THE QUANTUMMECHANICAL CORRECTION OF THE QUASICLASSICAL DENSITY OF STATES OF A PARTICLE IN A GAUSSIAN RANDOM POTENTIAL

ŠTEFAN BARTA*, RUDOLF DURNÝ*, PETER NAGY**, Bratislava

The expansion of the partition function and of the density of states in a power series of the Planck constant are found. The proposed method gives the corrections for an arbitrary autocorrelation function. Numerical results are also presented.

КВАНТОВОМЕХАНИЧЕСКИЕ ПОПРАВКИ К КВАЗИКЛАССИЧЕСКОЙ ПЛОТНОСТИ СОСТОЯНИЙ ЧАСТИЦЫ В СЛУЧАЙНОМ ГАУССОВСКОМ ПОТЕНЦИАЛЕ

В работе найдены разложения функции распределения и функции плотности состояний в степенные ряды по постоянной Планка. Предлагаемый метод даёт поправки для произвольной функции автокорреляции. Приведены также численные результаты.

I. INTRODUCTION

Many physical problems of noncrystalline solids are solvable in the one electron approximation. The appropriate use of the Hamiltonian enables us to compute the statistical sum and the density of states (d.s.), which latter represents an important quantity, because it defines all thermodynamical properties of the system and is further closely related to the optical and transport properties. The density of states of a particle in the random potential is known only in some special cases. In the deep tails d.s. can be computed by the "minimum counting method" [1]. The quasiclassical approximation [2], [3] can be utilized for positive and small negative energies. In this paper our aim is to use the method of Yaglom [4] in order to calculate the quantum mechanical corrections of the quasiclassical d.s. and to find out the region of validity of these corrections.

* Department of Physics, Slovak Technical University, Gottwaldovo nám. 19, CS-880 19 BRATISLAVA.

** Institute of Physics, Slovak Acad. Sci., Dúbravská cesta, CS-899 30 BRATISLAVA.

II. MODEL

An electron with the effective mass m in a random potential $U(\boldsymbol{r})$ will be described by the Hamiltonian

$$H=\frac{\boldsymbol{p}^2}{2m}+U(\boldsymbol{r}).$$

Providing the potential $U(\boldsymbol{r})$ is Gaussian, then it is statistically determined by the first two correlation functions

$$\langle U(\boldsymbol{r})\rangle_u=0;\quad \langle U(\boldsymbol{r}_1)U(\boldsymbol{r}_2)\rangle_u=\eta^2 W\left(\left(\frac{\boldsymbol{r}_1-\boldsymbol{r}_2}{L}\right)^2\right). \tag{1}$$

The relations (1) express explicitly the fact that the potential $U(\boldsymbol{r})$ is macroscopically homogeneous and isotropic. The parameter η^2 is the mean square potential fluctuation and L is the correlation length. The function W is defined so that $W(O)=1$. The symbol $\langle\ \rangle_u$ means the configurational average over all possible values of the potential $U(\boldsymbol{r})$.

It can be shown that the dimensionless parameter defined by

$$\hbar^{*2}=\frac{\hbar^2}{mL^2\eta} \tag{2}$$

does not depend on the choice of units for L, m, η, therefore in the next calculations we use the convention

$$L=m=\eta=1.$$

$\hbar^*$ is the only parameter which determines the shape of d.s.

III. THE FUNCTIONAL AVERAGE

In this section our purpose is to expand the statistical sum in the power series of the parameter $\hbar^*$ (2). Doing that we use the path-integral representation of the statistical sum [5].

$$\langle Z(\beta)\rangle_u= \tag{3}$$

$$=\int_{r_a}^{r_a}\mathscr{D}\boldsymbol{r}(u)\exp\left\{-\frac{1}{2\hbar^*}\int_0^{\hbar^*\beta}\dot{\boldsymbol{r}}^2(u)\,du+\frac{1}{2\hbar^{*2}}\int_0^{\hbar^*\beta}\int_0^{\hbar^*\beta}W((\boldsymbol{r}(u)-\boldsymbol{r}(u'))^2)\,du\,du'\right\}.$$

Here the Gaussian behaviour of the potential $U(\boldsymbol{r})$ has been utilized. The last path-integral can be expressed using the Wiener measure. Similarly as in paper [4] we obtain the statistical sum in the following form

$$\langle Z(\beta)\rangle_u=(2\pi\hbar^2\beta)^{-3/2}\left\langle\exp\left\{\frac{1}{2}\beta^2\int_0^1\int_0^1 W(\hbar^*\beta(\boldsymbol{\varrho}(u)-\boldsymbol{\varrho}(u'))^2)\,du\,du'\right\}\right\rangle_{\varrho}. \tag{4}$$

The symbol $\langle\ \rangle_{\varrho}$ means the average over the multigaussian random vector function $\boldsymbol{\varrho}(u)$. The different vector components are statistically independent. The first two correlations are

$$\langle\varrho(u)\rangle_{\varrho}=0 \tag{5}$$

$$\langle\varrho_x(u)\varrho_y(u')\rangle_{\varrho}=\delta_{xy}(\mathrm{Min}(u,u')-uu').$$

Here $\varrho_x(u)$ means the x-th component of the vector $\boldsymbol{\varrho}(u)$.

IV. EXPANSION OF THE STATISTICAL SUM AND d.s. IN TERMS OF THE POWER SERIES OF $\hbar^*$

According to the results of Yaglom [4], we shall express the statistical sum in the form

$$\langle Z(\beta)\rangle_u=(2\pi\hbar^{*2}\beta)^{-3/2}\left\{\sum_{n=0}^{\infty}\hbar^{*n}Z_n(\beta)\right\}. \tag{6}$$

The factor $(2\pi\hbar^{*2}\beta)^{-3/2}$ is the statistical sum of the free electron. Expanding the exponential function in formula (4) we get

$$\langle Z(\beta)\rangle_u=(2\pi\hbar^{*2}\beta)^{-3/2}\exp\left(\frac{1}{2}\beta^2\right)\times \tag{7}$$

$$\times\left\{1+\frac{1}{2}\hbar^{*2}\beta\langle W_1\rangle_{\varrho}+\frac{1}{4}\hbar^{*4}\left(\beta^4\langle W_2\rangle_{\varrho}+\frac{1}{2}\beta^6\langle W_1W_1\rangle_{\varrho}\right)+\right.$$

$$\left.+\frac{1}{12}\hbar^{*6}\left(\beta^5\langle W_3\rangle_{\varrho}+\frac{3}{2}\beta^7\langle W_2W_1\rangle_{\varrho}+\frac{1}{4}\beta^9\langle W_1W_1W_1\rangle_{\varrho}\right)+\ldots\right\}.$$

The quantities W_m are in close connection with the derivatives of the autocorrelation function (1) and they are defined by

$$W_n\equiv\frac{\mathrm{d}^n}{\mathrm{d}x^n}\int_0^1\int_0^1 W(x(\boldsymbol{\varrho}(u)-\boldsymbol{\varrho}(u'))^2)\,du\,du'\Big|_{x=0}. \tag{8}$$

The averaged values of the types

$$\langle W_m\rangle_{\varrho},\quad \langle W_mW_n\rangle_{\varrho},\ldots. \tag{9}$$

define the numerical coefficients of the expansion (7). The method of computing them is shown in the Appendix. We calculate the respective d.s. from the well-known formula

$$g(E)=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\langle Z(\beta)\rangle\, e^{\beta E}\,d\beta.$$

(σ is a positive convergence parameter). For further calculations we shall use the integral [6]

$$\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}(2\pi\hbar^{*2}\beta)^{-3/2}\exp\left(\beta E+\frac{1}{2}\beta^2\right)\beta^n\,d\beta=\frac{1}{4\pi^2\hbar^{*3}}\times$$

$$\times\exp\left(-\frac{E^2}{4}\right)D_{n-3/2}(-E).$$

$D_\nu(z)$ is the function of the parabolic cylinder [7].

The density of states with the quantum mechanical corrections is then

$$g(E)=\frac{1}{4\pi^2\hbar^{*3}}\{g_0(E)+\hbar^{*2}g_1(E)+\hbar^{*4}g_2(E)+\hbar^{*6}g_3(E)+\ldots\} \tag{10}$$

The corrections $g_n(E)$ can be expressed using Eq. (7) in terms of the functions $D_\nu(-E)$. The zero-order approximation

$$\frac{1}{4\pi^2\hbar^{*3}}g_0(E)=\frac{1}{4\pi^2\hbar^{*3}}\exp\left(-\frac{E^2}{4}\right)D_{-3/2}(-E) \tag{11}$$

is known as the quasiclassical approximation.

V. THE NUMERICAL RESULTS

We shall not investigate the convergence of series (10) exactly. We can expect a good convergence of the series (10) in the energy region, where the quasiclassical approximation (11) is acceptable. From the paper [3], [8] it is evident that the quasiclassical approximation is not reasonable for energies

$$E<-(2\hbar^{*2})^{-1/3}\equiv E_c. \tag{12}$$

We divide the whole energy interval into three regions. a) $E<E_c$. The states from this interval are localized in deep potential wells [1]. The finite number of quantummechanical corrections cannot give the proper results. b) $E_c<E<1$. The physical interpretation of these states is not clear. The series (10) converges well. c) $E>1$. Electrons with these energies are extended and only a little scattered by the random potential. The higher order quatum mechanical corrections are negligible.

Table 1

The values of the parameters $\hbar^*$ and E_c

$\hbar^*$ E_c	$L=10$ nm	$L=5$ nm	$L=2$ nm	$L=1$ nm
$\eta=1.0$ eV	0.028 8.6	0.055 5.5	0.138 3.0	0.276 1.9
$\eta=0.5$ eV	0.039 6.9	0.078 4.3	0.195 2.4	0.390 1.5
$\eta=0.1$ eV	0.087 4.0	0.175 2.5	0.436 1.4	0.873 0.9
$\eta=0.05$ eV	0.123 3.2	0.247 2.0	0.617 1.1	1.234 0.7

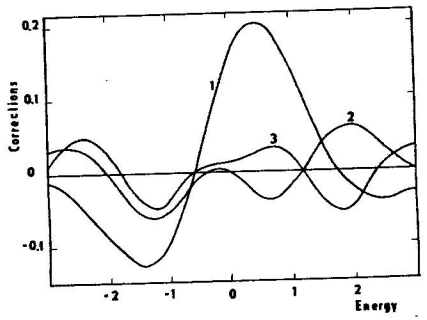

Fig. 1. The functions $g_1(E)$, $g_2(E)$, $g_3(E)$ versus energy in units η. The labelling of curves is equivalent to the order of the correction.

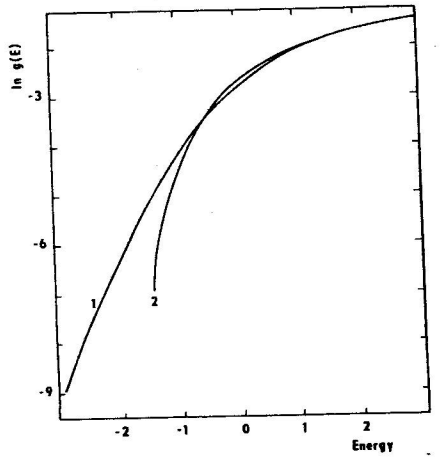

Fig. 2. The d.s. in unit states/ηL^3 versus energy in units for $\hbar^*=0.8$. Line 1 represents the quasiclassical approximation, line 2 represents d.s. with the first three corrections.

We need not discuss the results for different values of η, L, m, because the role of the quantum effects is determined by the parameter $\hbar^*$ (2).

The smaller $\hbar^*$ is, the better series (10) converges. The values of $\hbar^*$ and E_c for different L, and $m=m_e$ are shown in Tab. 1. We have used the formulae (2) and (12).

The first three corrections for the autocorrelation function $\langle U(r_1)U(r_2)\rangle_u=\exp(-(r_1-r_2)^2)$ have been calculated. The functions $g_1(E)$, $g_2(E)$, $g_3(E)$ are plotted in Fig. 1. For $\hbar^*=0.1$, 0.5 the corrections are negligible. Fig. 2 shows the comparison of the quasiclassical approximation with corrected d.s. for $\hbar^*=0.8$. The respective value of the critical energy E_c is $E_c=-0.92$. As it has been anticipated the quantum corrections decrease the d.s. for negative energies and increase them for positive energies, because the quantum effects shift the bound states energy levels to higher energies.

APPENDIX

THE COMPUTING OF AVERAGES OF THE TYPE $\langle W_m \rangle_\varrho$

In this appendix we shall use the simplified notation

$$\varrho_{11'} \equiv \varrho(u_1) - \varrho(u_2) \tag{A1}$$

$$w_{12} \equiv \langle (\varrho_x(u_1) - \varrho_x(u_1'))(\varrho_x(u_2) - \varrho_x(u_2')) \rangle .$$

The functions $\varrho(u)$ are statistically defined in Eq. (5). To compute the coefficients (9) we have to know the averages

$$\langle (-\varrho_{11'}^2)^n \rangle_\varrho , \quad \langle (-\varrho_{11'}^2)^m (-\varrho_{22'}^2)^n \rangle_\varrho , \ldots \tag{A2}$$

We define the generating function S_N of N variables

$$S_N(x_1 \ldots x_N) \equiv \left\langle \exp \left\{ -\sum_{i=1}^{N} x_i \varrho_{11'}^2 \right\} \right\rangle_\varrho . \tag{A3}$$

The averages (A2) can be expressed by means of derivates of the generating function, for example

$$\langle (-\varrho_{11'}^2)^n \rangle_\varrho = \frac{\partial^n S_1(x_1)}{\partial x_1^n} \bigg|_{x_1 = 0} \tag{A4}$$

and so on.

Since the random function ϱ is Gaussian, we find:

$$S_N(x_1 \ldots x_N) = D_N^{-3/2}(x_1 \ldots x_N), \tag{A5}$$

where $D_N(x_1 \ldots x_N)$ is a determinant of a matrix $\mathcal{A}$ of the order $N \times N$ with the matrix elements

$$A_{kl} = \delta_{kl} + 2\sqrt{x_k x_l}\, w_{kl} .$$

Using the formulae (8), (A1), (A4), (A5) we get the coefficients

$$\langle W_1 \rangle_\varrho = \int_0^1 \int_0^1 \langle -\varrho_{11'}^2 \rangle \, du_1 \, du_1' = -3 \int_0^1 \int_0^1 w_{11} \, du_1 \, du_1' = -\frac{1}{2}$$

and similarly

$$\langle W_2 \rangle = \int_0^1 \int_0^1 15 w_{11}^2 \, du_1 \, du_1' = \frac{1}{2}$$

$$\langle W_3 \rangle_\varrho = -\int_0^1 \int_0^1 105 w_{11}^3 \, du_1 \, du_1' = -\frac{3}{4}$$

$$\langle W_1 W_1 \rangle_\varrho = \int_0^1 \int_0^1 \int_0^1 \int_0^1 (9 w_{11} w_{22} + 6 w_{12}^2) \, du_1 \, du_1' \, du_2 \, du_2' = \frac{17}{60}$$

$$\langle W_2 W_1 \rangle_\varrho = -\int_0^1 \int_0^1 \int_0^1 \int_0^1 (45 w_{11}^2 w_{22} + 60 w_{11} w_{12}^2) \, du_1 \, du_1' \, du_2 \, du_2' = -\frac{9}{28}$$

$$\langle W_1 W_1 W_1 \rangle = -\int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 (27 w_{11} w_{22} w_{33} + 24 w_{12} w_{23} w_{13} -$$

$$- 54 w_{11} w_{23}^2) \, du_1 \, du_1' \, du_2 \, du_2' \, du_3 \, du_3' = -\frac{457}{2520} .$$

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