THE TEMPERATURE DEPENDENCE OF QUANTUM DISTRIBUTION FUNCTIONS

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In the present article we consider a method for obtaining the quantum distribution function in phase space given a specific choice of operator for a function of the coordinates and momenta. The temperature equation is written for this function. We obtain the operator expression for the temperature quantum distribution function in phase space.

As we know, it is possible in quantum theory to introduce a function of the coordinates and momenta \( f(r, p) \) in order to calculate the mean values by analogy with classical mechanics [1, 2]:

\[
\langle A \rangle = \int A(r, p) f(r, p) \, dr \cdot dp.
\]  

(1)

Just as in classical statistical mechanics, the function \( f(r, p) \) is called the distribution function in phase space. However, this function cannot be interpreted as a probability density because it cannot take negative values. By integrating with respect to the momenta or the coordinates it is possible to obtain from \( f(r, p) \) distribution functions for the coordinates or the momenta which are probability densities.

A certain ambiguity arises in defining the form of \( f(r, p) \) from quantum theory. This ambiguity is connected with the fact that there is in quantum theory itself no definition of an unambiguous correspondence between a physical quantity which is a function of the coordinates and momenta and an operator for calculating its mean value. A similar ambiguity in the choice of \( f(r, p) \) cannot be an argument against using that function, since this ambiguity is inherent not in the method of calculating the mean values (1), but in quantum theory itself, and appears in any formulation of it. In cases which are important in practice this ambiguity does not play a role. Thus it is convenient to choose for \( f(r, p) \) the simplest expression.

1. THE EXPRESSION FOR THE QUANTUM DISTRIBUTION FUNCTION

Let there be a physical quantity \( A \) which is a function of the coordinates and momenta of the system \( A = A(r, p) \). We decompose this function into a series or integral in terms of two complete systems of functions \( \{q_n(r)\}, \{\xi_m(p)\} \), one of which depends on the coordinates and the other on the momenta:

\[
A(r, p) = \sum_{n,m} a_{nm} \cdot q_n(r) \cdot \xi_m(p).
\]  

(2)

With the expression we associate the operator \( \hat{A} \) in the following way:

\[
\hat{A} = \sum_{n,m} \frac{1}{2} [a_{nm} \cdot \hat{q}_n(r) \cdot \hat{\xi}_m(p) + a_{nm}^* \cdot \hat{\xi}_m(p) \cdot \hat{q}_n(r)].
\]  

(3)

On the functions \( q_n(r) \), \( \xi_m(p) \) we impose the one restriction: the spectral decomposition must hold for the operators \( f_{q_n}(\hat{r}) \), \( f_{\xi_m}(\hat{p}) \). This is fulfilled for real \( q_n(r) \), \( \xi_m(p) \) and for \( \varphi_n(r) \) and \( \zeta_m(p) \) chosen in the form \( \varphi_n = e^{i\alpha_n r} \), \( \zeta_m = e^{i\beta_m p} \). Allowing for what has been said,

\[
q_n(r) = \int \varphi_n(r) \hat{r} \, dr; \quad \xi_m(p) = \int \zeta_m(p) \hat{p} \, dp.
\]  

(4)

Here \( \hat{r} \) and \( \hat{p} \) are the operators of projection onto states with a definite coordinate and momentum, respectively.

We now take a system of state of which is characterized by the statistical operator \( \hat{\rho} \). The mean value of the physical quantity \( A \) with the operator \( \hat{A} \) in the state \( \beta \) is equal to:

\[
\langle A \rangle = \text{spur} \hat{A} \cdot \hat{\rho}.
\]

(5)

We substitute (3) in (5) and taking (4) into account we then obtain

\[
\langle A \rangle = \text{spur} \int \frac{1}{2} [a_{nm} \cdot \varphi_n(r) \cdot \zeta_m(p) \hat{r} \cdot \hat{p} + \hat{r} \cdot \hat{p} \cdot \varphi_n(r) \cdot \zeta_m(p)] \, dr \cdot dp.
\]  

(6)

Allowing for the fact that

\[
\text{spur} \hat{r} \cdot \hat{p} = \text{spur} \hat{p} \cdot \hat{r}
\]

and for the fact that \( A(r, p) \) is real by its meaning, we find

\[
\langle A \rangle = \int A(r, p) \cdot \text{Re} \text{spur} \hat{r} \cdot \hat{p} \cdot \rho \, dr \cdot dp.
\]  

(7)

Comparing (6) with (1), we obtain the expression for \( f(r, p) \):

\[
f(r, p) = \text{Re} \text{spur} \hat{r} \cdot \hat{p} \cdot \rho = \text{Re} \text{spur} P_{r} \cdot P_{p} \cdot \rho = \text{Re} \text{spur} P_{r} \cdot P_{p} \cdot \rho.
\]  

(8)

In quantum theory there is a distribution function for the commuting variables \( \alpha \) and \( \beta \) which is a probability density. This function can be written as follows [3]:

\[
f(\alpha, \beta) = \text{spur} \hat{r} \cdot \hat{p} \cdot \rho.
\]  

(9)

Expression (10) was first proposed in [4-5]; however, it was not clear to what theory of noncom-
muting variables it corresponded. It should be noted that for expression (10) some equations are obtained in a somewhat simpler form than for the corresponding expression proposed by Wigner [1].

2. THE EQUATIONS FOR THE QUANTUM DISTRIBUTION FUNCTION

The kinetic equation for the function \( f(r, p) \) can be obtained by differentiating expression (9) with respect to the time and taking into account the equation for the statistical operator [3]. For a system of \( N \) nonidentical particles this equation looks like the following:

\[
\frac{\partial}{\partial t} f(r, p, t) + \sum_{j=1}^{N} \left( \frac{p_j}{m_j} \right) f(r, p, t) - \sum_{j=1}^{N} \left( \frac{\hbar}{m_j} \right) f(r, p, t) = 0
\]

\[
= \frac{1}{\hbar} \left\{ U(r) \cdot f(r, p, t) - \left( \frac{1}{2\pi} \right)^N \cdot \int f(r, p + z, t) \times \right.
\]

\[
\left. \sum_{j=1}^{N} \phi_j \cdot \frac{\hbar}{m_j} \cdot \left[ U(r + \hbar z) \cdot d^{N}y \cdot d^{N}z \right] \right\}.
\]

It is not simpler than the corresponding equation for the function obtained by Wigner [1]. However in the present article we shall be interested in the temperature equation for \( f(r, p) \).

Let there be a system of \( N \) nonidentical particles located in a state of thermodynamical equilibrium at a temperature \( T \). Assuming that \( \beta' \) is zero and taking into account the boundary, its normalized statistical operator has as we know the following form [3]:

\[
\hat{\rho} = e^{-\beta \hat{H}}; \hat{H} = U(r) + \sum_{j=1}^{N} \frac{p_j^2}{2m_j}; \beta = \frac{kT}{\hbar}.
\]

Allowing for this and expression (10), we obtain the temperature function in the following form:

\[
f(r, p; \beta) = \langle p | r \cdot e^{-\beta \hat{H}} \cdot \langle r | p \rangle,
\]

\[
= \left( \frac{1}{2\pi\hbar} \right)^N \cdot e^{\frac{\hbar}{2\beta}} \cdot \left[ \sum_{j=1}^{N} p_j \right] \cdot \left[ \begin{array}{c}
U(r) + \frac{1}{2m_j} \cdot \left( \frac{\hbar}{p_j} \cdot \phi_j \right) \end{array} \right].
\]

In order to obtain the equation we shall differentiate (13) with respect to \( \beta \):

\[
\frac{\partial f(r, p; \beta)}{\partial \beta} = -\langle p | r \cdot \hat{H} \cdot e^{-\beta \hat{H}} \cdot \langle r | p \rangle.
\]

We have from (13)

\[
e^{-\beta \hat{H}} \cdot \langle r | p \rangle = (2\pi\hbar)^N \cdot \langle r | p \rangle \cdot f(r, p, \beta).
\]

Substituting (15) in (14) and operating on (15) with the operator \( \hat{H} \), we obtain the equation for \( f(r, p, \beta) \) in the following form:

\[
\frac{\partial f(r, p, \beta)}{\partial \beta} = - \left[ U(r) + \frac{1}{2m_j} \cdot \left( \frac{\hbar}{p_j} \cdot \phi_j \right) \right] f(r, p, \beta).
\]

Equation (16) can be written in the more compact form

\[
\frac{\partial f(r, p, \beta)}{\partial \beta} = - \hat{H} \cdot f(r, p, \beta), \quad \hat{H} = U(r) + \sum_{j=1}^{N} \frac{p_j^2}{2m_j},
\]

where \( p_j = -i\hbar \phi_j \) is the momentum operator for the \( j \)-th particle.

Thus the temperature equation for the quantum distribution function can be obtained from the classical one on replacing \( p_j \) by \( p_j + \hat{\phi}_j \). Equation (17) by its simplicity has the advantage over the corresponding equation for the Wigner distribution function obtained in [6].

3. THE OPERATOR EXPRESSION FOR THE TEMPERATURE QUANTUM DISTRIBUTION FUNCTION

We now introduce the evolution operator from the temperature \( \beta' \) to \( \beta \):

\[
f(r, p, \beta) = \hat{U}(\beta, \beta') \cdot f(r, p, \beta').
\]

This operator corresponds to the boundary value condition \( U(\beta, \beta') = 1 \). Substituting (18) into (17), we obtain the equation for \( U(\beta, \beta') \):

\[
\frac{\partial U(\beta, \beta')}{\partial \beta} = - \hat{H} \cdot \hat{U}(\beta, \beta').
\]

Formally integrating this equation or, which is the same thing, solving it by the method of successive approximations, we obtain

\[
\hat{U}(\beta, \beta') = \exp \left[ -\beta \hat{H} \right].
\]

Consequently,

\[
f(r, p, \beta) = \exp \left[ -\beta \hat{H} \right] \cdot f(r, p, \beta').
\]

Assuming that \( \beta' \) is zero and taking into account the boundary value condition for \( f(r, p, \beta) \)

\[
f(r, p, \beta) = \left( \frac{1}{2\pi\hbar} \right)^N \cdot e^{-\beta \hat{H}},
\]

we obtain

\[
f(r, p, \beta) = \left( \frac{1}{2\pi\hbar} \right)^N \cdot e^{-\beta \hat{H}}, \quad 1 =
\]

\[
= \left( \frac{1}{2\pi\hbar} \right)^N \cdot \exp \left[ -\beta \hat{H} \right] \cdot \left[ U(r) + \sum_{j=1}^{N} \frac{p_j^2}{2m_j} \right].
\]

It can be seen from formula (23) that the quantum temperature distribution function is obtained from the classical one by replacing \( p_j \) by the operator quantity \( p_j + \hat{\phi}_j \). The transition to the classical limit is obtained in a natural way from (23) by neglecting the noncommutative nature of the momentum and coordinate operators. Applying the rules for handling functions of noncommuting operators [7], we can obtain from (23) decompositions in terms of powers of \( \hbar \) or powers of the interaction.

4. THE QUANTUM CORRECTIONS TO THE CLASSICAL EXPRESSION FOR \( f \)

We shall seek \( f(r, p, \beta) \) in the form of the following decomposition in terms of powers of \( \hbar \):