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EXACT AND QUASI-CLASSICAL DENSITY MATRIX AND WIGNER FUNCTIONS FOR A PARTICLE IN THE BOX AND HALF SPACE.

E. A. AKHUNDOVA

Institute of Physics Academy of Science of
Azerbaijan, Baku, 370143, Prospect Azizbekova, 33

V. V. DODONOV

P. N. Lebedev Physical Institute, Moscow, 117924, Leninsky
Prospect 53, USSR

V. I. MAN'KO

P. N. Lebedev Physical Institute, Moscow, 117924,
Leninsky Prospect 53, USSR.

The exact expressions for 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]. Correspondending Hamiltonians are quadratic forms of Euclidean coordinates and momenta. In this paper we consider the problem of one-dimensional free particle movement in the bounded region $0 < x < a$ (including the case $a = \infty$). For this problem the solutions of Schrödinger equation are well known:

$$\psi_n = (2/a)^{1/2} \sin(\pi n x / a), \quad E_n = (\pi n \hbar)^2 / (2ma^2), \quad n = 1, 2, 3, \ldots \quad (1)$$

Then the equilibrium density matrix can be calculated by formula

$$\rho(x, x', \beta) = \sum \psi_n(x) \psi^*(x') \exp(-\beta E_n) \quad (2)$$

Indroducing the expression (1) to (2) and mading some simple transformations we obtain two series, each of which

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is, practicallly the definition of teta-function [4]

$$\Theta_3(z|\tau)=1+2\sum_{n=1}^{\infty}\cos(2\pi nz)\exp(i\pi\tau n^2) \qquad (3)$$

As result we have the expression

$$\rho(x,x',\beta)=\frac{1}{2}\left[\Theta_3\left(\frac{x-x'}{2a}\Big|\frac{i\pi\hbar^2\beta}{2ma^2}\right)-\Theta_3\left(\frac{x+x'}{2a}\Big|\frac{i\pi\hbar^2\beta}{2ma^2}\right)\right] \qquad (4)$$

The replacement $\beta=it/\hbar$ transforms the expression (4) into the propogator of Schrödinger equation for the particle in a box obtained earlier by various methods in [3,5,7].

Evidently in the limit $\beta/a^2 \to \infty$ (i.e. low temperature and small size of a box) the density matrix can be good approximated 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 β/a^2 (high temperature and wide box).

The qualitive behaviour of the probability density $\rho(x,x,\beta)$ in this case is clear from physical consideration. It must be almoust constant at all points inside the box except very small region near the wall corresponding to de Brogle wave length. In this region the density matrix must leads 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 deflexion uniform distribution inside the box caused by quantum corrections. This problem can be solved using the equality [4] for teta-function

$$\Theta_3(z|\tau)\equiv (i/\tau)^{1/2}\exp(-\pi iz^2/\tau)\Theta_3(-z/\tau|-1/\tau) \qquad (5)$$

Due to the fact that in our case the parameter τ is pure

complex and restricting by the first term of expansion series (3) of the function $\Theta_3(-z/\tau|-1/\tau)$ when $\tau \to 0$ we obtain the following formula describing the quasi-classical behaviour of the density matrix

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

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

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

For the diagonal elements of probability density we have following expression

$$\rho(x,x',\beta)=(m/2\pi\beta\hbar^2)^{1/2}\left\{1-\exp[-2mx^2/\beta\hbar^2]+2\exp[-ma^2/\beta\hbar^2][1-\right.$$
$$\left.-\exp[-2mx^2/\beta\hbar^2]\operatorname{ch}[4mx/\beta\hbar^2])\right\}, \quad x\leq a/2, \quad ma^2/\beta\hbar^2 \gg 1 \tag{8}$$

The first two terms in figure brackets describe the probability density of particle position in the infinite half space right from the wall placed to the point $x=0$. The other terms give corrections caused by the-presence of the second wall. Note, that this corrections don't oscillate as it can be seemed from formulas (3) and (4).

In the centre of the box the density matrix is equal to

$$\rho(a/2,a/2,\beta)=\text{const} \langle 1-2\exp(-ma^2/2\beta\hbar^2)$$

and the half space case on the same distance from the coordinate centre we have an analogous expression but without two in front of exponent. The exact expression of

statistical sum have the form

$$Z(\beta)= \frac{1}{2}\left[\Theta_3\left(0\left|\frac{i\pi\hbar\,\beta^2}{2ma^2}\right.\right)-1\right] \tag{9}$$

It's quasi-classical expansion is

$$Z(\beta)=a(m/2\pi\beta\hbar^2)^{1/2}(1+2\exp\ [-2ma^2/\beta\hbar^2])-1/2,\ \ ma^2/\beta\hbar^2>>1 \tag{10}$$

From (4) one can obtained the Wigner function

$$W(p,q,\beta)=\int\rho(q+\xi/2,q-\xi/2,\beta)\ \exp(-ip\xi/\hbar)\ d\xi \tag{11}$$

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

$$W(p,q,\beta)= \frac{2}{a}\int_0^q \cos\ (2py/\hbar)\ \Theta_3\left(\frac{y}{a}\left|\frac{i\pi\hbar\,\beta^2}{2ma^2}\right.\right)dy-$$

$$-(\hbar/ap)\sin(2pq/\hbar)\Theta_3\left(\frac{q}{a}\left|\frac{i\pi\hbar\,\beta^2}{2ma^2}\right.\right) \tag{12}$$

but when $a/2 \le q \le a$ one have to use the equality

$$W(p,q,\beta) = W(p,a-q,\beta)$$

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

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