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Effect of partial ordering of a two-dimensional system of scatterers on the anisotropy of its kinetic coefficients

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The effect of partial ordering of impurities (correlated along one direction and uncorrelated along the other) on the kinetic coefficients is considered. It is shown that the geometry of the spatial impurity distribution by itself has no effect on the diffusion coefficient or conductivity for scattering by a spherically symmetric potential, and these coefficients remain the same as for an uncorrelated system of impurities.
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The way that scattering by randomly located impurities and impurities that randomly occupy sites in a periodic lattice affect conductivity is now well understood. However, the δ-doped layers that can now be grown on vicinal surfaces of semiconductors constitute a class of structures that differ from those considered previously, since they exhibit partial ordering of the scattering centers.[1] At the surface there is a periodic structure of monoatomic steps, and during doping impurities are deposited primarily on these steps, forming a system of parallel chains. Along such a chain the positions of impurities may be treated as completely uncorrelated. In this case, the chains themselves form a periodic lattice, whose period depends on the angle of misorientation of the surface relative to the principal crystal plane. In its geometry this system differs from any studied previously. Experimental studies show[2] that such layers have anisotropic electronic properties. In this paper we discuss how the geometry of the system of scatterers affects the anisotropy of the kinetic coefficients.

Consider the scattering of an electron localized in a δ-layer and freely moving only in the plane of the layer. In this case, we can write the collision integral in the Boltzmann equation, which determines the correction f_1 to the equilibrium distribution function f_0, in the form

$$I_{st}(\mathbf{k})=\int\frac{d^2\mathbf{k}'}{2\pi}W(\mathbf{k},\mathbf{k}')[f_1(\mathbf{k}')-f_1(\mathbf{k})]\delta(\varepsilon_k-\varepsilon_{k'}),\tag{1}$$

where $W(\mathbf{k},\mathbf{k}')\delta(\varepsilon_k-\varepsilon_{k'})$ is the probability for the electron to make a transition from state $\mathbf{k}$ to state $\mathbf{k}'$ as a result of elastic scattering. We are interested only in changes in the distribution function associated with spatial correlations in the impurity positions, and ignore the electron density near an impurity, which, in general, is needed to calculate kinetic coefficients. If we assume that the electron wave function in the plane of the layer is a plane wave, the probability $W(\mathbf{k},\mathbf{k}')$ can be written in the form

$$W(\mathbf{q})=\frac{2\pi}{\hbar}\left|\int dxdydz\,e^{iq_xx}e^{iq_yy}V(\mathbf{r})\varphi^2(z)\right|^2,\quad \mathbf{q}=\mathbf{k}-\mathbf{k}',$$

where $\varphi(z)$ is the quantum-well wave function along the direction z, and

$$V(\mathbf{r})=\sum_j^N v(\mathbf{r}-\mathbf{R}_j)$$

is the impurity potential (where $\mathbf{R}_j$ is the coordinate of the jth impurity). It is easy to show[3] that

$$W(\mathbf{q})=\frac{2\pi}{\hbar}|v(\mathbf{q})|^2S(\mathbf{q}),$$

where $v(\mathbf{q})$ is the Fourier transform of the effective two-dimensional impurity potential, which for a Coulomb potential is

$$v(q)=\frac{2\pi e^2}{\varepsilon q}\int\exp(-q|z|)\varphi^2(z)dz,$$

while $S(\mathbf{q})$, the so-called structure factor

$$S(\mathbf{q})=\left|\sum_j^N e^{i\mathbf{q}\mathbf{R}_j}\right|^2,\tag{2}$$

which contains all the information about the system geometry. Assuming that the positions of the impurities are entirely uncorrelated along a chain (the x direction), and that the chains themselves are positioned on a periodic lattice (the y direction), we obtain for the structure factor averaged over impurity positions

$$\langle S(\mathbf{q})\rangle=N\left[1+\frac{(2\pi)^2}{a}\nu\delta(q_x)\sum_n\delta\left(q_y-\frac{2\pi}{a}n\right)\right],\tag{3}$$

where N is the total number of impurities in the entire plane, and ν is the average number of impurities per unit length of chain. The quantity $\langle S(\mathbf{q})\rangle$ differs from the structure factor for completely uncorrelated impurities only at $q_x=0$. Qualitatively, this behavior of $S(\mathbf{q})$ is connected with the fact that for $q_x\neq 0$ the average number of impurities at the plane-wave front is constant, and only for $q_x\neq 0$ will oscillations begin in the averaged number of impurities at this front.

Equation (3) has a symbolic meaning to a certain extent, since when we substitute it into Eq. (1), we obtain the product of three δ-functions, which after integration formally gives the indeterminate expression $\delta(0)$. In order to assign a meaning to such an expression, we must recall that it was obtained from the sum (2), in which the total number of impurities N is assumed to be a large but finite number. Then

$$2\pi\nu\delta(0)=\overline{N_x^2}-\overline{N_x}, \tag{4}$$

where $\overline{N_x}$ is the average number of impurities on one chain.

Substituting expression (3) into Eq. (1), we obtain

$$\begin{aligned}I_{st}=N\int\frac{d^2k'}{2\pi}|v(\mathbf{k}-\mathbf{k}')|^2(f_1(\mathbf{k}')-f_1(\mathbf{k}))\,\delta(k-k')\,\frac{m}{k'}\\+\frac{2\pi\nu}{a}\delta(k_x-k_x')\sum_{n=-\infty}^{\infty}\delta\left(k_y-k_y'-\frac{2\pi}{a}n\right)|v(\mathbf{k}-\mathbf{k}')|^2\\\times(f_1(\mathbf{k}')-f_1(\mathbf{k}))\,\delta(k-k')\,\frac{m}{k'}.\end{aligned} \tag{5}$$

The first term on the right side of Eq. (5) corresponds to the collision integral for uncorrelated impurities, and the entire contribution from spatial correlations is contained in the second (singular) term.

Next, we will discuss scattering by a potential with circular symmetry, i.e., $v(\mathbf{k})=v(k)$. Then the correction to the distribution function is conveniently cast in the form of a sum:

$$f_1(k,\varphi)=f_1^+(k,\varphi)+f_1^-(k,\varphi),$$

where

$$f_1^+(k,\varphi)=f_1^+(k,-\varphi),$$

and

$$f_1^-(k,\varphi)=-f_1^-(k,-\varphi).$$

After substituting the quantities f_1^+ and f_1^- into Eq. (5) and integrating, the expression for the collision integral takes the form

$$\begin{aligned}I_{st}=N\int\frac{d\varphi'}{2\pi}|v(k,\varphi-\varphi')|^2(f_1^+(k,\varphi')+f_1^-(k,\varphi')\\-f_1^+(k,\varphi)-f_1^-(k,\varphi))+\frac{|v(2k|\sin\varphi|)|^2}{k|\sin\varphi|}\\\times 2f_1^-(k,\varphi)\sum_{n=1}^{\infty}\delta\left(2k|\sin\varphi|-\frac{2\pi}{a}n\right).\end{aligned} \tag{6}$$

If the field-dependent part of the Boltzmann equation is an even function of angle (for example, proportional to $\cos\varphi$, as happens when we calculate the conductivity in a uniform electric field), then the equations for f_1^+ and f_1^- separate. This can be seen, e.g., if we replace φ by $-\varphi$ in the Boltzmann equation, and then add and subtract the resulting equations. As a result, we find that the function f_1^+ satisfies the Boltzmann equation without the singular term in the collision integral, and that f_1^- satisfies the homogeneous equation:

$$\begin{aligned}\int\frac{d\varphi'}{2\pi}|v(k,\varphi-\varphi')|^2(f_1^-(k',\varphi')-f_1^-(k,\varphi))\\+\frac{|v(2k|\sin\varphi|)|^2}{k|\sin\varphi|}2f_1^-(k,\varphi)\sum_{n=1}^{\infty}\delta\left(2k|\sin\varphi|-\frac{2\pi}{a}n\right)=0.\end{aligned} \tag{7}$$

We emphasize that this separation of the equations for f_1^+ and f_1^- is directly related to the fact that the equation $v(k,\varphi)=v(k,-\varphi)$ is valid for the potential. Since f_1 is the correction for the distribution function caused by external perturbation, while Eq. (7) does not contain the perturbation, we must assume that $f_1^-\equiv 0$.

Thus, in calculating the conductivity or diffusion coefficient for any spherically symmetric potential, the contribution from the singular part of the collision integral equals zero and correlated positions of impurities in itself has no effect on these coefficients.

From these considerations, it does not follow, of course, that the kinetic coefficients in this system are the same as coefficients in the uncorrelated system. For an exact calculation, let us say, of the conductivity, it is necessary to take into account the nonuniform distribution density of the electrons, which immediately leads to anisotropy of the kinetic coefficients.

We note that the probability of scattering, as we should expect, contains the singular part. If we calculate the residence time for elastic scattering in this system of impurities

$$\tau^{-1}(\mathbf{k})=\frac{2\pi}{\hbar}\int\frac{d^3\mathbf{q}}{(2\pi)^3}|V(\mathbf{q})|^2\delta[E(\mathbf{k})-E(\mathbf{k}-\mathbf{q})],$$

as was done in Ref. 4 for a three-dimensional periodic lattice with randomly occupied sites, then according to Eq. (3) we obtain

$$\frac{1}{\tau(\mathbf{k})}=\frac{1}{\tau_r(\mathbf{k})}+\frac{1}{\tau_c(\mathbf{k})}.$$

The quantity τ_r is determined by scattering by randomly located impurities, while τ_c is determined by scattering at ‘‘Bragg’’ angles by the correlated chains:

$$\frac{1}{\tau_c}=\frac{N}{a\hbar}\sum_{n\neq 0,\frac{2\pi}{a}n\in[k_y-|k|,k_y+|k|]}\frac{m}{|k_x|}v\left(0,\frac{2\pi}{a}n\right)2\pi\nu\delta(0). \tag{8}$$

Expression (8) implies that for $k_y=(2\pi/a)n$ there is additional scattering that is enhanced by a factor of $(\overline{N_x^2}-\overline{N_x})/N_x$ compared to the incoherent scattering. In this sense, the situation is analogous to scattering by a crystal lattice: although an external beam (plane wave) gives rise to Bragg peaks [an analog to Eq. (8)], for an electron in the crystal with momentum much smaller than the size of the Brillouin zone the scattering by the lattice is not important at all, since the electronic states at the boundary of the Brillouin zone from which the scattering takes place are unoccupied due to the relatively small concentration of carriers in these states.

Thus, the geometry of impurity positions on δ-doped vicinal surfaces in itself has no effect on kinetic coefficients. Partial ordering in such a system can manifest itself in scattering of an external beam of particles (for example, in surface electron holography).

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