

Frequency dependence of the conductivity of random systems near the true spectral edge

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Expressions have been obtained for the frequency dependence of conductivity for one- and three-dimensional random systems when the electron Fermi level is close to the true spectrum end point. The frequency values for which the investigation is valid are bounded from below.

The paper derives the frequency dependences of the conductivity of one- and three-dimensional random systems for the case when the absorption is determined by particles, the energy of which lies near the true spectrum boundary. For the sake of argument, we have examined a situation when the particles occupy the levels near the bottom of the band and the positions of impurities with positive potential energies have a Poisson distribution. In this case the true spectrum boundary is the energy $E = 0$ (the energy is reckoned from the lower edge of the band in the absence of impurities).

Let v_0 be the characteristic value of the potential of an individual impurity, and let a be the characteristic range of the potential. Then the renormalized spectrum boundary (see [1]) is $E_0 = nv_0a$ in the one-dimensional case and $E_0 = nv_0a^3$ in the three-dimensional case (n is the impurity concentration). Hereafter we shall assume that the Fermi energy of the particles is $E_F \ll E_0$. As is well known (see, e.g., [1]), the energy levels for $E \ll E_0$ are determined by fluctuations in the impurity distribution.

We obtain below the frequency dependence of the conductivity due to such fluctuation levels (in Sec. 1 for the one-dimensional case and in Sec. 2 for the three-dimensional case).

1. ONE-DIMENSIONAL CASE

As indicated above, the spectrum near the true boundary $E = 0$ is due to the fluctuations of the impurity distribution; in other words, regions appear in which the impurity concentration is lower than the average. We confine ourselves to a situation similar to the one studied by the author and Dykhne [2]. It corresponds to a special case of energy-level quantization when it is possible to find not only the exponential in the level-density formula but also the pre-exponential factor. We now proceed to the description of this case.

Energy levels with $E \ll E_0$ appear in those places where there is a great distance between the nearest impurities. It is clear that the wave-function propagation range outside this well is $\delta \sim (mE_0)^{-1/2}$ ($\hbar = 1$) is Planck's constant. We impose the auxiliary condition $\delta n \ll 1$, which means that the energy levels can be obtained by quantization in a potential well with infinite walls. This condition can also be rewritten in the form $n/mv_0a \ll 1$. It is clear that there are many levels in such a well. For the sake of simplicity, however, we assume that the absorption is due to a transition between the first two levels.

The general expression for conductivity $\sigma(\omega)$ is

$$\sigma(\omega) = -\pi e^2 \int dE \frac{f(E+\omega) - f(E)}{\omega} \sum_{n,m} |v_{nm}|^2 \delta(E_n - E) \delta(E_m - E - \omega) \quad (1)$$

($f(E)$ is the particle distribution function and v_{nm} is the velocity-operator matrix element). The expression is easily estimated apart from a numerical coefficient. From the quantization condition it follows that the energy levels are $E_n = \pi^2 n^2 / 2mr^2$, where r is the distance between the nearest impurities. If we limit ourselves to absorption as a result of a transition between the first two levels, then ω is always equal to $3E$ thanks to the δ -functions in (1) (therefore it follows that the difference of distribution functions in (1) cannot be replaced by a derivative). The condition $\omega = 3E$ corresponds to a transition between the first two levels. Generally speaking, during a transition from the first level to the n -th level we have $\omega = E(n^2 - 1)$.

It is evident that $v_{nm} \sim \omega r$. The expression (1) should be averaged with the multiplier ne^{-nr} that determines the probability that the distance between the nearest impurities is r . It should be noted that the number of such pairs are proportional to the concentration of impurities n . Taking into account these considerations, it is easily found from (1) that

$$\sigma(\omega) = A \frac{n^2 e^2}{m^2 \omega^4} \exp(-nr_0), \quad (2)$$

where $r_0 = \pi(3/2\omega)^{1/2}$ and A is the numerical parameter.

The condition $nr_0 \gg 1$ permits us to confine ourselves to the transition between the first levels. We confined ourselves to the case $T = 0$. Consequently, since the integration with respect to energy takes place in the region $E \geq E_F - \omega$, a lower bound is imposed on the frequency ω :

$$\omega >^{3/4} E_F. \quad (3)$$

There is no upper bound, since transitions are possible not only between the first levels. In the event of a transition between the first and n -th levels we have

$$E_F(n^2 - 1) > \omega > (n^2 - 1)E_F/n^2.$$

We confine ourselves to a transition between the first levels. It should be noted here that the bound (3) is of a basic nature, since the splitting of levels due to the overlap of the wave functions in different potential wells drops considerably faster with a decreasing particle concentration ρ than the distance between the levels in an individual potential well. Utilizing the results of [2], the condition (3) can be rewritten as follows:

$$\omega > \frac{3n^2}{8m} \left(\ln \frac{n}{\rho} \right)^{-2}. \quad (4)$$

We note here that from the author's preceding paper [3] it follows that when $\omega = 0$ the conductivity is equal to

zero, but the dependence on ω as $\omega \rightarrow 0$ will, of course, differ from formula (2).

2. THREE-DIMENSIONAL CASE

Here, too, we assume that the energy levels determining the absorption are due to quantization in potential wells with endless walls. However, because the conditions differ from the one-dimensional case, we present the appropriate limitations on the parameters. The condition $n^{1/3}(mv_0 a^3 n)^{-1/2}$ means that the energy levels correspond to a potential well with endless walls. In this case (see [4]) the first level (for a sphere) is $E_1 = \pi^2/2mr^2$ and the second is $E_2 = \pi^2 \alpha^2/2mr^2$ (α is determined from the condition $x = \alpha\pi$, $x = \tan x$). Hence (taking into account the δ -functions in (1))

$$r_0 = \pi \left(\frac{\alpha^2 - 1}{2\omega} \right)^{1/2}. \quad (5)$$

Condition (3) goes over into

$$\omega > (\alpha^2 - 1) E_F / \alpha^2. \quad (6)$$

The probability that there are no impurities in the volume V is obviously ne^{-nV} . Obviously, the volume V should be minimal at the specified energy value. This is apparently achieved for a sphere. Similarly, as in the paper by Zittarz and Langer [5], the conductivity will be

proportional to the number of points where a minimum volume is achieved, as determined by the derivative $\partial V / \partial E$. However, since the investigated quantization method does not depend on the impurity density, the number of such cavities per unit of volume is $\sim V^{-1}$.

Taking these considerations into account, we obtain from (1) (B is a numerical parameter)

$$\sigma(\omega) = B \frac{ne^2}{m\omega} \exp\left(-\frac{4\pi}{3} nr_0^3\right), \quad (7)$$

where r_0 is given by formula (5). We again assume that $nr_0^3 \gg 1$, i.e., only the transition between the first levels is essential.

¹I. M. Lifshitz, Usp. Fiz. Nauk **83**, 617 (1964) [Sov. Phys.-Uspekhi **7**, 549 (1964)].

²Yu. A. Bychkov and A. M. Dykhne, ZhETF Pis. Red. **3**, 313 (1966) [JETP Lett. **3**, 202 (1966)].

³Yu. A. Bychkov, Zh. Eksp. Teor. Fiz. **65**, 427 (1973) [Sov. Phys.-JETP **38**, 209 (1974)].

⁴L. D. Landau and E. M. Lifshitz, Quantum Mechanics, Addison-Wesley, 1963.

⁵J. Zittarz and J. S. Langer, Phys. Rev. **148**, 741, 1966.

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