

Dynamics of a classical electron in a dense medium of disordered scatterers

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The motion of a classical electron in a dense medium of disordered scatterers is studied. The interaction of an electron with a single scatterer is described by a potential with an attractive polarization part and a repulsive short-range part. The electron-velocity autocorrelation functions for different values of the electron energy and of the density of the scatterers are found by a computer-experiment method. The electron conductivity is calculated as a function of the energy. A sharp increase of the electron conductivity is observed in a narrow energy band corresponding to opening of percolation channels.

The behavior of an electron in disordered systems has been studied in many papers. The theory of the electron states in disordered systems explains many electronic properties of strongly-doped semiconductors and amorphous solids and gives a correct description of phenomena occurring during the motion of an electron in substances as widely different, at first sight, as dense helium at cryogenic temperatures and dense plasmas of alkali metals and mercury at low degrees of ionization. By now, the problems of the theory of the density of states in a system of disordered scatterers have acquired a certain appearance of completion. The progress achieved in this field is reflected in the reviews^[1-3]. Whereas for the density of states there are methods of calculation and analytic expressions based on different strong inequalities between the parameters of the system, for properties determined by the dynamics of the electron, e.g., kinetic coefficients, the situation is significantly worse.

A systematic solution of the problem of the conductivity of an electron in a medium of disordered scatterers can be obtained only when the mean free time of the particle is much longer than the collision time. As a rule, this condition is not fulfilled in the above-mentioned systems, and the intuitive ideas of gas-kinetic theory do not work. At high densities of scatterers new qualitative phenomena arise that do not occur in rarefied systems. Belonging to this group are, e.g., the nonmonotonic energy dependence of the mobility, the appearance of percolation at negative electron energies, etc. (The mobility edge is the lowest energy value E_p of a classical particle situated in an arbitrary potential-energy relief $V(r)$ at which it is still possible to find a region of space with $V(r) < E$, going out to infinity in all directions.) To determine even such a comparatively simple characteristic of the motion of an electron in a dense medium as the mobility edge, complicated methods of numerical calculation are used. On the more subtle characteristics of the motion of an electron in disordered systems, such as, e.g., the temporal velocity autocorrelation function, there is practically no information at the present time, in the cases of both the quantum and the classical description of the system. In view of this, in the calculation of kinetic coefficients one has to confine oneself to phenomenological arguments, as, e.g., in^[4].

In the present paper the classical velocity autocorrelation functions of an electron moving in a medium of disordered scatterers are studied by a computer-ex-

periment technique. The energy dependences of the autocorrelation functions, relaxation time and conductivity of the electron are also obtained, for different densities of the scatterers. It is shown that in a dense medium of classical scatterers a sharp increase in the electron conductivity is observed in a narrow energy interval.

1. We shall consider the motion of a classical electron in a medium of disordered scatterers producing a field

$$V = - \sum_{i=1}^N u(\mathbf{r}_e - \mathbf{r}_i), \quad (1)$$

where \mathbf{r}_e is the electron coordinate, \mathbf{r}_i is the coordinate of a scatterer and N is the total number of scatterers. The interaction potential between the electron and a scatterer is prescribed in the form

$$\begin{aligned} u(r) &= 4e \left[\left(\frac{\delta}{r} \right)^6 - \left(\frac{\delta}{r} \right)^4 \right], & r > \delta, \\ u(r) &= \infty, & r \leq \delta. \end{aligned} \quad (2)$$

Inasmuch as (2) is a two-parameter potential, the law of corresponding states is valid for the system being studied.

The model under consideration has direct application to the description of the properties of an electron in a dense weakly-ionized mercury or cesium plasma. Under certain conditions in such a plasma the interaction between an electron and the neutral atoms is dominant^[5,6], and the interaction of the electrons with the ions and amongst themselves can be neglected. The free electrons and the electrons near the mobility edge are classical or else quasi-classical, and move in the field formed by the superposition of the polarization potentials of the neutral atoms interacting with the electrons. The appropriate criteria that enable us to regard the motion of an electron in a plasma as classical have been given by Khrapak and Yakubov^[7]. If we choose the parameters of the potentials in (2) such that $4e\delta^4$ be equal to the polarization constant $\alpha e^2/2$, and the quantity δ is the gas-kinetic radius of the atom, then our model corresponds to the situation in a plasma. We note that the behavior of the interaction potential between an electron and a neutral atom at short distances is not sufficiently well-known. However, it is clear that the principal features of the dynamics of an electron in a dense medium will be the same for a potential in the form (2) as for any other potential having an attractive part $\sim \alpha e^2/2r^4$ and a repulsive short-range part.

The static conductivity of the system under consideration is determined as follows:

$$\sigma_{xx} = ne^2 \beta Z^{-1} \int_{-\infty}^{\infty} e^{-\beta E} \rho(E) \sigma(E) dE, \quad (3)$$

where

$$Z = \int_{-\infty}^{\infty} e^{-\beta E} \rho(E) dE,$$

n is the number of carriers, $\rho(E)$ is the density of states,

$$\sigma(E) = \int_0^{\infty} \varphi_E(t) dt,$$

$\varphi_E(t)$ is the velocity autocorrelation function, defined in the following way:

$$\varphi_E(t) = \langle v_x(0) v_x(t) \rangle_E, \quad (4)$$

v_x is a component of the electron velocity, $\langle \dots \rangle_E$ denotes a microcanonical average, at a fixed total electron energy (the mass of a scatterer is infinite), over its initial momenta and coordinates, averaged over all possible configurations of the scatterers. In the present paper the quantities $\varphi_E(t)$ and $\sigma(E)$ will be calculated.

2. The velocity autocorrelation functions are found by the molecular-dynamics method^[8], into which only slight changes have been introduced. The quasi-classical corrections can be calculated in an analogous manner on the basis of^[9]. We shall briefly describe the scheme of the calculations.

N scatterers are placed in a cube with edge L . Two variants will be considered below. If we assume that the scatterers are not mutually correlated, the centers of the scatterers are assigned in a random manner by means of a random-number generator. In this variant it is possible in principle that the centers of several scatterers coincide. In the second variant the mutual correlation of the scatterers is taken into account, it being assumed that the scatterers interact with each other like hard spheres with radius δ . In the second variant the coordinates of the centers of the scatterers were assigned by the following scheme. First, the coordinates of one scatterer were generated in a random manner. Then the coordinates of the next scatterer were generated, again in a random manner. If the distance between the centers of the two scatterers was found to be less than 2δ , this state was rejected and the coordinates of the second scattering center were generated anew, until the sphere fell in unoccupied space. Then the coordinates of the third scattering center, etc., were found in an analogous manner.

After all the scatterers in the first or second variant had been placed in the cube, an electron with total energy E was placed at an arbitrary, randomly-selected point in the cube. As is usual in the molecular-dynamics method, periodic boundary conditions are imposed, i.e., it is assumed that the cell is surrounded by cells in which the configurations of the scatterers are the same. When the electron has been placed at an arbitrary point in the cell, the potential energy

$$V = \sum_{i=1}^N u(r_i - r_e)$$

is calculated at this point. In the calculation of the potential energy, here and below, one takes into account the interaction of the electron with all the particles situated in a cube of side L whose center coincides with

the location of the electron. Here, if $E < V$, a subsequent selection is performed until the electron falls in the classically accessible region $E - V = mv^2/2$ (we note that when this is done the configuration of the scatterers is also projected anew). The momentum obtained is the initial condition for the solution of the equations of motions of the electron in the cell. If as a result of the motion the electron leaves the cell under consideration through one of the sides, this is equivalent to the entry of an electron, with the same momentum as the one that left, at the corresponding point on the opposite side.

The equations of motion are solved by a numerical scheme analogous to that of^[10] but somewhat complicated by the necessity of taking into account the undifferentiable potential $u(r)$ at $r = \delta$. Since the solution of the dynamical equations gives the classical trajectory of the electron as a function of time, using the ergodic hypothesis we can replace the ensemble average in (4) by a time average, which must then be further averaged over the different configurations of the scatterers:

$$\varphi_E(t) = \lim_{M \rightarrow \infty} \frac{1}{M} \sum_{j=1}^M \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T v_x(t', R_j) v_x(t'+t, R_j) dt', \quad (5)$$

where R_j denotes the j -th configuration formed by the N scatterers in the cell and T is the averaging time along the trajectory of the system. It is clear that if the equations of motion were solved both for the electron and for the heavy particles, a single time-averaging would be sufficient. In this case the quantity T should be greater than the relaxation time of the heavy particles. In view of the fact that the electron relaxation time is incomparably shorter than the relaxation time for the heavy particles, to carry out such a scheme would require enormous expenditure of computer time. It is an entirely obvious approximation to assume that scatterers are immobile compared with the electrons. However, in this case, for negative energies it is possible that the electron will fall in a rarely-encountered random cluster of scatterers from which it cannot escape. In a real system, the motion of the scatterers leads sooner or later to the freeing of the electron from its chance captivity and makes the system ergodic. Therefore, the averaging over the different configurations of the scatterers, which models the motion of the heavy atoms, is necessary. For positive energies, when all regions of space are accessible, the further averaging over the configurations is, in addition, equivalent to increasing the averaging time T by a factor of M , and this is an important factor increasing the accuracy of the calculation^[11].

Most of the values of the quantity $\varphi_E(t)$ were calculated for $N = 200$, $M = 100$. Here we shall not dwell on the questions of the convergence with respect to T , M and N . The methods used in the present paper to check the convergence are practically the same as in^[10]. We note only that for $N = 50$, $M = 50$, the result already hardly differs from that for the case $N = 200$, $M = 100$. The calculations were performed on a BESM-6 computer. Since the interaction potential is a two-parameter potential, the law of corresponding states will be valid for all the quantities in (3); in view of this, the calculations were performed in dimensionless units. The potential depth ϵ was used as the unit of energy. The cube edge L was taken equal to unity. The quantity δ was measured in fractions of L . The dimensionless time $t' = tm^{-1} \delta^{-1} \epsilon^{1/2}$. The electron mass was taken

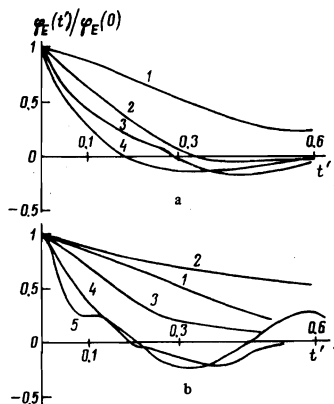


FIG. 1. a) The velocity autocorrelation function of an electron as a function of time for motion in the field of uncorrelated scatterers with density $\delta = 0.05$: curve 1—for $E = 5$; 2—for $E = 0$; 3—for $E = -0.5$; 4—for $E = -1.5$. b) Velocity autocorrelation function of an electron as a function of time for motion in the field of correlated scatterers with density $\delta = 0.04$: 1—for $E = 10$; 2—for $E = 5$; 3—for $E = 0$; 4—for $E = -0.5$; 5—for $E = -1.1$.

equal to unity. It is clear that changing the quantity δ is equivalent to changing the density of the system.

3. Figure 1a shows the behavior, calculated for $\delta = 0.05$, of the quantity $\varphi_E(t')/\varphi_E(0)$ as a function of t' for various E for the case of uncorrelated scatterers. The same quantity in the case of correlated scatterers for $\delta = 0.04$ is plotted in Fig. 1b. At this density the potentials of the scatterers are strongly overlapping. (For $\delta = 0.05$ the average potential equals -1). For high values of E the particle moves in a very dense gas of hard spheres and the attractive part of the overlapping potentials is a perturbation. The densities are such that, even for high energies, the behavior of the autocorrelation function as a function of time differs from the exponential behavior that is characteristic for a rarefied gas. With decreasing energy of the electron a negative minimum—an echo of the oscillatory motion of the electron—appears in the function $\varphi_E(t')$, i.e., the electron is, as it were, localized for a certain time, until it finds an opening in the potential barrier. Here the integral

$$\int_0^{\infty} \varphi_E(t) dt,$$

characterizing the conductivity at a fixed energy is still essentially nonzero. On further decrease of the energy, in the region of large negative energies the electron is localized and

$$\int_0^{\infty} \varphi_E(t) dt = \sigma(E) = 0.$$

This definition of a localized electron coincides with that proposed by Mott^[12].

Localization of electrons at high densities occurs at several scatterers. This fact is best observed by considering Fig. 2. In this figure the behavior of the quantity $\varphi_E(t')/\varphi_E(0)$ is presented as a function of time for the energy $E = -0.5$ for various densities of correlated scatterers. The quantity $t' = t\delta^{-1}\epsilon^{1/2}$ with $\delta = 0.03$ is taken as the unit of measurement of the time. (This is done to make it possible to compare the characteristic times of the oscillations.) At low densities the electron is localized on one scatterer (the classical analog of a negative ion), and the correlator has a clearly pronounced oscillatory character. On increase of the density the characteristic times of the oscillations increase, the electron is localized at several scatterers (if the localization occurred at one scattering center the period would remain constant) and, finally, at $\delta = 0.05$ the quantity $\varphi_E(t')$ is noticeably damped, conduction channels appear, and the electron is not localized. The

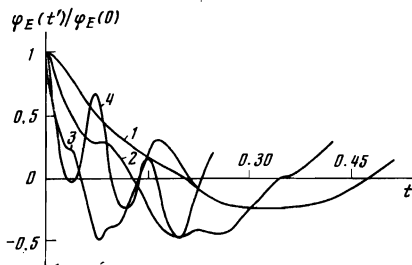


FIG. 2. Velocity autocorrelation function of an electron as a function of time for motion in the field of correlated scatterers for $E = -0.5$ and various density values: curve 1—for $\delta = 0.05$; 2—for $\delta = 0.03$; 3—for $\delta = 0.02$; 4—for $\delta = 0.01$.

possibility of localization at one scatterer is manifested at moderate densities ($\delta = 0.03$, $\delta = 0.02$) in beats with the frequency of the oscillations that characterize the motion at negative energies in the field of one scatterer. At such densities the numbers of configurations for which an electron with negative energy can be localized either by one center or by a cluster of centers are comparable.

We now consider the behavior of

$$\tau(E) = \frac{1}{\varphi_E(0)} \int_0^{\infty} \varphi_E(t) dt.$$

This quantity has the physical meaning of a relaxation time for monotonically decreasing correlators only. Indeed, for oscillating correlators corresponding to localized electrons, the relaxation time is extremely long, whereas

$$\int_0^{\infty} \varphi_E(t) dt = 0.$$

However, inasmuch as an analog of $\tau(E)$ appears in the phenomenological theories, it is meaningful to give its energy dependence. Figure 3 shows the behavior of $\tau(E)$ as a function of E for $\delta = 0.05$ and $\delta = 0.04$ in the cases of correlated and uncorrelated scatterers. The character of the dependence on E is analogous to the phenomenological results of^[4]. We note that the behavior of the quantity $\tau(E)$ at negative energies for uncorrelated scatterers is not the same as that for correlated scatterers. For correlated scatterers $\tau(E)$ increases steeply from a value of zero at $E = E_p$, where E_p is the mobility edge; for uncorrelated scatterers the dependence on E is significantly smoother. The tail of $\tau(E)$ for negative energies E in the case of uncorrelated scatterers extends into the region of larger negative energies. This situation arises because the probability of formation of conduction channels as a result of a density fluctuation is higher in the case of uncorrelated scatterers than for correlated scatterers, and percolation appears at high negative energies.

For high positive energies E the quantity $\tau(E)$ begins to fall, and this is explained by the decrease of the time between collisions on increase of the velocity. The values of $\tau(E)$ at high energies are higher for uncorrelated than for correlated scatterers, since the possibility of superimposing several scatterers at one point effectively decreases the scattering. Naturally, with decreasing density the difference in $\tau(E)$ for correlated and uncorrelated scatterers should decrease, and this can be seen by comparing the figures.

With decrease of E the accuracy of the calculation of $\tau(E)$ and, consequently, of $\sigma(E)$ falls, despite the fact

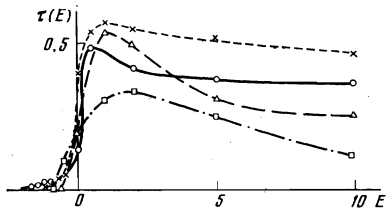


FIG. 3. Conventional relaxation time of an electron as a function of energy: X—uncorrelated scatterers, $\delta = 0.04$; O—uncorrelated scatterers, $\delta = 0.05$; Δ —correlated scatterers, $\delta = 0.04$; \square —correlated scatterers, $\delta = 0.05$.

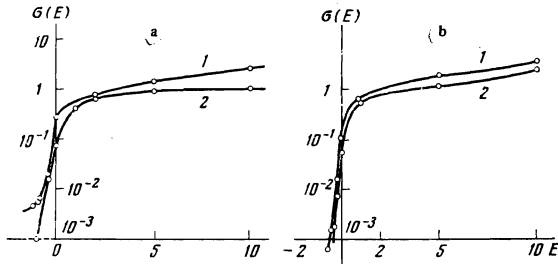


FIG. 4. (a) The dependence $\sigma(E)$ for density $\delta = 0.05$: curve 1—uncorrelated scatterers, 2—correlated scatterers. (b) The dependence $\sigma(E)$ for density $\delta = 0.04$: curve 1—uncorrelated scatterers, 2—correlated scatterers.

that the error in the calculation of $\varphi_E(t)$ is not higher than 5%. The error in the calculation for negative E arises as a consequence of the numerical integration of the oscillating functions, whose behavior at large times we have not calculated, because of the large expenditure of machine time necessary for this. Despite the fact that for $E \sim E_p$ the error in the calculation can be comparable with the quantity $\tau(E)$ itself, the above-mentioned difference in the behavior of $\tau(E)$ for correlated and uncorrelated scatterers can be traced sufficiently clearly. In addition, it is clear that the given method of calculation does not permit us to determine exactly the value of the mobility edge E_p , and, although the fraction of the classically accessible volume Ω_c has been calculated as a function of the electron energy in our work, it has not been possible to establish an exact correspondence between E_p and $\Omega_c(E_p)$.

Of most interest, from our point of view, is the dependence $\sigma(E)$. Figure 4 shows the quantity $\sigma(E)$ for the two density values $\delta = 0.05$ and $\delta = 0.04$ respectively.

For both densities of scatterers, $\sigma(E)$ increases by several orders of magnitude in a narrow range of energies. For lower densities the increase is steeper, since the conduction channels are opened at high energies and the value of E_p for lower densities is shifted to the right. Such a sharp increase in conductivity could also be expected on the basis of the results of model calculations of the quantity $p(E)^{[13]}$, which represents the fraction of conduction electrons in the total number of electrons. After all regions of space have become accessible (except, of course, the regions occupied by hard cores), the conductivity $\sigma(E)$ increases smoothly, like \sqrt{E} approximately.

In conclusion we express our deep gratitude to I. M. Lifshitz for useful discussion of the work.

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