density operator in coordinate presentation

$$\langle x|\hat{\rho}|x'\rangle \tag{12}$$

can be presented in terms of the coherent states as

$$\langle x|\hat{\rho}|x'\rangle = \frac{1}{\pi^2}\iint \langle x|z\rangle\langle z|\hat{\rho}|z'\rangle\langle z'|x'\rangle\,\mathrm{d}^2z\,\mathrm{d}^2z'. \tag{13}$$

This relation directly follows from the completeness of the coherent states and the expansion

$$\hat{1} = \frac{1}{\pi}\int |z\rangle\langle z|\,\mathrm{d}^2z$$

of the unit operator is used; $\mathrm{d}^2z = \mathrm{d}\,\mathrm{Re}\,z \cdot \mathrm{d}\,\mathrm{Im}\,z$ and $z = \frac{1}{\sqrt{2m\hbar\omega}}(m\omega x + ip)$.

For the calculation of the integral (13) we need to evaluate $\langle x|z\rangle$ and $\langle z|\hat{\rho}|z'\rangle$. By using relation (7) for $\langle x|z\rangle$ one has

$$\langle x|z\rangle = \langle x|e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}|n\rangle = e^{-\frac{1}{2}|z|^2}\sum_{n=0}^{\infty}\frac{z^n}{\sqrt{n!}}\langle x|n\rangle. \tag{14}$$