

Corrections to diffusion and conductivity in the field of randomly distributed force centers

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The question of the frequency dependence of the conductivity $\sigma(\omega)$ at low frequencies and of the corrections to the diffusion law $\langle r^2(t) \rangle \propto Dt$ is considered for particles moving in a system of randomly distributed force centers. It is shown that besides the usual terms proportional to integral powers of ω the series for $\sigma(\omega)$ or the diffusion coefficient $D(\omega)$ contains terms $\sim \omega^{3/2}$ in three-dimensional, or $\sim \omega \ln \omega$ in two-dimensional, space, which corresponds to corrections to the diffusion law $\sim t^{-1/2}$ for $d=3$ and $\sim \ln t$ for $d=2$ (d is the dimension of the space). In the quasi-unidimensional situation, i.e., when the transverse dimensions of the system are small, but finite, the nonregular corrections considerably exceed the classical corrections and turn out to be $\sim \sqrt{\omega}$ for $\sigma(\omega)$ and $\sim \sqrt{t}$ for $\langle r^2(t) \rangle$. These corrections lead to a situation in which at large t the velocity correlator for the diffusing particles $\propto t^{-(d+2)/2}$. The presence of nonregular terms in the expressions for $\sigma(\omega)$ and $\langle r^2(t) \rangle$ is due to the existence in the perturbation-theory series for the diffusion coefficient of intermediate states containing diffusion poles corresponding to quasi-particles: "diffusions." The coefficients in the nonregular corrections are computed in the limit of weak interaction and low scatterer concentration. The anomalous corrections are of a quantum nature, i.e., they vanish in the classical limit.

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1. INTRODUCTION

The problem of the motion of a particle in the field of randomly distributed force centers has been investigated in a large number of papers (see, for example, the review by Lifshitz^[1]). It is well known that if the particle energy is sufficiently high, then the particle propagates like a weakly damped plane wave; if, on the other hand, the energy is small, then the wave is heavily damped, and there arises the difficult problem of finding the energy spectrum near the band edge, a problem which has not been completely solved.

In this paper we shall investigate the spatial and temporal distribution of the particle density. It is clear from physical arguments (this will be rigorously proved below) that in the limit of large times and distances the particle density satisfies the diffusion equation

$$\frac{\partial}{\partial t} \rho_E(r, t) = D_E \nabla^2 \rho_E(r, t), \quad (1)$$

where ρ_E is the density of particles of energy E and D_E is the diffusion coefficient for these particles (since the centers are static, energy is conserved in scattering by them, and we neglect the particle-particle interaction; therefore, particles with energy E diffuse with a diffusion coefficient D_E). In the general case D_E is a complex function of the energy. We can only assert that in the limit of large energies

$$D_E^{(d)} = 2E/d\gamma_{tr}^{(d)}, \quad (2)$$

where $\gamma_{tr} = \gamma - \gamma_1$ is the "transport attenuation factor" for the particle and d is the dimension of the space; we are using a system of units in which $\hbar = 2m = 1$ (it should be noted that, according to Mott^[2], diffusion in one-dimensional systems is impossible; therefore, in (2) $d = 2, 3$; the last section of the paper is devoted to a discussion of diffusion in the quasi-unidimensional situation, i.e., when the wavelength of the particles is comparable to the transverse dimensions of the system).

To the equation (1) corresponds the usual law,

$$\langle r^2(t) \rangle^{(d)} = 2dD_E^{(d)} t, \quad (3)$$

according to which the particle density spreads out in time and which corresponds to the random-walk picture. The diffusion law (3) is valid only at the limit $t \rightarrow \infty$. Let us discuss the nature of the possible corrections to the expression (3), i.e., assuming in (3) that $D_E^{(d)} = D_E^{(d)}(t)$, let us elucidate the behavior of the diffusion coefficient at large $t \neq \infty$. On account of the Einstein relations, the diffusion coefficient is proportional to the conductivity, and, knowing its dependence on the frequency of the electromagnetic field, $\sigma(\omega)$, we could, in principle, determine the dependence $D_E(t)$. Since it is known that at low frequencies $\sigma(\omega)$ can be expanded in powers of the quantity $(\omega \tau_{tr})$, where $\tau_{tr} = \gamma_{tr}^{-1}$ is the "transport time" between collisions of the particle with an impurity, the diffusion coefficient at large t should also be expandable in powers of (τ_{tr}/t) . These regular corrections are not connected with the quantum properties of the particle, and, if they are large, then this means that the system simply has not yet reached the diffusion regime, which obtains at $t \gg \tau_{tr}$.

In the present paper we show that there exist, besides the classical corrections, other corrections to the diffusion law that arise precisely at times larger than the microscopic times and that contain a quantum parameter—the ratio of the particle wavelength to the mean free path. Let us briefly explain the mechanism leading to the appearance of the nonregular—in t —corrections to the diffusion. The diffusion process can be treated as the propagation of a distinctive slow quasi-particle with a purely imaginary mass: a diffusion. This diffusion is formed as a result of the random walk of the particles from one center to another. In such wanderings the rare processes in which the particles return to the force centers with which they had earlier interacted (multiple scattering) are possible. If the rescattering events occur after times comparable to τ_{tr} , then this leads to some renormalization of the constants in the expansion of $\langle r^2(t) \rangle$ in powers of (τ_{tr}/t) . If, on the other hand, the particle returns to the center after many wanderings, i.e., after a time $t \gg \tau_{tr}$, during which it traverses a

distance much longer than the mean free path, then such a return can be described as a slow process of diffusion scattering by impurities, a process which renormalizes the effective interaction ensuring a diffusion process such that there appear in it terms nonregular in ω .

The form of these quantum corrections depends on the dimension of the space. The dominant of them in the law $\langle \mathbf{r}^2(t) \rangle$ for the three-dimensional case is $\sim t^{-1/2}$ or $\sim \omega^{3/2}$ for $D(\omega)$, while for the two-dimensional case we respectively have $\ln t$ and $\omega \ln \omega$. The correction to the conductivity in the three-dimensional case can be observed at low temperatures against a background of the first standard correction ($\omega \tau_{tr}^{(3)}$). For the two-dimensional case it is clear that for sufficiently low frequencies (or at large times in $D(t)$) the indicated correction becomes larger than the regular correction ($\omega \tau_{tr}^{(2)}$). It turns out to be especially large in the quasi-unidimensional case, where the contribution to the diffusion coefficient is of the order of $\sqrt{\omega}$, which corresponds to the appearance of a term $\sim \sqrt{t}$ in the diffusion law (3).

In conclusion of this section, let us note that the non-regular corrections to diffusion have been discussed in a paper by one of the present authors^[3], as well as in other papers^[4,5]. In contrast to^[3-5], in our case we are able not only to ascertain the form and the physical cause of the resulting corrections in the general form, but also to carry through the computations for some concrete examples at the microscopic level.

2. THE GENERAL STRUCTURE OF THE CORRECTIONS TO DIFFUSION

In this section we discuss the structure of the perturbation-theory series for the particle-density propagation function, as well as the mechanism underlying the appearance of the corrections to diffusion and the conductivity.

The analysis is based on the usual diagrammatic techniques for a particle in the field of randomly distributed force centers (see, for example, the book by Abrikosov, Gor'kov, and Dzyaloshinskiĭ^[6]). For the study of diffusion, it is necessary to consider the retarded Green function, $K^R(\mathbf{k}, \omega)$, for the particle density, this function being the analytic continuation to the real axis from above of the corresponding function of the discrete frequencies:

$$K(\mathbf{k}, i\omega_n) = \int_0^{1/\tau} d\tau \langle T_\rho(\rho_{\mathbf{k}}(\tau) \rho_{-\mathbf{k}}(0)) \rangle \exp i\omega_n \tau = T \sum_{iE} K(\mathbf{k}, iE, i\omega_n), \quad (4)$$

where $\rho_{\mathbf{k}}(\tau)$ is the Fourier transform of the particle-density operator. The first few diagrams for K are shown in Fig. 1, where the lines with arrows correspond to the exact particle Green functions, the wavy lines correspond to the Fourier transform of the potential of the interaction with a center, and a point denotes a force center. To each point corresponds a factor n , the concentration of the force centers, and the law of conservation of momentum is satisfied at each vertex. Since the centers are static in all the diagrams, to the upper lines corresponds an energy $iE + i\omega$, while to the lower lines corresponds an energy iE ; the function K is an analytic function of the variables $iE + i\omega_n$ and iE , and has branch cuts along the lines $\text{Im}(iE + i\omega_n) = 0$ and $\text{Im}(iE) = 0$. Taking this circumstance, as well as the fact that $i\omega_n = 2\pi nT$, into account, we can easily carry out the analytic continuation (4) in the general form (see Ginzburg's paper^[7]):

$$K^R(\mathbf{k}, \omega + i\delta) = \frac{1}{2\pi i} \int dE \{ [n(E + \omega) - n(E)] \tilde{K}(\mathbf{k}, E + \omega + i\delta, E - i\delta) + n(E) \tilde{K}(\mathbf{k}, E + \omega + i\delta, E + i\delta) - n(E + \omega) \tilde{K}(\mathbf{k}, E + \omega - i\delta, E - i\delta) \}, \quad (5)$$

where $n(E)$ is the Fermi or Bose distribution function, depending on the statistics of the particles under consideration. It is evident that the formula (5) is valid for any distribution function of the particles over energy that does not correspond to thermodynamic equilibrium. Thus, as was to be expected, the problem has been reduced to the study of the behavior of the density of particles with a fixed energy. Now in the diagrams of Fig. 1 the arguments of the upper and lower Green functions are respectively $E + \omega$ and E . Further, if the imaginary correction to the energy is positive, then to a line corresponds the retarded Green function $G_p^R(E) = G_p^R(E + i\delta)$, while if the correction is negative, then $G_p^A(E - i\delta) = G_p^*(E)$.

It is not difficult to verify by considering the perturbation-theory series for $\tilde{K}(\mathbf{k}, E + \omega + i\delta, E + i\delta)$ that in the limit when $\mathbf{k}, \omega = 0$ (cf.^[7])

$$\tilde{K}(0, E + i\delta, E + i\delta) = -\frac{1}{(2\pi)^d} \int dp \frac{\partial}{\partial E} G_p(E). \quad (6)$$

Using this relation and the analogous formula for $\tilde{K}(0, E - i\delta, E - i\delta)$, we obtain from (4) for small \mathbf{k} and ω :

$$K^R(\mathbf{k}, \omega + i\delta) = \frac{1}{2\pi i} \int dE \frac{\partial n(E)}{\partial E} \left\{ \omega \tilde{K}(\mathbf{k}, E + \omega + i\delta, E - i\delta) + \frac{2i}{(2\pi)^d} \int dp \text{Im} G_p(E) \right\} = \int dE \left(-\frac{\partial n(E)}{\partial E} \right) K(\mathbf{k}, E, \omega + i\delta). \quad (7)$$

On account of the law of conservation of the total particle number, $\rho_{\mathbf{k}} = 0(t)$ does not depend on the time, and, therefore, $K^R(\mathbf{k} = 0, \omega + i\delta) \equiv 0$. This implies the validity of the exact equality

$$K(\mathbf{k} = 0, E + \omega + i\delta, E - i\delta) = \frac{2\pi i \rho(E)}{\omega}, \quad (8)$$

$$\pi \rho(E) = -\frac{1}{(2\pi)^d} \int dp \text{Im} G_p(E).$$

Here $\rho(E)$ is the usual density of states of particles with energy E . As shown below, at finite \mathbf{k}, ω in the denominator of (8) is replaced by $\omega + iD_{\mathbf{k}} k^2$, and, as a result, we obtain:

$$K^R(\mathbf{k}, \omega + i\delta) = \int dE \left(-\frac{\partial n}{\partial E} \right) \rho_{\mathbf{k}} \frac{D_{\mathbf{k}} k^2}{-i\omega + D_{\mathbf{k}} k^2}. \quad (9)$$

To derive this formula and obtain the corrections to it, we shall need some general relations connecting $K^R(\mathbf{k}, \omega)$ with the retarded current correlator

$$P^R(\mathbf{k}, \omega) = \frac{i}{k^2} \langle [(\mathbf{k} \mathbf{j}_{\mathbf{k}}), (\mathbf{k} \mathbf{j}_{-\mathbf{k}})] \rangle_{\omega}^R$$

(Einstein's relations). These relations are easily derived by differentiating the function $K^R(\mathbf{r}_1 - \mathbf{r}_2, t_1 - t_2)$ with respect to t_1 and t_2 and substituting into the Fourier

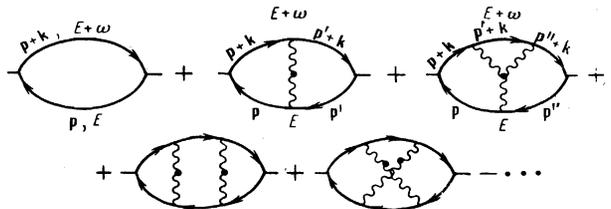


FIG. 1

$$\tilde{K}(k, E+i\delta, E-i\delta) = \text{Diagram 1} + \text{Diagram 2}$$

$$U = \text{Diagram 3} + \text{Diagram 4} + \text{Diagram 5} + \text{Diagram 6} + \text{Diagram 7} + \dots$$

FIG. 2

transform of the expression for $\hat{\rho}$ obtained from the equation of continuity $\hat{\rho}\omega, \mathbf{k} = -i\mathbf{k}j\omega, \mathbf{k}$:

$$-\frac{i\omega}{k^2} K^R(\mathbf{k}, \omega) = \frac{1}{i\omega} [P^R(\mathbf{k}, \omega) - 2N]. \quad (10)$$

According to [6], the right-hand side of (10) is the conductivity $\sigma(\mathbf{k}, \omega)$. To compute $P^R(\mathbf{k}, \omega)$, we can easily introduce analytic-continuation formulas similar to (7). The quantity $k^2 P^R(\mathbf{k}, \omega)$ is described by the same set of diagrams that describe $K^R(\mathbf{k}, \omega)$, the only difference being that at the right and left vertices of each of the loops stands a scalar product of the vector \mathbf{k} and the sum of the momenta of the lines converging at these vertices. Using the Ward identity

$$P(k=0, E+i\delta, E+i\delta) = \frac{2}{d} \frac{1}{(2\pi)^d} \int d\mathbf{p} \mathbf{p} \frac{\partial}{\partial \mathbf{p}} G_p(E), \quad (11)$$

which is obvious from the diagram series in Fig. 1, we can, in analogy to (7), write:

$$P^R(\omega) = \frac{1}{2\pi i} \int dE \left(\frac{\partial n}{\partial E} \right) \omega \bar{P}(E+i\delta, E-i\delta) - \frac{2}{\pi} \int dE n(E) \frac{1}{(2\pi)^d} \int d\mathbf{p} \text{Im} G_p(E).$$

Since the last term in (12) is simply $-2N$, from (9), (10), and (12) follows the Kubo formula for the diffusion coefficient

$$D(\omega) = \int dE \left(-\frac{\partial n}{\partial E} \right) \rho(E) D_E(\omega) = \frac{1}{i\omega} [P^R(\omega) - P^R(0)] = \frac{\sigma(\omega)}{e^2}. \quad (13)$$

Let us return to the derivation of the formula (9). In Fig. 2 we graphically represent the equality connecting $\tilde{K}(\mathbf{k}, E + \omega + i\delta, E - i\delta)$ with the quantity L , the complete four-point function, for which we have the equation

$$L_{pp'}(\mathbf{k}, E, \omega+i\delta) = U_{pp'}(\mathbf{k}, E, \omega+i\delta) + \frac{1}{(2\pi)^d} \int d\mathbf{p} U_{pp_i}(\mathbf{k}, E, \omega+i\delta) G_{p+\mathbf{k}}(E+\omega) G_{p'}(E) L_{pp'}(\mathbf{k}, E, \omega+i\delta), \quad (14)$$

where U is an irreducible four-point function, which cannot be divided into two parts by cutting only two lines corresponding to particles.

In the case of point centers, we have in the lowest order in the concentration n and in the interaction V the expressions

$$U(\mathbf{q}) = nV^2(\mathbf{q}), \quad V(\mathbf{q}) = \int d^d r e^{i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{r}), \\ G_p(E) = (E - p^2 + i\gamma^{(d)})^{-1}, \\ \gamma^{(3)} = -\text{Im} \Sigma^{(3)} = n\sigma\sqrt{E} = \frac{\sqrt{E}}{16\pi^2} \int d\Omega U(\mathbf{p}-\mathbf{p}') = \frac{\sqrt{E}}{4\pi} U_0, \\ \gamma^{(2)} = -\text{Im} \Sigma^{(2)} = \frac{1}{8\pi} \int d\varphi U(\mathbf{p}-\mathbf{p}') = \frac{U_0}{4}. \quad (15)$$

Here Σ is the self-energy part of G in the lowest approximation and, like $U_{pp'}$, does not depend on the momenta.

$$\Sigma = \text{Diagram 8} + \text{Diagram 9} + \text{Diagram 10} + \dots$$

FIG. 3

The equation for L is easy to solve:

$$L(\mathbf{k}, \omega) = U \left[1 - \frac{U}{(2\pi)^d} \int d^d \mathbf{p} G_{p+\mathbf{k}}(E+\omega) G_{p'}(E) \right]^{-1} \approx \frac{l^{(d)}}{-i\omega + D_E^{(d)} k^2}; \\ D_E^{(d)} = \frac{2E}{d\gamma^{(d)}}, \quad l^{(d)} = \frac{2\gamma^{(d)}}{I_0^{(d)}}, \quad I_0^{(d)} = \frac{1}{(2\pi)^d} \int d^d \mathbf{p} |G_p|^2, \quad (16) \\ I_0^{(3)} = \sqrt{E}/4\pi\gamma^{(3)}, \quad I_0^{(2)} = 1/4\gamma^{(2)}.$$

The approximate equality on the right-hand side of the first formula in (16) obtains if we neglect the higher terms of the expansion in powers of k^2 and ω . As follows from (8), the cancellation of the constant term in the denominator in (16) is a consequence of the law of conservation of the total particle number. In the general case an analogous cancellation is realized owing to the following exact relation:

$$\text{Im} \Sigma_p(E) = \frac{1}{(2\pi)^d} \int d^d \mathbf{p}' U_{pp'}(0, E, 0) \text{Im} G_{p'}(E). \quad (17)$$

The validity of (17) can easily be verified by considering the sequence of irreducible diagrams for the self-energy part, Σ , of the Green function G (see Fig. 3). If we compute $\text{Im} \Sigma$ with the aid of the equality $\text{Im}(AB) = A \text{Im} B + (\text{Im} A)B^*$, then the contribution to $\text{Im} \Sigma$ from each of the diagrams will consist of several terms, in each of which one of the internal Green functions will be replaced by $\text{Im} G$; the Green functions standing along the solid line to the left of this Green function do not change, while those standing to the right are replaced by G^* . As a result, each such term will have the form of an integral operator acting on $\text{Im} G$. Further, each diagram corresponding to such an operator coincides with one of the diagrams for $U_{pp'}(0, E, 0)$. As can easily be verified, in such a procedure all the diagrams for $U_{pp'}$ are reproduced, and there are no superfluous ones; for example, the three simplest diagrams in Fig. 3 reduce to the six simplest diagrams shown in Fig. 2. Equation (17) is, essentially, a unitarity condition for G and ensures the singularity of $L(\mathbf{k} = 0, \omega = 0)$. In order to verify this, let us write Eq. (14) in the operator form as follows:

$$L(\mathbf{k}, \omega) = U(\mathbf{k}, \omega) + U(0, 0) |G|^2 L(\mathbf{k}, \omega) + \Delta[U(\mathbf{k}, \omega) (GG^*)_{\mathbf{k}, \omega}] L(\mathbf{k}, \omega), \\ \Delta[U(\mathbf{k}, \omega) (GG^*)_{\mathbf{k}, \omega}] = U(\mathbf{k}, \omega) (GG^*)_{\mathbf{k}, \omega} - U(0, 0) |G|^2. \quad (18)$$

If now we let an integral operator with a kernel $\text{Im} G$ act on this equation from the left, then we arrive at the equality

$$-\text{Im} \Sigma - \text{Im} G \Delta[U(\mathbf{k}, \omega)] = \text{Im} G \Delta[U(\mathbf{k}, \omega) (GG^*)_{\mathbf{k}, \omega}] L(\mathbf{k}, \omega). \quad (19)$$

$\Delta[U(\mathbf{k}, \omega) (GG^*)_{\mathbf{k}, \omega}]$ tends to zero as $\mathbf{k} \rightarrow 0, \omega \rightarrow 0$, from which it necessarily follows that $L(0, 0) = \infty$. Taking into account the symmetry of $L_{pp'}$ with respect to interchange of \mathbf{p} and \mathbf{p}' , as well as Eqs. (8) and (13), we can easily understand that the solution (18) in the lowest approximation in \mathbf{k} and ω has the form

$$L_{pp'}(\mathbf{k}, \omega) = 2i \frac{\text{Im} \Sigma_p(E) \text{Im} \Sigma_{p'}(E)}{\pi \rho(E)} \frac{1}{\omega + iD_E k^2}, \quad (20)$$

which corresponds with the formula (9).

To compute D_E , we must expand $\Delta[UGG^*]$ in (18) in powers of k up to the k^2 term and substitute into it the

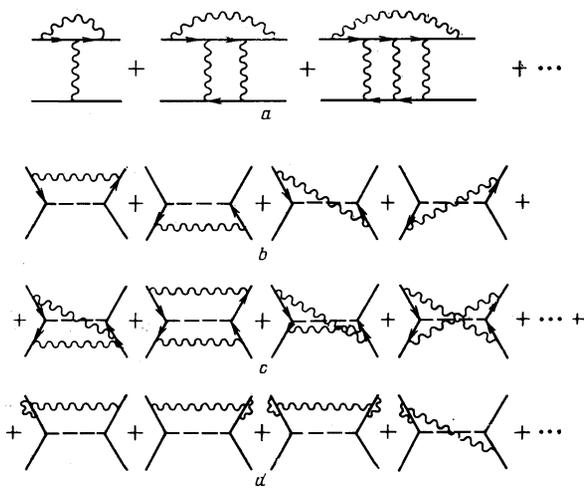


FIG. 4

expression (20). We can similarly find the corrections to (20). For this purpose, we should expand U and (GG^*) in (18) up to the powers of interest to us, substitute into the resulting expression (20), in which the unit term in the numerator and D_E in the denominator should be replaced by some functions $l_{pp'}(\mathbf{k}, \omega)$ and $D_E(\mathbf{k}, \omega)$ expanded in the appropriate series, and equate the coefficients attached to identical powers in the expansion, requiring the fulfillment of the condition (19) for each of the powers. We obtain a system of integral equations, for which the conditions (19) are simply conditions for their solubility. The execution of this program requires the knowledge of the form of the expansion of $(UGG^*)_{\mathbf{k}, \omega}$. First of all, it is clear that for $k^2, \omega \ll E$

$$G_{p+p'}(E+\omega)G_p^*(E) = |G_p(E)|^2 + g_{1p}(E)\omega + g_{2p}(E)\mathbf{k} + g_{3p}^{(2)}(E)k_\alpha k_\beta + \dots \quad (21)$$

Therefore, the direct expansion of the function G does not lead to any nonregular corrections to the diffusion.

The simplest diagrams for $U_{pp'}$, which are shown in Fig. 2, also do not contain terms that are nonregular in \mathbf{k} and ω . We can, however, make, for example, the fifth diagram in Fig. 2 more complex, as shown in Fig. 4a. As a result of such a complication, the internal sequence of diagrams is gathered into an expression having a diffusion pole, and the corresponding contribution to $U_{pp'}(\mathbf{k}, E, \omega + i\delta)$ can be represented at small \mathbf{k} and ω in the form

$$\int d\mathbf{q} \frac{F(\mathbf{p}, \mathbf{q}, \mathbf{k}, \mathbf{p}')}{-i\omega + Dq^2} = \int d\mathbf{q} \frac{F(\mathbf{p}, \mathbf{q}, \mathbf{k}, \mathbf{p}')}{Dq^2} + i\omega \int d\mathbf{q} \frac{F(\mathbf{p}, 0, 0, \mathbf{p}')}{Dq^2(-i\omega + Dq^2)} + \dots = a + b\sqrt{i\omega} + ck + d\omega + e\omega^{3/2} + \dots \quad (22)$$

in three-dimensional space. In the two-dimensional case the square root branchings in this series are replaced by logarithmic ones.

Thus, we see that the presence in the internal parts of the diagrams for $U_{pp'}$ of sequences, the summation of which gives rise to a diffusion pole, leads to the appearance in the expression for $U_{pp'}$ of terms that are nonregular in ω . We shall represent the propagation of such a diffusion pole, or, in other words, of such a quasiparticle with an imaginary mass—a diffusion—by a dashed line. The simplest diffusion diagrams are shown in Fig. 4. It is precisely the appearances of such diffu-

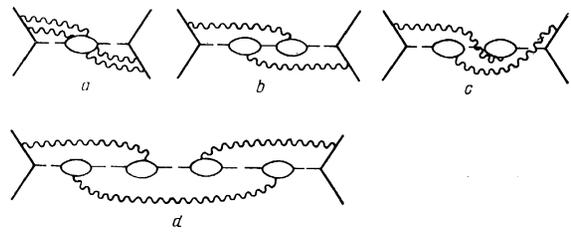


FIG. 5

sion intermediate states in the expression for $U_{pp'}$ that constitute the return effects discussed in the Introduction. Besides the single-diffusion diagrams shown in Fig. 4, it is clear that there also exist multidiffusion diagrams in which the diffusing density more than once is gathered into a diffusion. Some of these diagrams are shown in Fig. 5, it being clear that, for example, the diagram in Fig. 5a gives a singularity of the same order as the one given by the diagrams in Fig. 4, whereas the diagrams in Figs. 5b and 5c have singularities $\sim \ln(-i\omega + Dk^2/9)$, the five-diffusion diagram in Fig. 5d already contains a singularity $\sim (-i\omega + Dk^2/25)^{-1/2}$, etc. It is precisely the appearance of similar large terms in the expression for $\Sigma_p(E)$ at low energies that is the source of the difficulties that are encountered in the study of the energy spectrum of particles near the band edge and that were mentioned in the Introduction^[1]. But we know that the quantity entering into (17) is finite. This means that there exists a mechanism that ensures the absence of such large terms. Moreover, even if we make use of the simplest type of complication (Fig. 4) and attempt to solve Eq. (18), $L(\omega)$ turns out to be proportional to $\omega^{-1/2}$, instead of the dependence, ω^{-1} , that follows from the law of conservation of particle number, (8). This fact means that there should also occur here certain cancellations that are such that they at least ensure the absence in $L(\omega)$ of terms that decrease the order of its divergence as compared to ω^{-1} . In other words, since the above-described procedure for computing the density correlator leads to the formula

$$K(\mathbf{k}, E, \omega + i\delta) = \rho(E) \frac{f(\omega) iD_E(\mathbf{k}, \omega) k^2}{\omega f(\omega) + iD_E(\mathbf{k}, \omega) k^2}, \quad (23)$$

the expansion of $f(\omega)$ should, in any case, begin with unity. On the other hand, there are two circumstances that allow us to avoid the indicated difficulties.

Our aim is to study the dependence on ω of the experimentally observable value of the conductivity $\sigma(\omega)$ and of the asymptotic behavior at large times of the quantity $\langle \mathbf{r}^2(t) \rangle$. For the computation of $\sigma(\omega)$, we have the formulas (13), while $\langle \mathbf{r}^2(t) \rangle$ is defined according to standard rules^[3] as

$$\langle \mathbf{r}^2(t) \rangle = \frac{\int d\mathbf{r} r^2 \int d\omega \text{Im} K^R(\mathbf{r}, \omega) \omega^{-1} e^{-i\omega t}}{\int d\mathbf{r} \int d\omega \text{Im} K^R(\mathbf{r}, \omega) \omega^{-1} e^{-i\omega t}} \quad (24) = \int dE \left(-\frac{\partial n(E)}{\partial E} \right) \cdot 2d \left\{ D_E(0)t - \frac{1}{2\pi} \int \frac{d\omega}{\omega^2} e^{-i\omega t} \Delta_n D(\omega) \right\},$$

i.e., both the conductivity and the mean square distance are determined only in terms of the \mathbf{k} -independent part of the diffusion coefficient $D_E(\omega)$, and, in this sense, $f(\omega)$ does not carry any information. On the other hand, the homogeneous part of the dynamical diffusion coefficient can be directly computed, using the formulas (18). Before proceeding to do this, let us note that, because of

the vectorial nature of the vertices of the current-density correlator $\mathbf{pR}(\omega)$, the ω singularities do not strengthen as larger and larger numbers of diffusions are put in the intermediate states. To verify this, let us write out the obvious—from the diagram series for D and the formula (13)—equations determining the diffusion coefficient:

$$D_E(\omega)k^2 = \frac{1}{(2\pi)^d} \int d\mathbf{p} (2\mathbf{pk})^2 G_p(E+\omega) G_p^* \Phi_p(E, \omega), \quad (25)$$

$$2\mathbf{pk} \Phi_p(E, \omega) = 2\mathbf{pk} + \frac{1}{(2\pi)^d} \int d\mathbf{p}_1 U_{\mathbf{pp}_1}(E, \omega) G_{\mathbf{p}_1}(E+\omega) G_{\mathbf{p}_1}^*(E) \cdot 2\mathbf{p}_1 \mathbf{k} \Phi_{\mathbf{p}_1}(E, \omega).$$

For $\omega = 0$ the solution to these equations will give the static diffusion coefficient, while the expansion of $G_p(E + \omega)$ and $U_{\mathbf{pp}_1}(E, \omega)$ will lead to equations determining the dynamical corrections to it. The function Φ_p is determined by the quantity $U_{\mathbf{pp}_1}(E, \omega)$ multiplied by \mathbf{p} the cosine of the angle between \mathbf{p} and \mathbf{p}_1 and integrated over this angle; therefore, upon the substitution of the formula (22) into (25), only the term bilinear in $(\mathbf{p} \cdot \mathbf{q})(\mathbf{p}_1 \cdot \mathbf{q})$ makes a contribution. In fact, let us consider the single-diffusion diagrams shown in Fig. 4. For the diagrams in Fig. 4b this fact is obvious. The series of diagrams with two interaction lines joining nondiffusion blocks (of the type shown in Fig. 4c) is distinguished by the fact that the terms in it with nonintersecting interaction lines are canceled out after integration by terms for which these lines intersect. This phenomenon can also be observed in the case of diagrams with any number of interaction lines joining the nondiffusion blocks. Similarly, in multidiffusion diagrams each of the blocks not containing diffusion insertions should be expanded up to the first order in all the ingoing (into it) and outgoing (from it) diffusion momenta, and only the first-order (and nonzero) terms of the expansion will contribute to the nonregular corrections. But then it is clear that, being interested in only the dominant terms in the nonregular correction, we need to take only the single-diffusion intermediate states into account. The correction to D in the three-dimensional case is then proportional to $\omega^{3/2}$:

$$D_E^{(3)}(\omega) = D_E^{(3)}(0) [1 + i\omega\tau_{tr}^{(3)} + B_E^{(3)} i(\omega)^{3/2} + \dots], \quad (26)$$

while in the two-dimensional case it is proportional to $\omega \ln \omega$:

$$D_E^{(2)}(\omega) = D_E^{(2)}(0) [1 + i\omega\tau_{tr}^{(2)} + B_E^{(2)} i\omega \ln(\omega_0/\omega) + \dots],$$

which corresponds to corrections to the diffusion law that are proportional to $t^{-1/2}$ in three-dimensional space, or to $\ln t$ in two-dimensional space:

$$\begin{aligned} \langle r^2(t) \rangle_E^{(3)} &= 6D_E^{(3)} [t + B_E^{(3)} (\pi t)^{-1/2} - \tau_{tr}^{(3)} + \dots], \\ \langle r^2(t) \rangle_E^{(2)} &= 4D_E^{(2)} \left[t - \frac{B_E^{(2)}}{2} \ln(\omega_0 t) - \tau_{tr}^{(2)} + \dots \right], \end{aligned} \quad (27)$$

where ω_0 is some characteristic cutoff frequency.

3. CORRECTIONS TO DIFFUSION IN PERTURBATION THEORY

The entire analysis, carried out in the preceding section, of the corrections to the diffusion law and the conductivity did not depend on the magnitude of the interaction and the concentration of the scatterers. The results obtained there were based only on the smallness of \mathbf{k} and ω and the fact of the appearance in the diagrams for $U_{\mathbf{pp}'}$ of diffusion intermediate states. Therefore, the as-

sertions made about the behavior of $\sigma(\omega)$ and $\langle r^2(t) \rangle$ are valid in the entire region of energies E where infinite particle motion occurs. In the present section we compute with the aid of perturbation theory the coefficients in the frequency-dependent terms in the expansion of $D_E(\omega)$ and the coefficients in the higher-order corrections to $\langle r^2(t) \rangle$, assuming that the concentration of the scatterers is low and that the particle-scatterer interaction is a weak interaction. Accordingly, we shall restrict ourselves to only the simplest diagrams.

Since $V_{\mathbf{p}-\mathbf{p}'}$ is small, according to (15) and (17), the pole of the Green function lies near the real axis, and the dominant contribution to the computations will be made by momenta close in magnitude to \sqrt{E} , while the principal parameter of the perturbation theory will be the quantity $(E\tau)^{-1} \ll 1$. When $U_{\mathbf{pp}'}(E, \omega) = V_{\mathbf{p}-\mathbf{p}'}$, the Eqs. (25) are easy to solve, and it turns out that

$$D_E(\omega) = D_E(0) [1 - i\omega\tau_{tr}]^{-1}, \quad (28)$$

where $D_E(0)$ is determined by the formula (2); $\tau_{tr} = \gamma_{tr}^{-1}$; and, according to (15), in which \mathbf{p} should be set equal to $E^{1/2}$, $U = U_{tr}$. To this standard expression for the low-frequency diffusion coefficient should now be added terms arising from the diffusion renormalization of $U_{\mathbf{pp}'}(E, \omega)$. It is not difficult to see that it is necessary to take into account only the diagrams in which the non-diffusion blocks are joined by one interaction line. Diagrams of the type shown in Fig. 4c are small, since the requirement that all the momenta lie close to the energy surface leads to the restriction of the integration domain to the range of variation of one of the angles between them. This does not, however, mean that we can restrict ourselves to the diagrams in Fig. 4b. In the first place, it is necessary to complicate the right and left vertices of the nondiffusion blocks, which means that with these vertices must be associated the function $2\mathbf{pk} \Phi_p$. In the second place, if we sum up the four diagrams in Fig. 4b, then it turns out that the dominant—with respect to $(E\tau)^{-1}$ —corrections in them cancel out (notice that cancellation occurs also in the summation of diagrams with two interaction lines between blocks). Therefore, it is necessary to take into account the diagrams in which the ends of the interaction lines are made complicated (in the simplest fashion), as shown in, for example, Fig. 4d. It is also clear that for the computation of the diffusion correction the formula for the diffusion (20), which contains only the maximum singularity with respect to \mathbf{k} , is not enough, i.e., with a dashed line in the diagrams in Fig. 4 should be associated the expression

$$L_{\mathbf{pp}'}(E, \omega, \mathbf{q}) = \frac{2}{\pi\rho(E)} \frac{(l_p + l_{p'} 2\mathbf{pq})(l_{p'} + l_{p'} 2\mathbf{p}'\mathbf{q})}{-i\omega + D_E q^2}. \quad (29)$$

Here $l_p = \text{Im } \Sigma_p$ and for l_{1p} we clearly have the equation

$$\begin{aligned} 2\mathbf{pq}l_{1p} &= \frac{1}{(2\pi)^d} \int d\mathbf{p}_1 [U_{\mathbf{pp}_1}(k) G_{\mathbf{p}_1+\mathbf{k}} G_{\mathbf{p}_1}^* - U_{\mathbf{pp}_1}(0) |G_{\mathbf{p}_1}|^2] l_{p_1}, \\ &+ \frac{1}{(2\pi)^d} \int d\mathbf{p}_1 U_{\mathbf{pp}_1}(0) |G_{\mathbf{p}_1}|^2 2\mathbf{p}_1 \mathbf{q} l_{1p_1}. \end{aligned} \quad (30)$$

Of interest to us in the expansion of the free term of this equation are the terms linear in \mathbf{q} . Thus, the formula for the computation of the diffusion coefficient and connected with the rescattering of the diffusion will have the form

$$\Delta D_E'(\omega)k^2 = \frac{1}{(2\pi)^d} \int_{q \leq \xi} d\mathbf{q} \frac{1}{-i\omega + D_E q^2} \frac{2}{\pi\rho(E)}$$

$$\times \left\{ \frac{1}{(2\pi)^d} \frac{1}{k^2} \int dp |G_p|^2 (2pk)^2 (qk) \Phi_p \Lambda_p \right\}^2 V(0),$$

$$\Lambda_p = 2 \operatorname{Re} \left[G_p \left(1 - \frac{\partial \Sigma_p}{\partial E} \right) \right] l_{1p} + 2i \operatorname{Im} \left[G_p \left(1 - \frac{\partial \Sigma_p}{\partial E} \right) \right] l_p. \quad (31)$$

In the region of applicability of the perturbation theory, the Eqs. (25) for Φ_p and (30) for l_{1p} are easy to solve:

$$l_{1p} = \frac{i\sqrt{E} \gamma_t}{2 \gamma_{tr}}, \quad \Phi_p = \frac{\gamma}{\gamma_{tr}} - \frac{p - \sqrt{E}}{p} \frac{\gamma_t}{\gamma_{tr}}. \quad (32)$$

The limitation in (31) to the domain of integration with respect to q is connected with the fact that the diffusion in the form (20) exists when $q \leq \xi \ll \gamma/\sqrt{E}$. Since we shall not be interested in a minor renormalization of the static diffusion coefficient and in the renormalization of the regular corrections to it, this limitation is of no importance to us. The same result can be obtained with the aid of two ($d=3$) or one ($d=2$) subtraction. Substituting the expressions from (15) and (32) into (31), we obtain after simple calculations the expressions:

$$B_E^{(3)} = -D_E^{(3)}(0) \frac{2}{3} \frac{U(0)}{4\pi\sqrt{E}} \frac{1}{(D_E^{(3)}(0)E)^{3/2}},$$

$$B_E^{(2)} = -D_E^{(2)}(0) \frac{U(0)}{4\pi E} \frac{1}{D_E^{(2)}(0)E}, \quad B_E^{(d)} \sim (D_E^{(d)}(0))^{-d/2} (\kappa)^d. \quad (33)$$

It should be noted that, while in the computation of the principal order of the self-energy part and of the static diffusion coefficient in the region of applicability of the perturbation theory the nature of the dependence of the interaction U_{pp} on the momenta was not very important, in the computation of the corrections with the aid of the formula (31) this dependence cannot, generally speaking, be ignored. Thus, if in the equations determining $\operatorname{Im} \Sigma_p$, Φ_p , and l_{1p} we allow, in first order, for the deviation of the momenta from the square root of the particle energy $p = \sqrt{E}$, i.e., if we represent γ_p and γ_{1p} as

$$\gamma_p = \gamma + \gamma'(p - \sqrt{E}), \quad \gamma_{1p} = \gamma_t + \gamma'_t(p - \sqrt{E}), \quad (34)$$

then the values of $B_E^{(d)}$ should be multiplied by the quantity $(1 - D_E^{(d)}(0)/D_E'^{(d)}(0))$, where $D_E'^{(d)}(0)$ is determined by the formula (2) with γ_{tr} replaced by γ'_{tr} .

4. QUASI-UNIDIMENSIONAL DIFFUSION

According to Mott^[2], in a one-dimensional system of scattering centers all the particle states should be localized, and, in view of this, there should be no diffusion. In the present paper we shall not prove this fact in its general form on the basis of the formula (13), but shall discuss only the question of diffusion in a system of point centers under the condition that $E/\gamma \gg 1$. (The question of diffusion in such a system in the purely one-dimensional situation has been investigated by Berezinskiĭ^[8].) In our method of description, the vanishing of the diffusion coefficient is connected with the fact that in the one-dimensional case the cross diagrams for $P(\mathbf{k}, \omega)$ make, in order of magnitude, the same contribution as the diagram without interaction lines (which alone makes the dominant contribution to the coefficient of diffusion by point centers). This occurs on account of two circumstances. The first is that the cross diagrams in the one-dimensional case do not contain small terms that arise as a result of the smallness of the phase volume, a smallness which obtains in three and two dimen-

sions; the second is that, because of the oddness of the vertex in $P(\mathbf{k}, \omega)$ the contributions from the integration domains near $+\sqrt{E}$ and $-\sqrt{E}$ add up and not cancel each other out, as happens in the case of the computation of, say, the imaginary part of the self energy. On the other hand, let us imagine a system infinite in the direction of the z axis and bounded by a barrier in the perpendicular directions. In such a system the energy is quantized in the transverse directions and has an arbitrary value in the direction of the z axis, and for the Green function we obtain:

$$G(E, \epsilon_{nm}, p) = (E - \epsilon_{nm} - p^2 + i\gamma)^{-1}, \quad p = p_z. \quad (35)$$

The two-particle Green function will now be a matrix with components corresponding to the values of the quantized—in the transverse directions—energy. We shall be interested in only the component of this matrix that contains zero transverse energy, since only this component has a singularity at $\omega = 0$. For the computation of the diffusion coefficient from the formula (13), all the integrals over p_x and p_y in (25) should be replaced by sums over ϵ_{nm} , the summation being restricted by the condition $\epsilon_{nm} < E$, since the terms of the sums with $\epsilon_{nm} > E$ strongly cancel each other out after integration over p , and the contribution from them turns out to be $\gamma|E - \epsilon_{nm}|^{-1}$ times smaller than the contribution from the terms with $\epsilon_{nm} < E$; we assume the particle wavelength to be comparable to the dimensions of the system, and therefore we can neglect this contribution.

On the face of it, it seems that the same difficulty encountered in the one-dimensional situation in connection with the cross diagrams obtains here, since only the diagonal terms in these diagrams are important, and it is as if we have the one-dimensional case for each term of the series. This, however, is not the case because the diagonal elements alone are not enough to compensate the smallness resulting from two extraneous interaction lines. In other words, as in two- and three-dimensional spaces, the cross diagrams are small because of the smallness of the phase volume of that region where they themselves are large, the phase volume of that region where they themselves are large, the phase volume being now represented by a number of large terms of the series. If the number of terms with $\epsilon_{nm} < E$ is not large, but greater than one (this is the most interesting case), then it is not possible to obtain a closed expression for the diffusion coefficient. We can only say that it has a normal order of magnitude $D_E^{(1)} \sim E\gamma^{-1}$.

In such a quasi-unidimensional model, all our arguments employed above in the two- and three-dimensional systems about the corrections to the diffusion coefficient that arise as a result of diffusion scattering are valid. It is not difficult to see that this correction is now proportional to $\sqrt{\omega}$:

$$D_E^{(1)} = D_E^{(1)}(0) [1 + iB_E^{(1)} \sqrt{i\omega} + i\omega\tau_{tr}], \quad B_E^{(1)} \sim \frac{V(0)}{E'} - \frac{1}{(ED_E^{(1)}(0))^n}, \quad (36)$$

and, at small ω , considerably exceeds the first regular correction $\sim \omega$. Correspondingly, there arises in the conductivity $\sigma(\omega)$ in a quasi-unidimensional system a term that depends anomalously on the frequency: $\sigma(\omega) = \sigma(0)[1 + \sigma' \sqrt{i\omega} + \dots]$. It is interesting to note that if we construct, in accordance with the diffusion law in a quasi-unidimensional system

$$\langle r^2(t) \rangle_E^{(1)} = 2D_E^{(1)} \left[t - \frac{2B_E^{(1)}}{\sqrt{\pi}} \sqrt{t} + \dots \right] \quad (37)$$

the graph for the root-mean-square distance $R = \langle \mathbf{r}^2(t) \rangle^{1/2}$ traversed by the particle in the process of diffusion (at large t) and joint it to the asymptotic form, it does not go through zero, but cuts off on the ordinate axis an intercept $R_0 = -2B_E^{(1)}\sqrt{D_E^{(T)}}$.

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156