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Effect of Impurity Scattering of a Tunneling Electron on Variable-Range Hopping Conduction

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Variable-range hopping conduction in semiconductors is determined by the asymptotic behavior of impurity wave functions on distances much larger than mean interimpurity separation. Scattering of an impurity electron by the other impurities situated near its tunneling path is shown to result in a correction Δa to electron localization length a. This correction depends on the impurity scattering length and impurity concentration N and may be of the order of $a(Na^3)$ or $a(Na^3)^{1/2}$.

KEY WORDS: Impurity; hopping conduction; tunneling.

In 1979 Lifshitz and Kirpichenkov[1] studied tunnel transparency of films with randomly spaced impurities. Our paper is devoted to application of their ideas to the theory of the hopping conduction.

In the case of variable-range hopping conduction an electron typically hops between two impurities 1 and 2 with close energies, separated in space by a distance much larger than the average interimpurity distance $N^{-1/3}$. The hopping probability depends on the overlap of two wave functions of such impurities $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r})$. Let us assume that for an isolated impurity $\psi(\mathbf{r}) \propto e^{-r/a}$. This wave function may be considered the probability amplitude of the electron tunneling through the barrier of the height which is equal to the ionization energy of the impurity.

We show below that in a light doped semiconductor ($Na^3 \ll 1$) scattering of the tunneling electron by many impurities situated between impurities 1 and 2 results in the correction to the localization length a:

$$a(N) = a + \Delta a = a[1 + C(Na^3)^{\alpha}]$$

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Numerical coefficient C may be positive or negative and the exponent α may be equal 1 or 1/2.

In spite of the fact that the small correction Δa may considerably affect variable-range hopping conductivity it is difficult to find such correction using experimental data on the concentration dependence of variable range hopping. Investigation of the effect of magnetic field on Δa is more promising from the experimental point of view but the theory of magnetoresistance is beyond the scope of this paper.

We consider the wave function of an electron in eigenstate with the energy $\varepsilon < 0$ localized on the impurity 1. Other impurities are supposed to have short-range potentials with the ground state energies randomly distributed in the narrow range $\varepsilon_0 - \Delta$, $\varepsilon_0 + \Delta$ where $\varepsilon_0 < 0$ and $\Delta \ll |\varepsilon - \varepsilon_0| \ll \varepsilon_0$. We assume that there are no electrons on the other impurities, so that we deal with the one-electron problem.

Lifshitz and Kirpichenkov[1] have shown that the wave function of impurity 1 modified by the scattering may be written in the form of the expansion

$$\psi_1(\mathbf{r}) = \psi_1^0(\mathbf{r}) + \sum_i \frac{\mu \psi_i^0(\mathbf{r}_i)}{|\mathbf{r}_i - \mathbf{r}|} \exp\left(-\frac{|\mathbf{r}_i - \mathbf{r}|}{a}\right) + \sum_{ij} \psi_1^0(\mathbf{r}) \frac{\mu^2}{|\mathbf{r}_i - \mathbf{r}_j|} \exp\left(-\frac{|\mathbf{r}_i - \mathbf{r}_j|}{a}\right) \frac{1}{|\mathbf{r}_j - \mathbf{r}|} \times \exp\left(-\frac{|\mathbf{r}_j - \mathbf{r}|}{a}\right) + \cdots \tag{2}$$

where

$$\psi_1^0 = \frac{1}{r(2\pi a)^{1/2}} \exp\left(-\frac{r}{a}\right)$$

is the wave function of the isolated impurity 1, $a = \hbar/(2m|\varepsilon|)^{1/2}$, $\mathbf{r}_i$, $\mathbf{r}_j$ are coordinates of the scatterers and

$$\mu = \frac{a\varepsilon_0}{\varepsilon_0 - \varepsilon} \tag{3}$$

is the scattering length which is supposed to have approximately the same value for all impurities. Each term of the expansion (2) may be described by some path (see Fig. 1). Owing to the negative sign of the energy ε the length of the important path should be as small as possible. That is why backward scattered waves can be neglected.

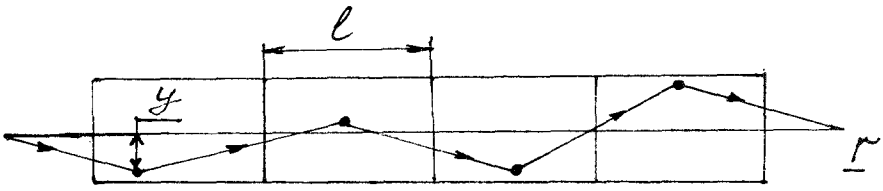

Fig. 1. Tunneling path with four points of scattering.

It is clear that the wave function $\psi_1(\mathbf{r})$ depends on the random distribution of impurities in space around the vector $\mathbf{r}$. In this sense $\psi_1(\mathbf{r})$ is a random variable. The averaging procedure depends on the physical problem under the study.[2,3] Lifshitz and Kirpichenkov[1] studied tunnel transparency of a film with the thickness d. In this case a plane wave of energy ε falls on a barrier with impurities and the tunnel transparency is proportional to

$$\langle |\psi(d)|^2 \rangle = \exp\left(-\frac{2d}{a+\Delta a_f}\right) \tag{4}$$

where the correction Δa_f describes the effect of impurity scattering, $\langle ... \rangle$ means the averaging over the impurity coordinates.

In the theory of hopping conduction the magnitude

$$\langle \ln |\psi|^2 \rangle \equiv \frac{2r}{a+\Delta a} \tag{5}$$

is of interest which is two times the typical value of the exponent of wave function $\psi(\mathbf{r})$.[2,3] Here we consider just this value. In principle the correction Δa_f may exceed Δa owing to chains of densely packed impurities which penetrate (rarely) through the film and determine its tunnel transparency. On the other hand, if relative fluctuations of wave function are small the correction Δa_f is equal Δa.

Lifshitz and Kirpichenkov (see Section 4 of Ref. 1) we have shown that the relative fluctuations of ψ are determined by the parameter $B = (N\mu^2 a)^{1/2}$. At $B \ll 1$ fluctuations of $\psi(r)$ are small and the result obtained by Lifshitz and Kirpichenkov for Δa_f is valid for Δa:

$$\Delta a = \Delta a_f = \mu N a^3 \tag{6}$$

At $B \gg 1$ relative fluctuations of ψ are large. According to the Ref. 1 in this case Δa_f is not small and $\Delta a_f \simeq a$. We show below that at $B \gg 1$ the correction Δa has the form

$$\Delta a \simeq a(Na^3)^{1/2} \ln^{3/2} B \tag{7}$$

and is much smaller than Δa_f. At $B \simeq 1$ Eqs. (6) and (7) give the same result. Below we refer to the case $B \gg 1$ as the fluctuation regime and to the case $B \ll 1$ as the homogeneous regime. It is seen from the Eq. (6) that in the homogeneous regime the correction Δa has the sign of $\varepsilon_0 - \varepsilon$ and is proportional to the impurity concentration. Therefore it may be considered a result of the shift of the bottom of a conduction band or of a correction to an effective mass. On the other hand, in the fluctuation regime Δa is independent of the sign of $(\varepsilon_0 - \varepsilon)$.

We begin with the derivation of the Eq. (6) at $\mu > 0$. The following derivation of the Eq. (6) is less rigorous than the original one of the Ref. 1 but it is just in the same level of arguments as the following derivation of the Eq. (7) which we cannot do more rigorously.

Let us consider the contribution to the wave function from one term in the expansion (2) which corresponds to n scatterings (Fig. 1). We have stressed above that for negative energies scattering is mainly in the forward direction. So a typical distance between two scattering points along the direction of $\mathbf{r}$ is equal to $l = r/n$. Let y be a typical deviation of a scattering point in the direction perpendicular to the vector $\mathbf{r}$ (see Fig. 1). Then the contribution of one path from the point 1 to the point $\mathbf{r}$ by the order of value is equal to

$$\frac{\mu^n}{l^n} \exp\left(-\frac{r}{a} - n\frac{y^2}{la}\right) \tag{8}$$

where y^2/l is the increase of the distance between two scatterings due to the transverse deviation of the path. The total number of such paths may be estimated as $(Ny^2l)^n$, where Ny^2l is the number of impurities in the cylinder of the height l and the base surface y^2 which we refer to as the cylinder of scattering. Then for the contribution of all the paths with n scatterings one obtains

$$(Ny^2\mu)^n \exp\left(-\frac{r}{a} - n\frac{y^2}{la}\right) = \exp\left[-\frac{r}{a} + f(n, y)\right] \tag{9}$$

where

$$f(n, y) = n \ln(Ny^2\mu) - \frac{n^2y^2}{ra} \tag{10}$$

The next step is to sum contributions (9)over all n. To this end we estimate values of n and y which provide the maximum value of $f(n, y)$:

$$n_{\max} \simeq N\mu ra, \qquad y_{\max} = \frac{1}{(\mu N)^{1/2}} \tag{11}$$

Substituting Eq. (11) into Eq. (10) we obtain Eq. (6). Evidently, Eq. (6) is valid if there are many impurities in the typical cylinder of scattering, i.e., $Ny^2l \gg 1$. Using Eq. (11) we see that this inequality is identical to the inequality $B \ll 1$.

Now we consider the opposite case $B \gg 1$. In this case there are no impurities in the typical cylinder with parameters of Eq. (11). It means that the typical wave function cannot be determine by paths with such parameters. Typical paths should have one impurity in the cylinder of scattering. It gives

$$Ny^2l \simeq 1 \tag{12}$$

Using Eq. (12) for the contribution of one path to $\psi(r)$ we obtain from Eq. (8)

$$\left(\frac{n\mu}{r}\right)^n \exp\left(-\frac{r}{a} - \frac{n^3}{Nr^2a}\right) = \exp\left[-\frac{r}{a} + \varphi(n)\right] \tag{13}$$

where

$$\varphi(n) = -\frac{n^3}{Nr^2a} + n \ln\left(\frac{n\mu}{r}\right) \tag{14}$$

The function $\varphi(n)$ is maximal at

$$n = n_{\max} \simeq \frac{r}{a}(Na^3)^{1/2} \ln^{1/2} B \tag{15}$$

Substituting Eq. (15) into Eqs. (14) and (13) we obtain Eq. (7). In this derivation only one typical path was taken into account. The total number of such paths may be roughly estimated as Z^n, where Z is a number of neighboring cylinders of scattering which is of the order of several units. It is seen easily that inclusion of the factor Z^n into Eq. (13) does not change the main term of the correction Δa given by Eq. (7).

Thus far we have considered the case $\mu > 0$. If $\mu < 0$ in the homogeneous regime $B \ll 1$ the correction Δa changes the sign owing to the cancellation of terms for different n and Eq. (6) is valid. In the fluctuation regime this cancellation results in an exponentially small factor which, however, does not change the main term of Eq. (7).

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