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Spatial Variation of Currents and Fields Due to Localized Scatterers in Metallic Conduction

Abstract: Localized scatterers can be expected to give rise to spatial variations in the electric field and in the current distribution. The transport equation allowing for spatial variations is solved by first considering the homogeneous transport equation which omits electric fields. The homogeneous solution gives the purely diffusive motion of current carriers and involves large space charges. The electric field is then found, and approximate space charge neutrality is restored, by adding a particular solution of the transport equation in which the electric field is associated only with space charge but not with a current. The presence of point scatterers leads to a dipole field about each scatterer. The spatial average of a number of these dipole fields is the same as that obtained by the usual approach which does not explicitly consider the spatial variation. Infinite plane obstacles with a reflection coefficient r are also considered. These produce a resistance proportional to $r/(1-r)$.

1. Introduction

In the solution of the transport equation in modern treatments of the electrical conductivity process, it is customary to assume that the distribution of electrons in momentum space is the same throughout the specimen (or at best has only a macroscopic variation due to temperature gradients, et cetera). Coupled with this is an assumption that the applied field is uniform. The applied field then produces a motion of the electronic distribution in momentum space. Scattering by lattice waves and obstacles tends to restore the original distribution, and equilibrium is established between the scattering and the accelerating field. The current density is then computed by taking a sum over the states of the undisturbed crystal and weighting the current associated with each state by its probability of occupation. This process ignores the off-diagonal elements of the current matrix. These off-diagonal elements do not contribute to the space average of the current density, but they can represent local fluctuations in the current distribution. The current due to each of the diagonal terms has the periodicity of the crystal. The spatial uniformity of current can, therefore, be regarded as a consequence of the assumed field uniformity and of the neglect of the off-diagonal matrix elements.

We wish to point out that the uniformity of the field and current density are assumptions which may frequently be well justified, but whose validity in general is not apparent. If the intensity of scattering is not uniformly distributed over the material, but is concentrated in well localized scattering centers, as is the case in the residual resistivity caused by impurities at low temperatures, then it seems in fact reasonable that the field should be concentrated near the points where the scattering is actually produced, so as to enable the current to pass around these obstacles. We shall, therefore, in this paper solve the transport equations in two simple cases without neglecting the relevant spatial variations. We shall consider the case of highly localized point scatterers and also the case of scattering by specular reflection at planes of infinite extension.

Despite the fact that the ordinary viewpoint neglects spatial variations it will, in most cases, lead to a correct answer. The quantities which have spatial variations may be characterized by suitably defined average values, which then can be used in the usual formalism. Some care must be exercised in this averaging process. If the averaging is carried out in too naive a manner, incorrect results can be obtained, as will be shown in the case of plane obstacles treated in Section 8.

In constructing our solution we do not wish to assume a uniform field and initially do not know the correct field distribution. It will, instead, be assumed that at the boundaries of the specimen the number of electrons which are moving into the interior of the specimen are so controlled as to maintain the proper current flow in and out of the

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material. If there were no scattering in the specimen, the current carriers could move unhampered, and the maintenance of the current at the surfaces of the specimen would not produce a field. An obstacle in the path of the current will result in a pile-up of electrons on one side of the obstacles and a deficit on the other side. This dipole moment will grow until the resultant electric field enables the incident current to pass the obstacle at the same rate at which further charges arrive. It is a superposition of many such dipole fields which will then constitute the electric field associated with the current flow, and it is the space average of these dipole fields which enter into a conductivity measurement.

In the usual discussions of the residual resistivity of metals, the conductivity is evaluated with the aid of the electron acceleration law, $d\mathbf{k}/dt = -e\mathbf{E}/\hbar$. Since the electric field is spatially inhomogeneous and highly concentrated about positions where the periodicity of the lattice potential is disturbed, the use of this relation is questionable. The transport equation, as used in the subsequent discussion, will naturally involve a term closely related to the electron acceleration law. It will be seen, however, that the term can be modified at positions close to the scatterers without affecting our evaluation of the conductivity.

2. General form of treatment

All the complications due to the real crystalline nature of the medium will be neglected in this treatment, and we will assume that our medium is isotropic. Its crystalline nature will be acknowledged only through the fact that the density of states in energy, dn/dU, at the spherical Fermi surface, and the wave number k_0 associated with this Fermi surface, will be taken as independent quantities. Except for the use of Fermi statistics our considerations will be classical, and we shall assume that at each point in space there is a well-defined distribution of electrons in $\mathbf{k}$ space. ($\mathbf{k}$ is the wave vector which determines the wave-function variation in going from cell to cell.) In the presence of a current, the number of electrons per unit volume moving within a solid angle $d\Omega$ about the direction $\boldsymbol{\Omega}$ (a unit vector) will differ from the number that moves in that direction in the undisturbed metal by an amount $N(\boldsymbol{\Omega})d\Omega$. We shall restrict ourselves to sufficiently low temperatures so that the distribution changes represented by $N(\boldsymbol{\Omega})$ are contained in a sufficiently narrow energy range to give all the $N(\boldsymbol{\Omega})$ extra (or deficit) electrons the same velocity and scattering cross sections. The transport equation for the steady state can then be written in the form

$$\partial N(\boldsymbol{\Omega}, r)/\partial t = 0 = -\alpha\boldsymbol{\Omega}\cdot\mathbf{E} - \nabla N\cdot\mathbf{v} + (\partial N/\partial t)_S. \tag{2.1}$$

In this equation the first term on the right-hand side represents the acceleration by the field. In terms of the electronic charge e and the Fermi-surface wave number k_0, we have $\alpha = ek_0^2/4\pi^3\hbar$. The second right-hand term represents spatial gradients, and $\mathbf{v} = \hbar^{-1}\boldsymbol{\Omega}\, dU/dk$. The last term represents the effect of the scatterers which cause the resistance.

Eq. (2.1), considered as an equation for N, is a linear inhomogeneous equation. Such equations can be solved by taking a particular solution and then adding to it solutions of the homogeneous equation to satisfy the boundary conditions. We shall use this procedure and shall use a particularly simple solution of Eq. (2.1) for the particular solution. Eq. (2.1) always has a solution in which the electric field produces spatial variations in electronic density but does not cause a current. This is a solution in which $N(\boldsymbol{\Omega}, \mathbf{r})$ is independent of $\boldsymbol{\Omega}$. In that case, we can expect the term $(\partial N/\partial t)_S$ to vanish. Using $\mathbf{E} = -\nabla V$, we then find for Eq. (2.1) the form

$$\alpha\boldsymbol{\Omega}\cdot\nabla V = v\boldsymbol{\Omega}\cdot\nabla N, \tag{2.2}$$

which has the solution

$$N(\mathbf{r}) = \frac{\alpha}{v}V(\mathbf{r}) + c = \frac{1}{4\pi}\frac{dn}{dU}eV(\mathbf{r}) + c, \tag{2.3}$$

where c is independent of $\mathbf{r}$, and dn/dU is the density of states at the Fermi surface.

The boundary conditions which determine the current entering and leaving the specimen must then be satisfied by a solution of the homogeneous transport equation. The homogeneous equation represents the motion of particles subject only to scattering and therefore gives the purely diffusive motion of the carriers.

3. Neutrality condition

Let $N_D(\boldsymbol{\Omega}, \mathbf{r})$ represent the solution to the homogeneous equation. Let $N_V(\boldsymbol{\Omega}, \mathbf{r})$ be the particular solution as given by Eq. (2.3). N_D will be determined by the boundary conditions and the diffusive motion. To determine N_V and V, we have to use Poisson's equation in addition to Eq. (2.1). This states

$$\nabla^2 V = 4\pi e\int(N_D + N_V)d\boldsymbol{\Omega}. \tag{3.1}$$

Now let

$$n_D = \int N_D d\boldsymbol{\Omega} \quad \text{and} \quad n_V = \int N_V d\boldsymbol{\Omega}. \tag{3.2}$$

If in (2.3) we choose the origin of the potential such that $N(\mathbf{r}) = 0$ where $V(\mathbf{r}) = 0$, it becomes

$$n_V(\mathbf{r}) = \frac{dn}{dU}eV(\mathbf{r}). \tag{3.3}$$

Combining (3.3), (3.2), and (3.1), we find

$$n_V - l^2\nabla^2 n_V = n_D, \tag{3.4}$$

with $1/l^2 = 4\pi e^2 dn/dU$. The distance l is the range to which the electronic screening in this medium permits electric fields to penetrate. In a typical good conductor, if we are concerned with variations existing over a distance of several atomic cells, then we can neglect the term $l^2\nabla^2 n_V$ in Eq. (3.4) and find

$$n_V = -n_D, \tag{3.5}$$

$$(dn/dU)eV = -n_D. \tag{3.6}$$

4. Point scatterer

We shall now analyze in detail the case of a point scatterer embedded in a spatially uniform background scattering. This is immediately suggestive of an impurity embedded in

a material which is scattering thermally. As we shall see later, however, other interpretations are possible.

Before entering into the details of our argument we would like to clear up one frequent misconception concerned with the relative importance of the physical dimensions, e.g., the radius a of a point scatterer and its quantum mechanical scattering cross section σ. We will assume that both a and $\sqrt{\sigma}$ are small compared to the mean free path. The localized obstacle will disturb the otherwise uniform current flow. If we are at a distance several times a from the center of the obstacle, then the disturbances set up there by the obstacle will depend only on the number of electrons that have had their direction changed by the obstacle—i. e., on the differential cross section of the obstacle. The physical size of the obstacle and the potential variation within its physical extension are primarily relevant to an evaluation of the disturbances in the volume of the obstacle itself. These will not concern us, except for some auxiliary discussions.

In solving the problem of the point scatterer, we shall use Eq. (2.1) in the form

$$-\alpha\boldsymbol{\Omega}\cdot\mathbf{E}-\boldsymbol{\nabla}N\cdot\mathbf{v}+(\partial N/\partial t)_B=0, \tag{4.1}$$

where $(\partial N/\partial t)_B$ denotes the background scattering. Eq. (4.1) is then satisfied everywhere except at the obstacle which is taken to be at $\mathbf{r}=0$. We shall satisfy the scattering conditions at $\mathbf{r}=0$ by superposing two solutions of Eq. (4.1). One solution represents the motion of the electrons without the obstacle, and the other represents the corrections due to the changed motion of the carriers after their incidence on the obstacle.

We shall restrict the nature of the scattering, both for the obstacle and for $(\partial N/\partial t)_B$. In both cases the probability of scattering will be taken as a function only of the angle through which the electron is deflected, and not as a function of the incident direction. In that case[1], the usual theory of conductivity which neglects spatial variations permits the background scattering to be characterized by a single conductivity relaxation time τ_B, and also permits the medium which has only a distribution of obstacles to be characterized by a single conductivity relaxation time τ_O. Furthermore, in that case the combined effects of both types of scattering can also be described by a single relaxation time in accordance with Matthiessen's rule.[2]

It is to be particularly noted that the assumption of differential scattering cross sections which are functions only of the angle through which the particle is scattered, leads to a simple timewise exponential relaxation for the disturbance produced by an electric field. For these same scattering cross sections, there will be many other possible disturbances from equilibrium which do not show a relaxation characterized by a single time constant.

In the ensuing discussion we shall use the symbol $\mathbf{i}$ to denote a current measured in numbers of electrons crossing a unit area in unit time. The electrical current $\mathbf{j}$ will then be given by $\mathbf{j}=-e\mathbf{i}$. We shall take the particular situation in which $\mathbf{i}$ far away from the obstacle has only a z component denoted by i_∞. If $v=\hbar^{-1}dU/dk$ is the velocity at the Fermi surface far away from the obstacle, we will have

$$N(\boldsymbol{\Omega})=3i_\infty\cos\theta/4\pi v, \tag{4.2}$$

where θ is the angle between $\boldsymbol{\Omega}$ and the z-axis. This current is accompanied by a field which can be determined from Eq. (4.1). Omitting the second term in Eq. (4.1) gives

$$E_z=-3i_\infty/4\pi v\alpha\tau_B, \tag{4.3}$$

which corresponds to a conductivity

$$\sigma_B=-\frac{ei_\infty}{E_z}=\frac{e^2k_0^2}{3\pi^2\hbar^2}\frac{dU}{dk}\tau_B. \tag{4.4}$$

If $N(\boldsymbol{\Omega})$ and $E(\mathbf{r})$, as given by Eqs. (4.2) and (4.3), are presumed to hold for all $\mathbf{r}$, then Eq. (4.1) is satisfied everywhere. The effect of the localized obstacle will in that case be ignored. Let us assume that the obstacle has a differential scattering cross section, $f^2(\theta)d\Omega$, for scattering through the angle θ into a range $d\Omega$ of solid angle. If Eq. (4.2) is correct in describing the number of electrons incident on the obstacle, then the rate at which electrons are scattered by the obstacle into an angular range $d\Omega$ about the direction $\boldsymbol{\Omega}_f$ is, through the use of (4.2),

$$d\Omega\int f^2(\boldsymbol{\Omega}_f,\boldsymbol{\Omega}_i)N(\boldsymbol{\Omega}_i)vd\boldsymbol{\Omega}_i=d\Omega\frac{3i_\infty}{4\pi}\int f^2(\boldsymbol{\Omega}_f,\boldsymbol{\Omega}_i)\cos\theta_i d\boldsymbol{\Omega}_i. \tag{4.5}$$

In Eq. (4.5), $f^2(\boldsymbol{\Omega}_f\boldsymbol{\Omega}_i,)$ denotes $f^2(\theta)$ where θ is the angle between the incident direction $\boldsymbol{\Omega}_i$ and the scattered direction $\boldsymbol{\Omega}_f$. θ_i denotes the angle between the direction of incidence and the z-axis. θ_f will similarly locate the scattered direction relative to the z-axis. With a little spherical trigonometry, the right-hand side of Eq. (4.5) can be put into the form

$$d\Omega\frac{3i_\infty}{4\pi}\cos\theta_f\int f^2(\theta)\cos\theta\, d\boldsymbol{\Omega}, \tag{4.6}$$

where the integral is now independent of $\boldsymbol{\Omega}_f$. Expression (4.6) gives the rate at which electrons are scattered into $\boldsymbol{\Omega}_f$, but it has not had subtracted from it the rate at which electrons which were originally moving within a range $d\Omega$ of the direction $\boldsymbol{\Omega}_f$ are scattered out of this range. The latter rate will be

$$d\Omega N(\boldsymbol{\Omega}_f)v\int f^2(\theta)d\boldsymbol{\Omega}=d\Omega\frac{3i_\infty}{4\pi}\cos\theta_f\int f^2(\theta)d\boldsymbol{\Omega}. \tag{4.7}$$

Subtracting the right hand side of Eq. (4.7) from (4.6), we find that the number of electrons per second leaving the obstacle in the range $d\Omega$ exceeds the number specified in Eq. (4.2) by

$$-d\Omega\frac{3i_\infty}{4\pi}(\cos\theta_f)\int f^2(\theta)(1-\cos\theta)d\boldsymbol{\Omega}. \tag{4.8}$$

The integral in (4.8), in which deflections are weighted by the factor $(1-\cos\theta)$, is the scattering cross section found relevant in the usual theory of conductivity and we will label it S_O. Then (4.8) can be written

$$-d\Omega\frac{3i_\infty}{4\pi}(\cos\theta_f)S_O. \tag{4.9}$$

We shall now construct a solution of Eq. (4.1) which has

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as its source electrons issuing from the obstacle as specified by (4.9). Furthermore, we shall require that the solution $N_S(\Omega,\mathbf{r})$ generated by this source vanish at infinity. The superposition, then, of N_S on the spatially uniform solution given by Eq. (4.2) and (4.3) satisfies both Eq. (4.1) and the scattering conditions imposed by the obstacle. This is actually not quite correct. The solution N_S contains electrons which can, after some scattering by the background, return again to the obstacle at $\mathbf{r}=0$. Since N_S is a strict solution of Eq. (4.1), it does not take into account scattering by the obstacle when the electron returns to the obstacle a second (or later) time. If, however, the mean free path determined by the background is large compared to the effective dimensions of the scatterer (i. e., the square root of its scattering cross section), the probability of multiple scatterings by the obstacle will be small, and we will therefore restrict our further considerations to this case.

We shall deal with the scattered solution $N_S(\Omega,\mathbf{r})$ by first treating the purely diffusive motion, thus finding $N_{SD}(\Omega,\mathbf{r})$, and then using Eq. (3.6) to find the accompanying field.

5. Diffusive motion about point scatterer

The diffusive motion about a point scatterer is schematized in Fig. 1. Line A shows a direction in which the number of incident carriers exceeds the equilibrium number. Similarly, line B shows a direction in which fewer than the equilibrium number are moving. A and B represent the spatially uniform solution (4.2) which gives the number of electrons incident on the obstacle. Line C shows a direction along which there is an excess of scattered electrons. Along line D there is a deficit. After a number of scatterings by the background the electrons which initially move away from the obstacle along C and D will have their velocity completely randomized. Their motion will then obey the diffusion equation. This diffusion current is schematically indicated by the broad arcs, which finally show the recombination of the electron excess and deficit.

Consider first the diffusion current generated by all the electrons which start their motion away from the scattering center in directions that lie within $d\Omega_f$ of the direction Ω_f. Far away from $\mathbf{r}=0$ at a position in space denoted by (r, ω), where r is the distance from the scattering center and ω is a unit vector pointing from the scatterer to the point involved, the diffusion current will establish a concentration $C(\Omega_f,\omega,r)d\Omega_f$ of electrons, all of which were originally travelling away from $\mathbf{r}=0$ in the direction Ω_f. This concentration obeys the steady state diffusion equation $\nabla^2 C=0$. Up to terms of order $1/r^2$ this has the solution

$$C(\Omega_f,\omega, r)=a/r+\mathbf{p}\cdot\omega/r^2, \tag{5.1}$$

with a and $\mathbf{p}$ arbitrary. The radial current density (in electrons/cm²sec) far from the origin due to the a/r term is $d\Omega_f D_B a/r^2$ where D_B is the diffusion coefficient of electrons in the presence of the background scattering. The integrated flow out of a large sphere is then $4\pi D_B a d\Omega_f$ electrons /sec. The other term $\mathbf{p}\cdot\omega/r^2$ does not contribute to the integrated flow. Equating $4\pi D_B a d\Omega_f$ to (4.9) gives

$$a(\Omega_f)=-\frac{3i_\infty(\cos\theta_f)S_O}{(4\pi)^2 D_B}. \tag{5.2}$$

To terms of order $1/r^2$, the right-hand side of Eq. (5.1) has the form $a/|\mathbf{r}-\mathbf{r}_f|$ with $\mathbf{r}_f=\mathbf{p}/a$. The term $\mathbf{p}\cdot\omega/r^2$ simply serves to displace the effective source away from the origin in the direction of $\mathbf{p}$. The average position of the particles described by Eq. (5.1) is therefore $\mathbf{r}_f=\mathbf{p}/a$. The average position of the particles can also be found by following a beam of particles issuing from $\mathbf{r}=0$ at $t=0$, and initially proceeding along Ω_f. The average position then is:

$$\mathbf{r}_f=\left\langle\int_0^\infty \mathbf{v}dt\right\rangle_{Av}=\int_0^\infty\langle\mathbf{v}\rangle_{Av}dt. \tag{5.3}$$

$\langle\mathbf{v}\rangle_{Av}$ as used in Eq. (5.3) is an average over electrons which initially left $\mathbf{r}=0$ in the direction Ω_f. $\langle\mathbf{v}\rangle_{Av}$ is therefore a function of Ω_f, but for the sake of typographical compactness this will not be explicitly indicated. $\langle\mathbf{v}\rangle_{Av}$ decays with time because of background scattering. The decay is generally not a simple exponential, since the initial velocity distribution, a collimated beam, is not the distribution involved in the usual definition of a relaxation time for the conductivity process. Since $\mathbf{p}=\mathbf{r}_f a$, combining (5.2) and (5.3) gives

$$\mathbf{p}=-\frac{3i_\infty(\cos\theta_f)S_O}{(4\pi)^2 D_B}\int_0^\infty\langle\mathbf{v}\rangle_{Av}dt. \tag{5.4}$$

To find the total concentration of diffused carriers we have to integrate (5.1) over all values of Ω_f. The integration over the a/r terms gives a vanishing result since the total number of carriers emitted at $\mathbf{r}=0$, according to (4.9), is zero. This leaves

$$n_D(\omega, r)=\int d\Omega_f C(\Omega_f, \omega, r)=\int d\Omega_f\mathbf{p}\cdot\omega/r^2$$

$$=-\frac{3i_\infty S_O}{(4\pi)^2 D_B}\frac{1}{r^2}\omega\cdot\int d\Omega_f(\cos\theta_f)\int_0^\infty\langle\mathbf{v}\rangle_{Av}dt. \tag{5.5}$$

After exchange of integrations this becomes

$$n_D(\omega, r)=-\frac{3i_\infty S_O}{(4\pi)^2 D_B}\frac{1}{r^2}\omega\cdot\int_0^\infty dt\int d\Omega_f(\cos\theta_f)\langle\mathbf{v}\rangle_{Av}. \tag{5.6}$$

The values of $\langle\mathbf{v}\rangle_{Av}$ which result from the electrons initially proceeding along Ω_f are now weighted with the factor $\cos\theta_f$. Therefore, Eq. (5.6) represents a timewise integration over a velocity distribution which is initially similar to the distribution produced by an electric field. Hence we can expect $\int d\Omega_f(\cos\theta_f)\langle\mathbf{v}\rangle_{Av}$ to decay as exp $(-t/\tau_B)$, where τ_B is the conductivity relaxation time for the background scattering. At $t=0$ we have an initial value

$$d\Omega_f\langle\mathbf{v}\rangle_{Av}\cos\theta_f=\int d\Omega_f\frac{1}{\hbar}\frac{dU}{dk}\Omega_f\cos\theta_f=\frac{4\pi}{3\hbar}\frac{dU}{dk}\mathbf{z}_1, \tag{5.7}$$

with $\mathbf{z}_1$ representing the unit vector in the z-direction. Combining (5.5) with (5.7) gives

$$n_D(\omega,r)=-\frac{i_\infty S_O}{4\pi D_B}\frac{1}{\hbar}\frac{dU}{dk}\frac{1}{r^2}\omega\cdot\mathbf{z}_1\int_0^\infty dte^{-t/\tau_B}$$

$$=-\frac{i_\infty\tau_B}{4\pi D_B}S_O\frac{1}{\hbar}\frac{dU}{dk}\frac{\cos\theta_\omega}{r^2}. \tag{5.8}$$

θ_ω is the angle between ω and the positive z-axis.

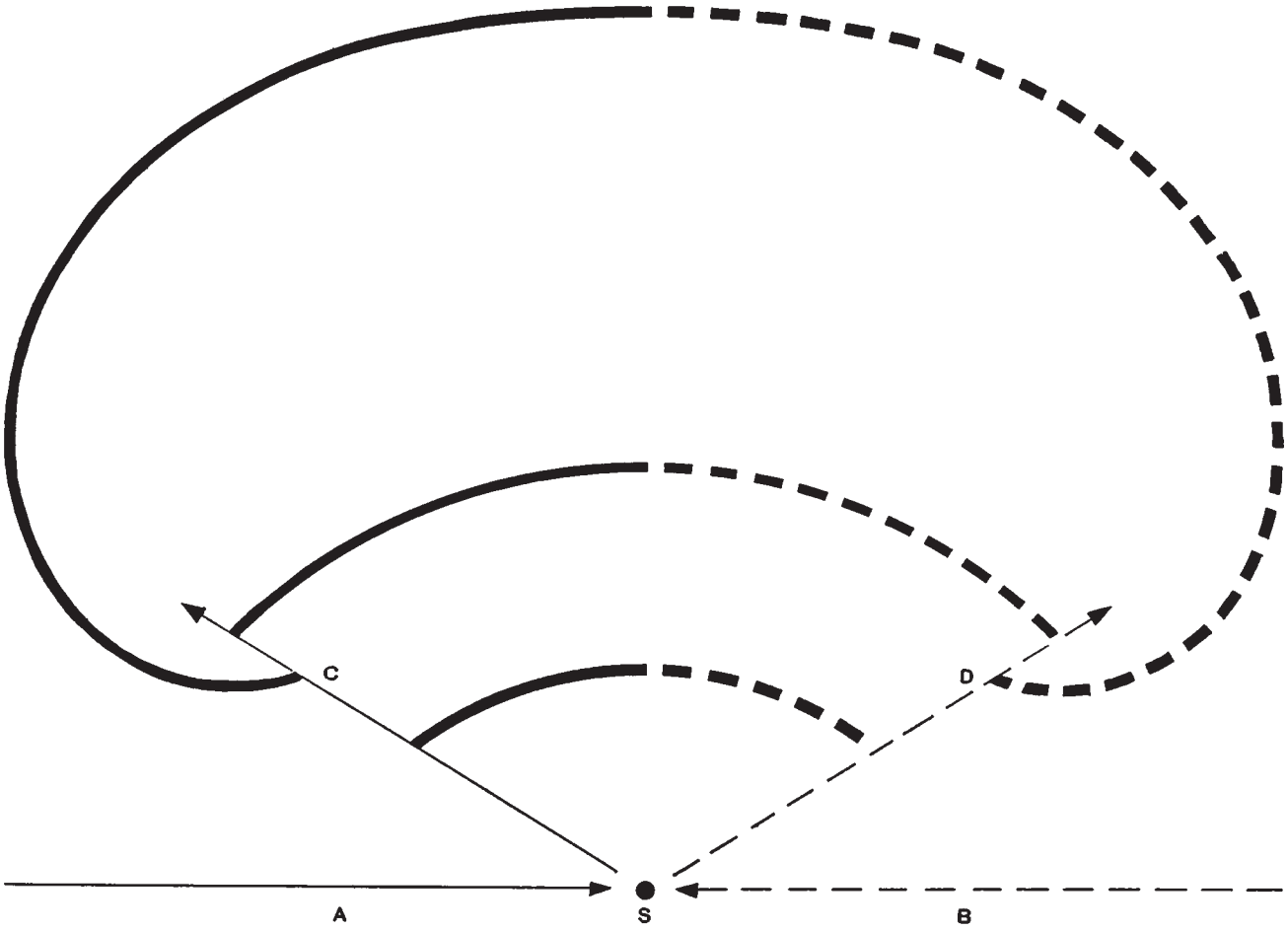

Figure 1 **Schematic representation of current flow disturbed by the scatterer** S.
Electrons in excess numbers are incident along A, then are scattered to C, then scattered by the background. The number of electrons incident along B is less than the equilibrium number. The deficit is scattered to D, then scattered by the background. The excess and deficit diffuse together and recombine along the arcs.

The diffusion coefficient D_B, as determined by the background scattering, and the conductivity σ_B, determined by the same scattering, are not independent. By considering the balance between diffusion currents and conductivity currents, in an equilibrium situation, we arrive at the "Einstein" relation for completely degenerate Fermi statistics in the same way as for semiconductors.[3] The resulting relation is

$$De^2 dn/dU = \sigma. \tag{5.9}$$

For our isotropic band structure and isotropic background scattering the conductivity in (5.9) is given by

$$\sigma_B = \frac{\tau_B}{3\pi^2}\frac{e^2}{\hbar^2}k^2\frac{dU}{dk}. \tag{5.10}$$

Hence we find

$$D_B = \frac{\tau_B}{3\pi^2}\frac{k^2}{\hbar^2}\frac{dU}{dk}\left(\frac{dn}{dU}\right)^{-1}. \tag{5.11}$$

This value for D_B can be introduced into Eq. (5.8) to give

$$n_D(\omega, r) = -\frac{3\pi i_\infty S_O \hbar}{4k^2}\frac{dn}{dU}\frac{\cos\theta_\omega}{r^2}. \tag{5.12}$$

Eq. (3.6) permits us to go from the above to the potential distribution

$$V = -\frac{n_D}{e}\left(\frac{dn}{dU}\right)^{-1} = \frac{3\pi i_\infty S_O \hbar}{4k^2 e}\frac{\cos\theta_\omega}{r^2}. \tag{5.13}$$

Eq. (5.1) which we used in the derivation of (5.12) and (5.13) is only an asymptotic expansion, and therefore we cannot on the basis of the above derivation expect (5.13) to be valid close to the scatterer. Consider the electrons close to the scatterer as specified by (4.9) and before they have been appreciably scattered by the background. The density $n_D(\omega, r)$ due to these electrons is easily evaluated and leads again to the expression (5.12). Since (5.12) is correct when we are much closer to the scatterer than a

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mean free path, and also when we are many mean free path lengths away from the scatterer, and since furthermore it is easily shown from (4.9) that $n_D(\omega, r)$ must vary as $\cos\theta_\omega$, for all values of r, we can expect that $n_D(\omega, r)$ is closely approximated by (5.12) for all r values. In computing an average field or conductivity, however, it is only the asymptotic behavior of (5.13) that matters, and this has been accurately justified.

Eq. (5.13) gives a potential associated with a dipole of moment

$$p = 3\pi i_\infty S_O \hbar / 4k^2 e. \tag{5.14}$$

If we have a density of $\mathfrak{N}$ obstacles per unit volume which are sufficiently far apart to be non-interacting, there will be a polarization $\mathfrak{N}\mathbf{p}$, and the space average of the dipole fields will be

$$E_z = -4\pi P_z = -3\pi^2 i_\infty S_O \hbar \mathfrak{N} / k^2 e. \tag{5.15}$$

The mean free time τ_O as used in the usual conductivity theory, and associated only with scattering by the obstacle is given by

$$\tau_O = 1/\mathfrak{N} S_O v. \tag{5.16}$$

This makes the space average field, as given in (5.15), equal to

$$E_z = -3\pi^2 i_\infty \hbar / k^2 e v \tau_O. \tag{5.17}$$

In terms of the electric current $j_\infty = -ei_\infty$, we find

$$E_z = \frac{3\pi^2\hbar^2}{k^2 e^2 \tau_O}\left(\frac{dU}{dk}\right)^{-1} j_\infty, \tag{5.18}$$

which is exactly the field associated with the obstacles, as found by the usual approach [e. g., compare with Eq. (5.10) which gives the connection between σ and τ resulting from the usual considerations]. The field given by (5.18) exists in addition to the background field of Eq. (4.3). Matthiessen's rule is satisfied; (5.18) does not depend on τ_B.

We would like to stress the extreme extent to which these dipole fields are really localized. To do this we must consider how the charges that are responsible for the dipole moment given by (5.14) are actually distributed. Let us assume for the moment that the charge density, in the (spherical) volume of the scatterer is of the form $\rho(r)\cos\theta_\omega$ and vanishes outside the scatterer. In computing an average field for the whole specimen we must evaluate $\int \mathbf{E} d\tau$, where the $\mathbf{E}$ includes the contributions of the particular dipole moment under discussion. Under the conditions specified above, 2/3 of this dipole contribution to $\int \mathbf{E} d\tau$ comes from the volume of the scatterer. Actually, of course, the dipole charges cannot be as well localized as we have assumed. [The screening length l of Eq. (3.4) is finite, the uncertainty principle also prevents an excessively localized charge. Furthermore, Eq. (5.12) is derived from a point model and cannot be expected to hold true up to the actual surface of the scatterer.] Therefore, only perhaps 1/3, instead of 2/3, of the voltage drop associated with the residual resistance is contained in the volume occupied by the impurity atoms.

Since such a large portion of the field is located where the crystalline potential has been disturbed, the use of the usual electron acceleration equation, $d\mathbf{k}/dt = -e\mathbf{E}/\hbar$, becomes questionable. Note that in our arguments the field is found as a result of screening considerations. The exact nature of the screening close to the impurity atom, is not relevant to the evaluation of an average field. That is, the nature of the first term in Eq. (2.1) can be modified, close to the impurity atoms, without appreciably affecting our asymptotic evaluation of the dipole potential. It is only necessary that (dn/dU), in Eq. (3.6) represent the actual density of states, in the dilute alloy, rather than the density in the pure solvent.

6. Interaction of obstacles

The preceding section has been concerned with a localized obstacle of cross section S_O embedded in a medium with a relaxation time τ_B. This is obviously applicable to the case of a single obstacle in a medium which otherwise has only thermal scattering. If we consider a medium which has a density of obstacles such that the obstacle scattering is comparable to the uniform scattering or larger, then we must invoke some supplemental considerations. First of all, the radial current scattered by a particular obstacle, as given by Eq. (4.9), will now be subject to scattering by other obstacles as well as by the uniform background. Let us confine our considerations to the most common case, that in which the mean free path (as determined by the combined scattering) is large compared to the distance between obstacles. Only a small portion of the radial current will then be scattered by any one obstacle and the radial current will therefore see a relaxation time τ_B which depends on both kinds of scattering. Therefore, as the density of obstacles is increased, the effective value of τ_B changes. The value of τ_B, however, does not affect the dipole field brought in with each additional obstacle. As the number of obstacles is increased, therefore, the space average of the electric field changes just as it does in the usual theory.

We have assumed in the preceding section that the electron velocity distribution incident upon the obstacle is equal to the average velocity distribution which exists far away from the obstacle. A localized scatterer disturbs the velocity distribution. Close to the obstacle there are the scattered radial currents as given by Eq. (4.9). Further away there are the diffusion currents. Both of these kinds of currents constitute deviations from the average velocity distribution. A second obstacle placed near the first will be exposed to the deviations caused by the first obstacle. An obstacle, however, will generally see the deviations caused by many obstacles, not just those caused by one. If we add the disturbances due to the many obstacles randomly placed within the vicinity of a given one, then we are doing the same thing as adding the disturbances due to a particular obstacle over many points in its environment, as long as the obstacles are uncorrelated in their positions. The mere fact that the obstacles are finite in extension will give them some correlation. Let us temporarily neglect this. It is easily shown that if we consider the deviations caused by a *single* obstacle, in a *particular* velocity class,

these deviations vanish after integration over all space. Hence, an obstacle which is exposed to the deviations caused by many other obstacles is exposed to the average velocity distribution.

The argument which has just been given relies on an integration which in turn strictly requires a point scatterer, as we have assumed. Let us take a more realistic view and give the scatterer an extension in space. Then the scatterers exclude (or diminish) the current within a small volume, and the average value of the current density at locations which are outside of the excluded regions is larger than the average taken over *all* space. It is this larger current density which an additional scatterer, placed among the previously existing ones, will see. In principle, therefore, one should apply corrections to find the correct "internal" velocity distribution in a manner similar to the use of Lorentz corrections in dielectric theory. If the volume occupied by the scatterers is small, as in a dilute solution, this is presumably a small effect. If the scatterers occupy an appreciable fraction of the volume, these corrections will very likely be overshadowed by the direct effect of the scatterers on the electronic structure of the medium. In the extreme case where the *complete* volume of the metal is occupied by the scatterers, as in the case of high temperature scattering by independently vibrating atoms, then again the incident velocity distribution must be the average velocity distribution.

7. Degree of localization required

The argument we have used in arriving at our dipole field relies upon the localization of the scatterer. Since the quantities entering into the transport equation vary on a scale comparable to the mean free path (associated with the background), it is only necessary that the scatterer be small compared to the mean free path. This condition will generally be satisfied for impurity scattering.

Actually, the localization of the background scattering is as relevant as that of the obstacle scattering. The use of Eq. (4.1) implies that the scattering depends only on the disturbance $N_D(\Omega, r)$ at the point $\mathbf{r}$ under consideration. Therefore, the obstacle and the background must be "localized" to the same extent. Scattering of electrons by phonons is generally sufficiently localized, since a wave packet of the representative thermally excited phonons is usually short compared to the electronic mean free path. The only apparent exception is the case of electron scattering by phonons at extremely low temperatures in an alloy where the scattering is almost completely determined by the lattice defects. At a sufficiently low temperature, the typical phonon wavelength will then exceed the mean free path. In this case, however, the phonon scattering will be an extremely small portion of the total scattering. Furthermore, this is a case in which any other theory would presumably have difficulties in correctly evaluating the contribution of the phonon scattering.

It might be thought that the spatial variations discussed here must disappear at very low temperatures since the small energy range of the order kT over which the probability of occupation varies from 1 to 0, does not permit the construction of very localized wave packets. This is, however, not relevant. One can, in principle, form stationary states which represent the multiple scattering of electrons by many obstacles, and thus find the probability of directional changes at various points in space. Such a solution specifies the scattered intensity as a function of direction of scattering within a few wavelengths of the scattering center. The relevant dynamic parameters for our theory are thus obtainable from solutions of the time-independent wave equation for a particular energy. (At least this is true for the cases where the time-wise variation of the lattice vibrations is not significant.)

The condition that one can construct highly localized wave packets, small compared to the mean free path, is the condition $\hbar/\tau < kT$, given by Peierls[4] long ago for the validity of the Bloch theory. This criterion was introduced as a consequence of the use of time-dependent perturbation theory and is a criterion only of the validity of time-dependent perturbation theory. If the probability of scattering is known correctly from some other treatment, this criterion has no relevance.

8. Reflecting walls

When there is a current impinging on a reflecting wall one can expect a voltage drop confined to the immediate vicinity of the reflecting plane. This is, in fact, taken for granted in the treatment of the contact resistance at the junction of two metallic conductors.[5] We have in mind a situation in which the current flow is perpendicular to the wall, and assume that the reflection is specular. A density of $\mathfrak{N}$ such planes per cm will be assumed without any additional source of electron scattering. These walls can be considered to be models of grain boundaries or of stacking faults. The reflection coefficient r will be assumed to be a function of the angle, θ, between the wall normal and the direction of incidence. We shall take the wall normal to be in the positive z-direction and θ to be the angle with this direction so that $r(\theta) = r(\pi - \theta)$, and shall first compute the conductivity according to the usual non-local viewpoint.

An electron travelling in a direction at an angle θ with the z-axis will pass $\mathfrak{N}|\cos\theta|$ walls per cm of its travel, and will therefore be incident upon $\mathfrak{N}|\cos\theta|v$ walls per second, where v is the velocity at the Fermi surface. At each of these collisions only a fraction $r(\theta)$ of the electrons are reflected. If there are n_+ electrons per unit volume moving in a certain direction, and n_- electrons in the reflected direction, we can expect that

$$dn_+/dt = -n_+\mathfrak{N}|\cos\theta|r(\theta)|v + n_-\mathfrak{N}|\cos\theta|r(\theta)|v, \tag{8.1}$$

$$dn_-/dt = -n_-\mathfrak{N}|\cos\theta|r(\theta)|v + n_+\mathfrak{N}|\cos\theta|r(\theta)|v. \tag{8.2}$$

If n_0 is the number of electrons travelling in the two directions concerned, in the absence of a current, then symmetry requires

$$n_+ - n_0 = n_0 - n_-. \tag{8.3}$$

If (8.3) is substituted in (8.2) and (8.1), we find

$$\frac{d}{dt}(n_+ - n_0) = -(n_+ - n_0)2\mathfrak{N}|\cos\theta|r(\theta)|v, \tag{8.4}$$

$$\frac{d}{dt}(n_- - n_0) = -(n_- - n_0)2\mathfrak{N}|\cos\theta|r(\theta)|v, \tag{8.5}$$

and therefore a relaxation time $\tau(\theta) = v/2\mathfrak{N}|\cos\theta|r(\theta)$. The usual conductivity theory then gives us a conductivity

$$\sigma = \frac{e^2k^2}{8\pi^3\mathfrak{N}\hbar}\int d\Omega|\cos\theta|r(\theta), \tag{8.6}$$

where the integration is over all directions of motion. Note that this value for the conductivity cannot be exact. As $r(\theta)$ is permitted to approach unity for all θ, all current flow must cease, yet Eq. (8.6) still yields a finite conductivity. This finite conductivity results from a finite relaxation time. The latter, in turn, is a result of the assumption of a uniform field. If the accelerating electric field is taken to be uniform, and the current flow is generated equally at all points in space, then it will take a finite time for portions of this current to reach the nearest reflecting barrier, and this is the relaxation time which can be obtained from (8.4) and (8.5), even if $r = 1$.

Instead of the treatment leading to Eq. (8.6), we can handle the problem by the methods we have already described. This requires that we have an expression for the distribution of electrons incident upon the wall. For any incident velocity distribution we can calculate a scattered current and a compensating charge. In general, however, these will be such that a second plane, parallel to the first, would be exposed to a different incident velocity distribution. We must therefore choose an incident velocity distribution such that the final resultant velocity distribution is the same on both sides of the plane at distances which are more than a screening length away from the plane. This leads, with a little calculation, to a velocity distribution (including incident electrons, reflected electrons, and compensating charge), of the form

$$N(\Omega,\mathbf{r}) = \beta\left(\frac{1-r(\theta)}{r(\theta)}\right)\frac{\cos\theta}{|\cos\theta|}, \tag{8.7}$$

where β is independent of θ. The conductivity resulting from the detailed localized treatment is

$$\sigma = \frac{e^2k^2}{8\pi^3\mathfrak{N}\hbar}\int d\Omega|\cos\theta|\frac{1-r(\theta)}{r(\theta)}. \tag{8.8}$$

This differs from (8.6) through the appearance in the integrand of the factor $(1-r(\theta))$. This factor serves to make the conductivity vanish as $r(\theta)$ approaches unity for all θ. The difference between (8.6) and (8.8) is therefore only important if the reflection probability is comparable to unity. In this connection it is interesting to note that some of the calculations for the reflection coefficient of stacking faults predict values for r which are not very small compared to unity.[6]

Note that the velocity distribution (8.7) does not vary with θ as $\cos\theta$. Therefore, there is no single relaxation time for the whole conduction process. If reflecting walls exist simultaneously with thermal scattering, Matthiessen's rule will not be satisfied. Even without thermal scattering, if we have a number of such walls with differing orientations, the scattering probabilities cannot just be added, since each orientation by itself would result in a different shape for the velocity distribution.

9. Multiple reflections by a single obstacle

In the treatment of point obstacles in Sections 4 and 5 we ignored the possibility of repeated reflections by the same localized obstacle, and found that the field associated with the point obstacles was linear in the scattering cross section S_O. In the treatment of plane reflectors in Section 8, our method did not ignore the multiple reflections and the resultant field was not linear in r, but varied as $r/(1-r)$. We shall here give a very rough argument to show that a more careful treatment of the point scatterer, taking into account the possibility of repeated reflection by the same obstacle, also leads to a resistivity which is non-linear in the scattering cross section S_O.

Consider the scattered current as given by Eq. (4.9). The z-component of the scattered current (measured in carriers per sec) is obtained by multiplying (4.9) by $\cos\theta_f$ and integrating over $d\Omega$. The resulting current has only a z-component given by $I_z = -S_O i_\infty$. This scattered current consists of electrons moving away from the obstacle in a radial direction for a distance of about λ, where λ is the mean free path determined by the background scattering. After moving through this distance λ, the electrons have their velocity randomized and follow a diffusive motion. After this randomization a fraction of them will be scattered again by the original obstacle. This fraction is roughly $S_O/4\pi\lambda^2$.

The total current incident on the obstacle at any one time is due to electrons which are incident for the first time and also due to electrons which have previously been scattered by the obstacle one or more times. The scattered current, integrated over all directions, is therefore of the form

$$\begin{aligned} i_z &= S_O i_\infty(1 + S_O/4\pi\lambda^2 + (S_O/4\pi\lambda^2)^2 + \ldots) \\ &= S_O i_\infty/(1 - S_O/4\pi\lambda^2). \end{aligned} \tag{9.1}$$

The diffusion charges, N_D, and the resulting potential will then vary with S_O as $S_O/(1-S_O/4\pi\lambda^2)$. This is comparable to the factor $r/(1-r)$ in the case of plane reflectors. It seems plausible, then, that in situations in which the mean free path is large enough so that multiple scatterings are negligible, we can expect the resistivity to vary linearly with scattering cross sections and can expect the usual formalism to be applicable. Thus, for example, in the case of highly localized, well separated cylindrical obstacles, we would expect that most of the carriers which are incident upon a given obstacle will be scattered only once by it, and that therefore the usual relations between resistance and scattering cross section are valid.

10. Conclusions

A detailed solution of the transport equation has shown that spatially localized scatterers produce spatially localized electric fields in the presence of current flow. In the case of point scatterers, these localized fields are dipole fields, one for each scatterer. The resistivity calculated on this basis

is the same as that given by the more usual calculations. The resistivity calculation has, however, been put on a more secure footing since the discussion that has been presented does not rely as intimately as the usual theory upon the only for uniform fields in strictly periodic crystals. In the case of a reflecting plane, the resistivity calculated from the localized fields is higher than that calculated from the usual equations, but the difference is significant only if the reflection coefficient is comparable to unity.

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