Effective Medium Theory for the Hall Effect in Disordered Materials*

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We present a classical effective-medium theory for the magnetoconductivity tensor in disordered materials which undergo a metal-nonmetal transition via a microscopically inhomogeneous transport regime.

The microscopic inhomogeneities[1] always present in disordered materials are a major source of difficulty in dealing with their transport properties. The inhomogeneities are associated with fluctuations[2-4] in, e.g., bonding configurations,[2] composition,[3] or local density,[4] which are independent of one another when separated by more than twice a correlation radius. The condition of the material is approximately constant within the correlation radius, i.e., within the fluctuation. These inhomogeneities give rise to potential fluctuations, which in turn can give rise to microscopic inhomogeneities in the electronic structure: randomly distributed localized states and extended states confined largely to semiclassical percolation[1,5-9] channels for energies near the mobility edges.[10,11] In the cases of interest to us, the phase coherence length is shorter than the amplitude coherence length for the relevant extended states.[12-14] The latter is essentially the correlation radius of the condition of the material. Thus, one can make a semiclassical approximation treating the system as having randomly distributed, locally uniform configurations and calculating the local properties semiclassically.[1,5-9] This approach has been carried out successfully by Eggarter and Cohen[6] for the calculation of the mobility of electrons in gaseous He. Cohen and Sak[8] have developed a theory of the metal-semiconductor transition in binary-alloy systems based on the same ideas.

Once one has made the semiclassical approximation, the transport problem becomes equivalent to that of conduction in a macroscopically inhomogeneous medium. There is a substantial body of theory for such media,[15-17] and Kirkpatrick[9,18] has pointed out its relevance to the present problems. The simplest and perhaps the most useful such theory is the effective-medium theory of Bruggeman[15] and Landauer.[16]

The problems we are dealing with, which arise near mobility edges during the course of metal-semiconductor transitions, relate to random systems in which a volume fraction C has a conductivity σ_0 and the remainder a conductivity σ_1 substantially less than σ_0. The results of the effective-medium theory for the conductivity σ of the material can then be expressed as[9,16]

$$\sigma = f\sigma_0, \tag{1}$$

$$f = a + [a^2 + \tfrac{1}{2}x]^{1/2}, \tag{2}$$

$$a = \tfrac{1}{2}[(\tfrac{3}{2}C - \tfrac{1}{2})(1-x) + \tfrac{1}{2}x], \tag{3}$$

$$x = \sigma_1/\sigma_0. \tag{4}$$

Equations (1)–(4) are not sufficient by themselves to establish that the material is microscopically inhomogeneous. Knight-shift data can be used[19] to establish values of C. Lacking these, thermodynamic data can be used[4] instead to estimate C. Even and Jortner[20] have shown that correlations among the conductivity, Hall constant, and Hall mobility are particularly helpful in drawing inferences about transport regimes. An effective-medium theory has not been constructed[21a] for the full magnetoconductivity tensor. Herring[21b] considered the somewhat different case of weak, continuous variations in the electrical properties. The closest available is the work by Juretschke, Landauer, and Swanson,[17] which gives both Hall effect and conductivity in several porous media ($\sigma_1 = 0$) in which the pores are sufficiently far apart to be nonoverlapping. This latter constraint restricts the validity of their results to first order in $\epsilon = 1 - C$. They find

$$R = R_0 \frac{1-\epsilon/4}{1-\epsilon}, \quad \sigma = \sigma_0 \frac{1-\epsilon}{1+\epsilon/2}. \tag{5}$$

Their result for σ does agree with the effective-medium result [Eqs. (1)–(4)] only to first order in ϵ.

In the present paper, we report the required effective-medium theory of the magnetoconductivity tensor. In any portion of the material there is a probability C that the magnetoconductivity tensor be $\overleftrightarrow{\sigma}_0(\vec{H})$, and a probability $1-C$ that it be $\overleftrightarrow{\sigma}_1(\vec{H})$. Excise a spherical portion of the material [of conductivity $\overleftrightarrow{\sigma}_I(\vec{H}) = \overleftrightarrow{\sigma}_0(\vec{H})$ or $\overleftrightarrow{\sigma}_1(\vec{H})$] and replace the material outside that portion by a uniform isotropic effective medium with magnetoconductivity tensor $\sigma(\vec{H})$. Asymptotically far from the excised portion, the field returns to the medium value $\vec{E}_m$. The electrostatic problem involved is exactly analogous to that of a dielectric sphere in a uniform field. Just as in that case, the field inside the sphere, $\vec{E}_I$, is constant and related to the asymptotic field $\vec{E}_m$ through

$$\vec{E}_I = \vec{E}_m - \tfrac{4}{3}\pi\vec{P}. \tag{6}$$

$\vec{P}$ is a fictitious polarization defined so that

$$P_n = \hat{r}\cdot\vec{P} \tag{7}$$

is identical to the surface-charge density on the boundary between the excision and the effective medium. Here $\hat{r}$ is the unit normal to the boundary at point $\vec{r}$ on the boundary. The field at points just inside the effective medium is

$$\vec{E}_{II} = \vec{E}_m + \tfrac{4}{3}\pi\vec{P}\cdot(3\hat{r}\hat{r} - \overleftrightarrow{I}). \tag{8}$$

The equation of continuity,

$$\nabla\cdot\vec{j} = 0, \tag{9}$$

requires that the normal component of current density $\vec{j}$ is unchanged across the boundary, or

$$\hat{n}\cdot\overleftrightarrow{\sigma}_I\cdot\vec{E}_I = \hat{n}\cdot\overleftrightarrow{\sigma}\cdot\vec{E}_{II}. \tag{10}$$

Now $\overleftrightarrow{\sigma}_I$ and $\overleftrightarrow{\sigma}$ will be of the general form

$$\overleftrightarrow{\sigma} = \sigma_d\overleftrightarrow{I} + \overleftrightarrow{\sigma}_a, \tag{11}$$

where σ_d has its $H=0$ value and $\overleftrightarrow{\sigma}_a$ is linear in $\vec{H}$ and antisymmetric:

$$\overleftrightarrow{\sigma}_a\cdot\vec{V} = A\vec{H}\times\vec{V}, \quad \vec{V}\cdot\overleftrightarrow{\sigma}_a = A\vec{V}\times\vec{H}, \tag{12}$$

where $\vec{V}$ is a general vector. Inserting (6) in the left-hand side and (8) in the right-hand side of (10), and using (11) and (12) leads to an equation which can be solved directly for $\vec{P}$ with the result

$$4\pi\vec{P} = (\sigma_d\overleftrightarrow{I} - \tfrac{1}{3}\overleftrightarrow{\sigma} + \tfrac{1}{3}\overleftrightarrow{\sigma}_I)^{-1}\cdot(\overleftrightarrow{\sigma}_I - \overleftrightarrow{\sigma})\cdot\vec{E}_m. \tag{13}$$

The conductivity tensors are treated as 3×3 matrices in (13).

The field both inside and outside the excised portion differs from $\vec{E}_m$ only through $\vec{P}$. If we choose $\overleftrightarrow{\sigma}$ such that $\vec{P}$ vanishes on the average, we shall have defined an effective medium within

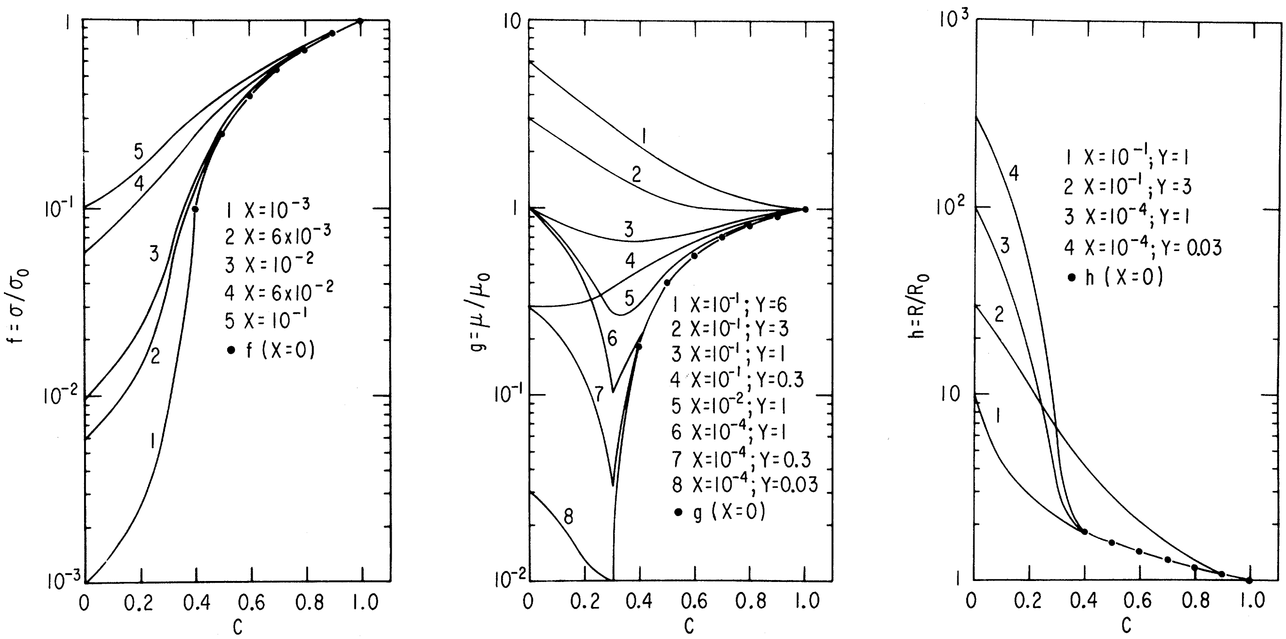

FIG. 1. Results of effective-medium theory for the electronic transport properties of a microscopically inhomogeneous system. (a) Electrical conductivity, Eqs. (1)–(4); (b) Hall mobility, Eqs. (17), (19), and (20); (c) Hall constant, Eqs. (16) and (18)–(20). The transport properties in the limit $x=0$ are presented for $C \geq 0.4$.

which fluctuations of the field from the medium value average to zero. This gives the effective-medium condition

$$\langle(\sigma_a \overleftrightarrow{I} - \tfrac{1}{3}\overleftrightarrow{\sigma} + \tfrac{1}{3}\overleftrightarrow{\sigma}_I)^{-1}\cdot(\overleftrightarrow{\sigma}_I - \overleftrightarrow{\sigma})\rangle = 0. \tag{14}$$

This is to be solved to first order in the field for $\overleftrightarrow{\sigma}_a$,

$$\overleftrightarrow{\sigma}_a = \frac{\langle \overleftrightarrow{\sigma}_{ia}/(\sigma_i + 2\sigma)^2\rangle}{\langle(\sigma_i + 2\sigma)^{-2}\rangle}. \tag{15}$$

In (15), σ_i is σ_0 with probability C and σ_1 with probability $1 - C$. Carrying out the averages gives

$$R = hR_0, \tag{16}$$

$$\mu = g\mu_0, \tag{17}$$

$$h = g/f, \tag{18}$$

$$g = f^{-1}\left[1 - \frac{(2f+1)^2(1-C)(1-xy)}{(2f+1)^2(1-C)+(2f+x)^2C}\right], \tag{19}$$

$$y = \mu_1/\mu_0. \tag{20}$$

Here R is the Hall constant and μ the Hall mobility. The significance of the subscripts is evident.

The results (16)–(20) agree with (5) to first order in ϵ for $x = 0$.

Plots of f, g, and h versus C are given in Fig. 1 for various values of x and y. They indicate several classes of behavior for materials undergoing a metal-nonmetal transition via an inhomogeneous transport regime.[19] We call attention to two patterns. For x and y both small, e.g., $x \sim 10^{-4}$ and $y \sim 10^{-2}$ as in metal-ammonia solutions,[3] σ and μ drop rapidly in the region $0.4 < C < 1$. For x somewhat larger and y of order unity, e.g., $10^{-2} \lesssim x \lesssim 10^{-1}$ and $1 \lesssim y \lesssim 3$, σ and R can vary strongly for $0.4 < C < 1$, whereas μ exhibits only weak variation, changing by ~30%, while σ changes by an order of magnitude. Such values of x and y are typical of high-temperature materials such as expanded liquid Hg[20,22] in the density range 9.3–8.0 g cm^{-3} and liquid Te[23-26] in the temperature range 670–1200°K, and the behavior of σ, R, and μ expected from (1)–(4) and (16)–(20) is observed experimentally. We expect, therefore, that the theory presented here will be of general utility in the analysis of similar materials.

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