

Quantum-interference component of the electron diffusion coefficient in a gas

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The quantum-interference component of the diffusion coefficient and of the conductivity of electrons in gases is discussed. At room temperature and a pressure of a few atmospheres, this component can reach a relative magnitude of a few tenths of 1%. Interatomic collisions provide an additional mechanism for the phase relaxation of the electron wave function. This mechanism is usually insignificant in a solid.

In this letter we report calculations of the quantum-interference component ΔD of the electron diffusion coefficient D as the electrons are scattered by the atoms of an inert gas. The diffusion coefficient $D = D_0 + \Delta D$ depends on the gas temperature T and the pressure P . It is related to the conductivity by the Einstein relation.

According to the classical theory, D_0 is determined by the mean free path l (or the mean free time τ) of the electrons. Our purpose here is to calculate the quantum component ΔD , which arises from an interference of the state of an electron which has been scattered repeatedly with the time-reversed state. We consider the case $pl \gg \hbar$, where p is a typical value of the momentum of the electron. In this case the relative magnitude of the quantum correction, $|\Delta D|/D_0$, is small.

Quantum corrections of this type were first studied in Refs. 1 and 2 in the case of dirty metals or semiconductors at low temperatures, where most of the scattering of electrons is caused by static defects, and where the electrons themselves obey Fermi statistics. Here we examine the diffusion of nondegenerate electrons in a three-dimensional gas. We assume—this is a particularly important assumption—that the gas temperature is high, and in calculating the correction we allow for the circumstance that the gas atoms can move. The quantum correction can be distinguished experimentally by imposing a magnetic field (Ref. 3 and the literature cited there).

For the relative correction we find the following expression, in complete analogy with Ref. 1:

$$\Delta D/D_0 \simeq - (\hbar/pl)^2 (\tau/\tau_\varphi)^{1/2}, \quad (1)$$

where $p \simeq \sqrt{mT}$ is the momentum of the electron, and τ_φ is the phase relaxation time of the electron wave function,³ which we are to determine.

Our calculation of the quantity in (1) (by a Matsubara diagram technique) can be explained by some graphic physical considerations. The field $U(\mathbf{r}, t)$, produced by the gas atoms that scatter the electrons, depends in a random way on the spatial coordinate \mathbf{r} and varies slowly over time. This variation is slow because the mass of an atom, M , is many times that of an electron, m . Electron paths with self-intersections

are known to be responsible for the quantum correction.^{1,2} For the existence of such a correction, the parameter $\omega\tau$ must be small,¹ where $\hbar\omega$ is the typical change in the energy of an electron, ϵ , in a collision. This change is, quite roughly, $(m/M)^{1/2}\epsilon$.

We denote by t the total time spent by an electron moving along a closed path, while s is the coordinate on this path, which we will write parametrically as a function of the time of motion along the path: $s_1 = s(t_1)$. The difference between the phases as an electron moves in the forward and backward directions is

$$\Delta\varphi = \hbar^{-1} \int_0^t dt_1 [U(s_1, t_1) - U(s_1, t - t_1)]. \quad (2)$$

We will then calculate the expectation value $\langle(\Delta\varphi)^2\rangle$, where the averaging is to be carried out over all realizations of the random field $U(\mathbf{r}, t)$. The time over which the expectation value reaches a value on the order of unity is the time τ_φ in which we are interested.

At each time, $U(s)$ depends on the spatial coordinate s in a random way. Correspondingly, we have $\langle U(s_1, t)U(s_2, t) \rangle \propto \delta(s_1 - s_2)$. Since the coordinate s is parametrized in terms of the time, we set

$$\langle U(s_1, t)U(s_2, t) \rangle = \alpha \delta(t_1 - t_2). \quad (3)$$

The parameter α is determined below on the basis of physical considerations. We note that there is no correlation between the random field and the rate at which it changes: $\langle U(s_1, t)\dot{U}(s_2, t) \rangle = 0$.

In the calculation of $\langle(\Delta\varphi)^2\rangle$ with the help of (2), different-time correlation functions of the type $\langle U(s, t_1)U(s, t_2) \rangle$ arise. The time dependence of this quantity stems from not only the free motion of the atoms but also their collisions, so that the correlation decays. We single out this decay as a special factor:

$$\langle U(s_1, t_1)U(s_2, t_2) \rangle = \langle U(s_1, t_1)U(s_2, t_2) \rangle_0 e^{-\gamma|t_1 - t_2|}, \quad (4)$$

where γ^{-1} is the mean free time of the atoms, and $\langle \rangle_0$ means an average over the free (collisionless) motion of the atoms.

We assume that the random field changes only slightly over the time t . Expanding the field $U(s, t)$ in powers of t in the calculation of $\langle(\Delta)^2\rangle$, and using

$$\langle \ddot{U}(s_1, t)U(s_2, t) \rangle_0 = - \langle \dot{U}(s_1, t)\dot{U}(s_2, t) \rangle_0,$$

we find²⁾

$$\langle(\Delta\varphi)^2\rangle = \frac{1}{3\hbar^2} \alpha \omega^2 \langle U^2 \rangle_0 t^3 + \frac{2\alpha}{\hbar^2} \gamma \langle U^2 \rangle_0 t^2, \quad t > 0. \quad (5)$$

Here we have used the order-of-magnitude relation $\langle \dot{U}^2 \rangle_0 = \omega^2 \langle U^2 \rangle_0$, where ω is the frequency introduced above, associated with the inelasticity of the electron-atom collisions. The quantity $\alpha \langle U^2 \rangle_0 / \hbar^2$ has the dimensionality of a reciprocal time, and by virtue of its derivation it refers to a single collision of an electron. In order of magnitude, it is equal to τ^{-1} . We finally find

$$\langle (\Delta\varphi)^2 \rangle = (t/\tau_\varphi^{(3)})^3 + (t/\tau_\varphi^{(2)})^2; \quad \tau_\varphi^{(3)} \simeq \tau^{1/3} / \omega^{2/3}; \quad \tau_\varphi^{(2)} \simeq \sqrt{\tau/\gamma}, \quad (6)$$

so that the quantity τ_φ in (1) is, in order of magnitude, the shorter of the times $\tau_\varphi^{(3)}$ and $\tau_\varphi^{(2)}$. We thus have two sources of phase relaxation. One is a direct result of the time variation of the random potential; the other results from the decay of the correlation of its fluctuations over time. The last term in (6) arises because as the electron moves along a loop in opposite directions it is scattered by the same atom at different times t_1 and $t - t_1$. If the atoms themselves collide with each other, the states of the system consisting of the electron plus an atom cannot be obtained from each other by time reversal, since there is an overwhelming probability that, if the time difference is sufficiently large, the atom will have a different momentum. A very important point here is that the collisions of the atoms make the system irreversible in time.

Interference effects exist if the following conditions hold: $\tau_\varphi^{(3)} \gg \tau$ (or, equivalently, $\omega\tau \ll 1$) and $\tau_\varphi^{(2)} \gg \tau$, i.e., $\gamma^{-1} \gg \tau$.

The dependence of ΔD on the magnetic field is found from the equations of Ref. 5. The only change we need to make in those equations is to incorporate the existence of the additional phase-relaxation mechanism involving the second term in (6).³⁾

We have made some numerical estimates for the case of Xe at $T = 300$ K and $P = 10$ atm. Here we have $m/M = 4.2 \times 10^{-6}$ and $\omega = (T/\hbar)(m/M)^{1/2} \simeq 10^{-11}$ s. The cross section for the scattering of an electron by the Xe atom at these energies is on the order of 6×10^{-14} cm²; we thus find $\omega\tau \simeq 10^{-2}$, $\tau/\tau_\varphi^{(3)} \simeq 4.5 \times 10^{-2}$, and $\tau \simeq 10^{-13}$ s. The time $\tau_\varphi^{(2)}$ turns out to be on the same order of magnitude as $\tau_\varphi^{(3)}$ if we assume that the cross sections for the scattering of atoms by each other and for scattering of electrons by atoms are comparable in magnitude. In this case we have $|\Delta D|/D_0 \simeq 2 \times 10^{-3}$ and $D_0 \simeq 3$ cm²/s; the critical magnetic field, at which the relative change ΔD is³⁾ on the order of its maximum value, is $H_c \simeq c\hbar/eD_0\tau_\varphi \simeq 3 \times 10^3$ Oe.

An experimental study of quantum corrections would make it possible to obtain important information on both the kinetics of electrons in gases and the kinetic processes in the gases themselves. It would be particularly interesting to raise the pressure and make the transition to the case in which these corrections are appreciable. A study of that case, for which we have no theory at this point, would cast light on kinetic processes in nonideal gases and liquids and on the mechanisms for the electronic conductivity under these conditions and thereby stimulate the development of new physical representations.

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¹⁾A corresponding condition for the interaction of electrons with phonons was given in Ref. 4, where the time $\tau_\varphi^{(3)}$ was also evaluated.

²⁾The existence of a mechanism of relaxation of the nondiagonal part of the density matrix, proportional to t^3 , was first pointed out by Kagan and Kononets.⁷

³⁾This dependence has yet to be observed in solids, since the condition $\omega\tau \gg 1$ has held in all the experiments. Under this condition, the phase relaxation occurs in a single collision, and the $\Delta D(H)$ dependence is different.

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