THE PROBLEM OF THE QUANTUM PARTICLE MOVEMENT IN BOUNDED SPACE IN COORDINATE AND WIGNER REPRESENTATION

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The exact expressions for the density matrix and Wigner function for the one-dimensional free particle movement in the bounded region $0 \le x \le a$ are obtained including the consideration of it's limits, $a \to \infty$.

The exact expression for the density matrix and Wigner functions of quantum systems are known only in special cases and, practically, all of them and their references are described in [1-3]. Corresponding Hamiltonians are quadratic forms of the coordinates and momenta. In this paper we consider the problem of one-dimensional free particle movement in the bounded region $0 \le x \le a$ (including the case $a \to \infty$).

For this problem the solutions of Schrödinger equation are well known

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n}{a} x\right), \quad E_n = \frac{\pi^2 n^2 \hbar^2}{2ma^2}, n = 1,2,3... \tag{1}$$

Then the equilibrium density matrix can be calculated by the formula

$$\rho(x, x', \beta) = \sum \psi_n(x) \psi_n^*(x') e^{\beta E_n} \tag{2}$$

Introducing the expression (1) to (2) and making some transformations we obtain two series, each of which is, practically, the definition of teta-function [4].

$$\theta_3(z|\tau) = 1 + 2\sum_{n=1}^{\infty} \cos(2\pi n z) e^{i\pi\tau n^2} \tag{3}$$

As result we have the following expression:

$$\rho(x, x'\beta) = \frac{1}{2a}\left[\theta_3\left(\frac{x - x'}{2a}\middle|\frac{in\hbar^2\beta}{2ma^2}\right) - \theta_3\left(\frac{x + x'}{2a}\middle|\frac{in\hbar^2\beta}{2ma^2}\right)\right] \tag{4}$$

The substitution $\beta = it/\hbar$ reduces the expression (4) to the propagator of Schrodinger equation for the particle in a box obtained earlier by various methods in [3, 5, 6].

Evidently in the limit $\beta/a^2 \to \infty$ (i.e. low temperature and the small size of the box) the density matrix can be approximated rather well only by the first order term of the expansion series (2). the question is in obtaining from the exact (but not very obvious) formula (4) the asymptotics of the density matrix in quasi-classical limit $\beta/a^2 \to 0$ (high temperature and the wide box). The qualitative behavior of the probability density $\rho(x, x, \beta)$ in this case is clear from physical considerations. It must be almost constant at all points inside the box except the very small region where the density matrix must be close to zero. However, it is interesting to obtain this result from the formula (4). More over we would like to know the character of the deflection uniform distribution inside the box caused by quantum corrections. This problem can be solved using the equality [4] for teta-function

$$\theta_3(z|\tau) = \sqrt{\frac{i}{\tau}} e^{\frac{-\pi i z^2}{\tau}} \theta_3\left(-\frac{z}{\tau}\middle| -\frac{1}{\tau}\right) \tag{5}$$

Due to the fact, that in our case the parameter τ is pure complex one and restricting the expansion series (3) by the first term of the function $\theta_3\left(-\frac{z}{\tau}\middle| -\frac{1}{\tau}\right)$, when $\tau \to 0$, we obtain the following formula, describing the quasi-classical behavior of the density matrix

$$\rho(x, x', \beta) = \sqrt{\frac{m}{2\pi\beta\hbar^2}} \left\{ \exp\left[\frac{-m(x-x')^2}{2\beta\hbar^2}\right]\left(1 + 2e^{-\frac{2ma^2}{\beta\hbar^2}} ch\left[\frac{2ma(x-x')^2}{\beta\hbar^2}\right]\right) - \right.$$
$$\left. - \exp\left[\frac{-m(x+x')^2}{2\beta\hbar^2}\right]\left(1 + 2e^{-\frac{2ma^2}{\beta\hbar^2}} ch\left[\frac{2ma(x+x')^2}{\beta\hbar^2}\right]\right)\right\} \quad (6)$$

This formula is correct in the region $|x \pm x'| \leq a$ (i.e. at the left half-space of the box). For the points outside of this region one have to use the properties following from (3) and (4)

$$\rho(x,x') = \rho(x',x), \rho(a-x, a-x') = \rho(x,x') \quad (7)$$

For the diagonal elements of probability density we have the following expression:

$$\rho(x,x,\beta) = \sqrt{\frac{m}{2\pi\beta\hbar}}\left\{1 - e^{\frac{-2mx^2}{\beta\hbar^2}} + 2e^{-\frac{2ma^2}{\beta\hbar^2}}\left[1 - e^{\frac{-2mx^2}{\beta\hbar^2}} ch\left(\frac{4\max}{\beta\hbar^2}\right)\right]\right\}, \quad (8)$$

$$x \leq a/2, ma^2/\beta\hbar^2 >> 1$$

The first two terms in figure brackets describe the probability density of particle position in the infinite right half-space from the wall ($x=0$.) The other terms give corrections caused by the presence of the second wall.

Note, that these correction don't oscillate as it can be seen from formulas(3) and (4). In the center of the density is equal to

$$\rho\left(\frac{a}{2}, \frac{a}{2}, \beta\right) = const\left(1 - 2e^{\frac{-ma^2}{2\beta\hbar^2}}\right),$$

and the half-space case on the same distance from the coordinate center we have an analogous formula but without the multiplier of the exponent expansion inside the brackets The exact expression of statistical sum has the form

$$z(\beta) = \frac{1}{2}\left[\theta_3\left(0\left|\frac{i\pi\hbar^2\beta}{2ma^2}\right.\right) - 1\right] \quad (9)$$

It's quasi-classical expression is as follows:

$$z(\beta) = a\sqrt{\frac{m}{2\pi\beta\hbar^2}}\left(1 + 2e^{\frac{-2ma^2}{\beta\hbar^2}}\right) - 1/2; ma^2/\beta\hbar^2 >> 1 \quad (10)$$

From (4) one can obtain Wigner function by the following formula:

$$W(p,q,\beta) = \int \rho\left(q + \xi/2, q - \xi/2\right) e^{\frac{-ip\xi}{\hbar}} d\xi \quad (11)$$

Taking into consideration that the integration region is bounded by the interval under the condition $0 \leq q \leq a/2$ we have [7]

$$W(p,q,\beta) = \frac{2}{a}\int_0^q \cos\left(\frac{2py}{\hbar}\right)\theta_3\left(\frac{y}{a}\left|\frac{i\pi\hbar^2\beta}{2ma^2}\right.\right)dy - \frac{\hbar}{ap}\sin\left(\frac{2pq}{\hbar}\right)\theta_3\left(\frac{q}{a}\left|\frac{i\pi\hbar^2\beta}{2ma^2}\right.\right) \quad (12)$$

but when $a/2 \leq q \leq a$ one has to use the equality $W(p,q,\beta) = W(p, a, -q, \beta)$.

The Wigner function for free particle in a half-space was originally exactly expressed by the error - function in [8].

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KOORDİNAT VƏ VİQNER TƏSVİRLƏRİNDƏ KVANT ZƏRRƏCİYİNİN MƏHDUD FƏZADA HƏRƏKƏTİ PROBLEMİ

Sərbəst Kvant zərrəciyinin birölçülü məhdud $0 \le x \le a$ oblastında hərəkət üçün sıxlıq matrisasının və Viqner funksiyasının aşkar ifadələri alınmışdır. Eləcə də onların $a \to \infty$ halında kvaziklassik düsturları tapılmışdır.

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ЗАДАЧА ДВИЖЕНИЯ КВАНТОВОЙ ЧАСТИЦЫ В ОГРАНИЧЕННОМ ПРОСТРАНСТВЕ В КООРДИНАТНОМ И ВИГНЕРОВСКОМ ПРЕДСТАВЛЕНИИ

Получены явные выражения для матрицы плотности и функции Вигнера для квантовой частицы, движущейся в ограниченной области $0 \le x \le a$, в одномерном случае. Также получены квазиклассические формулы для случая $a \to \infty$.

Дата поступления: 09.09.98 *Редактор: И.Г. Джафаров*