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# Diamagnetic current and positive Hall coefficients of disordered metals

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**Abstract.** Positive Hall coefficients of non-magnetic disordered metals are discussed in the light of an exact formula derived by Itoh in 1992. We re-examine the simplest tight-binding model of a random liquid with single  $s$  orbitals, in the single-site approximation adopted by Matsubara and Kaneyoshi. The exact formula leads to an additional contribution, which comes from the diamagnetic current and makes the Hall coefficient positive when the band is more than half-filled. The result is physically plausible and could explain the occurrence of positive Hall coefficients, without recourse to the concept of quasi-Bloch states due to local order or invoking a special mechanism such as skew scattering.

## 1. Introduction

The occurrence of positive Hall coefficients for non-magnetic disordered metals is a long-standing problem, in particular in connection with the electron transport in liquid [1] and amorphous [2] metals. Many materials in this category have been found, characterized by the feature that they all include either transition metal or rare-earth elements as constituent atoms. However, many of the earlier theoretical studies have suggested that the Hall coefficients of structurally disordered metals should always be electron-like, provided that the one-electron picture is valid and only the ordinary (i.e. non-magnetic) scattering is the dominant cause of the resistivity. In spite of the considerable efforts made so far, the problem has been left unresolved and the controversy is not yet settled.

In the case of  $s$ - $p$  electron metals, the basic understanding of the Hall conduction is already established. The structure of liquid or amorphous metals is characterized by their topological disorder. The system has homogeneity and isotropy in the statistical sense. If the potential scattering is sufficiently weak, the classical Boltzmann picture of transport holds. Due to the lack of periodicity in the structure, no ‘holes’ should exist in such systems. With all of the Bloch-band effects of the crystalline structure eliminated, the Hall coefficient is shown to become free-electron-like, i.e.  $R_H = -1/nec$ . Indeed, there exist no  $s$ - $p$  electron metals which exhibit hole-like conduction in their disordered states, even if the coefficient is positive in the corresponding crystalline states.

Theoretically, no substantial change results from quantum treatments, if the scattering is weak. The quantum corrections discussed by Fukuyama *et al* [3] and by Ballentine [4] have been shown to be cancelled [5], by the effective-mass renormalization found by Itoh and Watabe [6], and the above classical value is recovered. Some significant quantitative deviations from the free-electron model are found for several heavy-element materials, but

they are also described properly by the Boltzmann equation, by taking into consideration the skew scattering due to spin-orbit interactions [7]. Therefore, disordered s-p electron metals seem to be well described in the framework of the Boltzmann theory of transport.

In systems including transition metal or rare-earth elements, the d or the f electrons are relevant to the conduction, and the potential scattering becomes too strong to be treated as a perturbation to a free-electron Hamiltonian. Many of these materials do indeed show a positive sign of the Hall coefficients in their disordered states. Obviously, a full quantum treatment is essential for these cases, and model studies have been made by using tight-binding Hamiltonians and the Kubo formula. The Peierls approximation has been adopted to incorporate the effect of the magnetic field, and a single-s-band Hamiltonian has been studied [8–11]. These calculations show a definitive sign of the Hall conductivity, which is again electron-like.

The question has arisen, therefore, of whether the hole-like conduction in disordered metals is caused by a different mechanism, such as the skew scattering, or is still of ordinary type, such as a band-structure effect due to strong short-range order and/or the band hybridizations [12]. The skew scattering can also be caused by exchange interaction. In the case of liquid transition metals, its effect was examined again by Ballentine and Huberman [13], by extending their theory [7]. These authors conclude that neither the spin-orbit interaction nor the exchange scattering can yield sufficiently large skew scattering to account for the positive Hall coefficients of liquid Fe and Co. The argument seems valid for other positive-Hall-constant materials as well, although some authors still pursue this line [14].

In the present paper, we re-investigate the problem of a tight-binding single-band conduction, and introduce a different viewpoint to that adopted in the above studies. We will show that a simple tight-binding Hamiltonian can indeed yield a positive Hall coefficient, irrespective of the hybridization or skew scattering. The core of the problem is that the diamagnetic current plays an essential role for a system under a magnetic field, and the Peierls approximation adopted in the earlier studies can incorporate its effects only partially. The diamagnetic current is fully incorporated in the exact formula for the linear part of the Hall conductivity [15]

$$\sigma_{xy}/H = -\frac{\pi e^3 \hbar^2}{c} \int \frac{dE}{2\pi} \left( -\frac{\partial f}{\partial E} \right) \text{Im} \langle \text{Tr} [v_x G^+ v_y \delta(E - \mathcal{H}) v_x G^+ v_y \delta(E - \mathcal{H})] \rangle \quad (1)$$

where  $\mathcal{H}$  is the one-electron Hamiltonian,  $G^+$  is the retarded Green function operator,  $v_x$  and  $v_y$  are the  $x$ - and  $y$ -components of the current operator, and  $\langle \dots \rangle$  denotes the average over the atomic configurations. The above formula is valid for a general one-electron Hamiltonian, and we apply it in the present paper to the same single-s-band model as was studied earlier:

$$\mathcal{H} = \sum_{i \neq j} |i\rangle t_{ij} \langle j| \quad (2)$$

assuming that the orbitals are orthogonal to each other, and that the arrangement of atoms is completely random. It will then be revealed that the Hall conductivity changes its sign from negative to positive, as the Fermi energy is increased. The reverse of the sign occurs around the middle of the band, thus showing that the concept of a hole is not an issue which comes solely from the characteristics of a Bloch electron, but rather a general feature of electron transport in condensed matter.

## 2. Evaluation of the formula

The Hall coefficient  $R_H$  is given in terms of the dc and the Hall conductivities as

$$R_H = \sigma_{xy}/\sigma_{xx}^2 H \quad (3)$$

for an isotropic system, so we need to calculate both quantities. They should be treated in a consistent way, and we adopt the approximation scheme introduced by Matsubara and Toyozawa [16] for this purpose.

Diagrammatic analysis is involved in the calculation. Let us summarize the procedure. First the electron self-energy needs be calculated. The Matsubara–Toyozawa approximation avoids repeated scatterings between two atomic sites, and thus selects only ‘single-site diagrams’ for calculating the one-electron Green function. The self-energy is given by solving the following integral equation:

$$\Sigma = \int_k \frac{t_k^2}{E - t_k - \Sigma} \quad (4)$$

where  $t_k$  is the Fourier-transformed transfer integral. We have used the shorthand notation

$$\int_k = \rho^{-1} \int \frac{d\mathbf{k}}{(2\pi)^3} \quad (5)$$

where  $\rho$  is the atomic number density. Since we are dealing with a single-s-band Hamiltonian,  $t_k$  is a function only of  $k = |\mathbf{k}|$ . In this approximation the self-energy is a function only of the energy and is independent of the wavenumber. The Green function is then given by

$$G_k = \frac{1}{E - t_k - \Sigma}. \quad (6)$$

For the dc conductivity, they start from the Kubo–Greenwood formula

$$\sigma_{xx} = \pi e^2 \hbar \int dE \left( -\frac{\partial f}{\partial E} \right) \langle \text{Tr}[v_x \delta(E - \mathcal{H}) v_x \delta(E - \mathcal{H})] \rangle \quad (7)$$

and first substitute  $\delta(E - \mathcal{H}) = (i/2\pi)(G^+ - G^-)$  for the delta-function operator. Each of the Green function operators is then expanded into a perturbation series, and the dc conductivity tensor is expressed in terms of diagrams, each of which involves two current operators. Only diagrams that are topologically equivalent to those included in equation (6) are to be selected. The vertex corrections do not appear in this approximation and the conductivity is expressed as

$$\sigma_{xx} = \frac{2\pi e^2}{3\hbar} \int_k \left( \frac{dt_k}{dk} \right)^2 \left( -\frac{1}{\pi} \text{Im} G_k^+ \right)^2 \quad (8)$$

where  $G_k^+$  refers to the retarded Green function.

Now we proceed to the Hall conductivity, and apply exactly the same procedure to formula (1). The evaluation is very simple. The Hall conductivity is expressed in terms of the diagrams involving *four* current operators, instead of two. By selecting diagrams that are topologically equivalent to those for  $G_k$  and for  $\sigma_{xx}$ , we immediately notice that there exist no non-vanishing vertex corrections, so the result is simply given by replacing  $G^+$  and  $G^-$  in equation (1) by the corresponding averaged Green functions:

$$\begin{aligned} \sigma_{xy}/H &= \frac{e^3 \hbar^2}{4\pi c} \int dE \left( -\frac{\partial f}{\partial E} \right) \\ &\times \int \frac{d\mathbf{k}}{(2\pi)^3} \text{Im} \left( \frac{\partial t_k}{\partial k_x} G_k^+ \frac{\partial t_k}{\partial k_y} (G_k^+ - G_k^-) \frac{\partial t_k}{\partial k_x} G_k^+ \frac{\partial t_k}{\partial k_y} (G_k^+ - G_k^-) \right) \end{aligned} \quad (9)$$

where the minus sign in  $G_k^-$  refers to the advanced Green function. The four current operators have also been replaced by the derivatives of  $t_k$  with respect to the wavenumber components. The above expression can be simplified to

$$\sigma_{xy}/H = \frac{2\pi^2 e^3 \hbar^2}{3c} \int dE \left( -\frac{\partial f}{\partial E} \right) \times \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial t_k}{\partial k_x} \left\{ -2 \frac{\partial t_k}{\partial k_y} \frac{\partial^2 t_k}{\partial k_x \partial k_y} - \frac{\partial t_k}{\partial k_x} \frac{\partial^2 t_k}{\partial^2 k_y^2} \right\} \left( -\frac{1}{\pi} \text{Im } G_k^+ \right)^3 \quad (10)$$

by using the identity

$$\frac{\partial}{\partial \mathbf{k}} G_k^\pm = \frac{\partial t_k}{\partial \mathbf{k}} (G_k^\pm)^2. \quad (11)$$

Equation (10) is the major result of the present paper.

Starting from equation (1) represents a vast simplification of the calculation, compared to the earlier procedures given in [9–11], which are based on the Peierls approximation. In these calculations, the original Kubo formula for the off-diagonal part of the conductivity tensor has been used, and the effect of a magnetic field  $\mathbf{H}$  is incorporated by modifying the transfer integral as follows:

$$t_{ij} \rightarrow t_{ij} e^{-i\eta_{ij}} \quad (12)$$

where  $\eta_{ij}$  is the so-called Peierls phase factor:

$$\eta_{ij} \equiv (e/2\hbar c) \mathbf{H} \cdot (\mathbf{R}_i \times \mathbf{R}_j) \quad (13)$$

and  $\mathbf{R}_i$  denotes the position vector of the  $i$ th atom. The effect of a magnetic field on a current-matrix element is also taken into account through the Peierls phase:

$$\mathbf{v}_{ij} = \frac{1}{i\hbar} (\mathbf{R}_i - \mathbf{R}_j) t_{ij} e^{-i\eta_{ij}}. \quad (14)$$

Then the calculation follows in basically the same way as in the case of the dc conductivity. However, it is fairly involved. Close attention should be paid to the gauge invariance, when the field-linear part of  $\sigma_{xy}$  is extracted from each of the diagrammatic contributions.

It should be emphasized that the above conventional procedure generally yields a different result to starting from formula (1). This is clearly demonstrated by comparing equation (10) with the expression derived by Matsubara and Kaneyoshi [9] for the same model Hamiltonian:

$$\sigma_{xy}/H = \frac{2\pi^2 e^3 \hbar^2}{3c} \int dE \left( -\frac{\partial f}{\partial E} \right) \times \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\partial t_k}{\partial k_x} \left\{ \frac{\partial t_k}{\partial k_y} \frac{\partial^2 t_k}{\partial k_x \partial k_y} - \frac{\partial t_k}{\partial k_x} \frac{\partial^2 t_k}{\partial^2 k_y^2} \right\} \left( -\frac{1}{\pi} \text{Im } G_k^+ \right)^3. \quad (15)$$

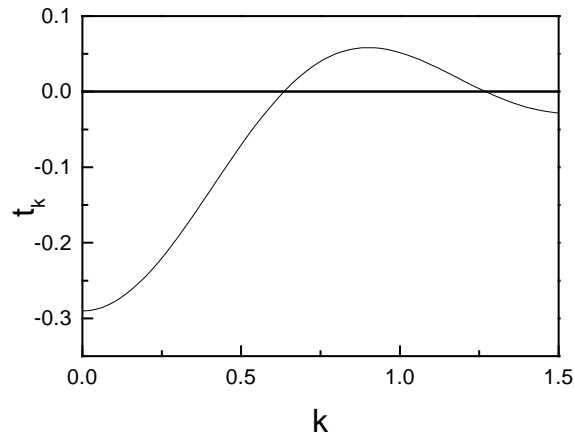
The result resembles equation (10) but differs in that the first term in the curly parentheses has a different magnitude and an opposite sign to the corresponding one in equation (10).

In fact the Peierls approximation (12), (13) and (14) involves more than a modification of the transfer integrals. Equation (12) is correct to first order in the field strength, but equation (14) neglects some part of the diamagnetic current, which is still linear in the field strength. A current operator is proportional to the commutator between the position operator and the Hamiltonian, and we have tacitly assumed in (14) that the former is diagonal with respect to the field-dependent basis orbitals. The same assumption has always been made in most conductivity calculations, but the off-diagonal elements are actually of first order

in the field strength. The effect is not necessarily small on the Hall conductivity, and can possibly make substantial contributions. Equation (10) should be more appropriate in this respect, since the full diamagnetic current is already included in formula (1).

### 3. Numerical results

In the actual calculation, we have assumed the transfer integral to decay with the distance, according to the form given by Harrison [17], adjusted with suitable parameters to simulate d–d transfers in liquid Fe. It is set equal to zero at a shorter distance than the ‘hard-core diameter’, which has been determined from the measured radial distribution function. At a longer distance, it is also truncated in between the second- and the third-nearest neighbours in the crystalline state, in order to yield an appropriate bandwidth. However, our choice of the parameters is not intended to simulate the real material closely. Except for the latter truncation, the model is practically the case studied numerically by Itoh and Watabe [10], although there is a fundamental difference in their theory as regards dealing with the average over atomic configurations.

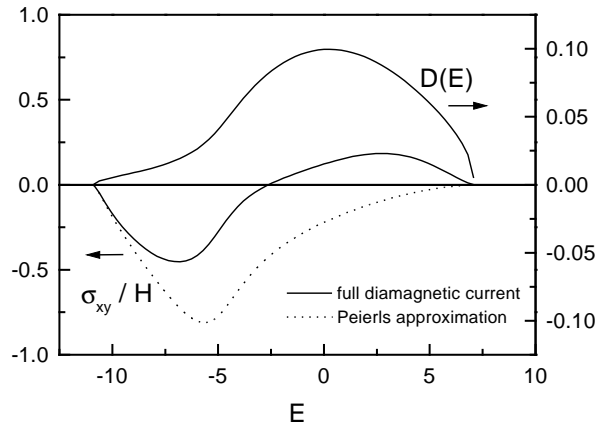


**Figure 1.** The Fourier-transformed transfer integral in arbitrary units, as a function of the wavenumber.

In figure 1 we have plotted the Fourier-transformed transfer integral as a function of  $k = |\mathbf{k}|$ . It is the only direct input quantity and serves as a ‘dispersion relation’ for an isotropically disordered system; its oscillation is caused by the truncation of the transfer integral. Figure 2 shows the comparison between the two calculations, i.e. equations (10) and (15), of the Hall conductivity. They are plotted as functions of the Fermi energy, and the electronic density of states is also shown. The present theory is seen to predict hole-like conduction in the upper half of the band, whereas the Peierls approximation always yields negative (electron-like) Hall conductivity throughout the whole band. The reason for the latter is readily understood by transforming equation (15) into

$$\sigma_{xy}/H = -\frac{2\pi^2 e^3 \hbar^2}{9c} \int dE \left( -\frac{\partial f}{\partial E} \right) \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{k^3} \left( \frac{dt_k}{dk} \right)^3 \left( -\frac{1}{\pi} \text{Im} G_k^+ \right)^3. \quad (16)$$

The above expression is expected to have a negative sign, provided that the dominant contributions to the integration come from the  $k$ -region where the dispersion  $t_k$  has a positive slope. Positive contributions come only from the limited negative-slope region; indeed it corresponds to the upper energy region of the band, but the relative magnitude of the spectral distribution  $-(1/\pi) \text{Im} G_k^+$  is not sufficiently large in this region to dominate the integration. A more detailed analysis of (16) is found in Itoh and Watabe’s work [10].



**Figure 2.** Two Hall conductivity functions calculated by using the Peierls approximation (dotted line) and equation (1) (solid line), as functions of the Fermi energy, in arbitrary units. The electronic density of states is shown for comparison.

Here, for a further comparison, we rewrite the two common terms appearing in both sets of curly parentheses in equations (10) and (15) as

$$\frac{\partial t_k}{\partial k_x} \frac{\partial t_k}{\partial k_y} \frac{\partial^2 t_k}{\partial k_x \partial k_y} = \frac{k_x^2 k_y^2}{k^5} \left( \frac{dt_k}{dk} \right)^2 \left( \frac{d^2 t_k}{dk^2} - \frac{1}{k} \frac{dt_k}{dk} \right) \quad (17)$$

$$\left( \frac{\partial t_k}{\partial k_x} \right)^2 \frac{\partial^2 t_k}{\partial k_y^2} = \frac{k_x^2 k_y^2}{k^5} \left( \frac{dt_k}{dk} \right)^2 \left( \frac{d^2 t_k}{dk^2} - \frac{1}{k} \frac{dt_k}{dk} \right) + \frac{k_x^2}{k^3} \left( \frac{dt_k}{dk} \right)^3 \quad (18)$$

apart from the numerical factors. The above recasting separates out two identical contributions, which represent the difference between the transport mass and the optical mass. They are cancelled out exactly in the combination of the terms in equation (15); in this case only the first derivative of the dispersion is relevant and the negative Hall conductivity results, as mentioned above. However, in equation (10) the combination is such that the contribution in question, i.e. the r.h.s. of equation (17), is not cancelled, but multiplied by three. Therefore it is the factor responsible for the positive Hall coefficient, and should be identified as representing that particular part of the diamagnetic current which has been missed out in the Peierls approximation.

The l.h.s. of equation (17) vanishes when the dispersion is purely parabolic (or more generally, when it is a sum of distinct single-variable functions of  $k_x$ ,  $k_y$  and  $k_z$ ). The r.h.s. consists of two competing terms. The first-derivative term (the second term in the parentheses) always has hole-like contributions throughout the first rise of the dispersion, whereas the second-derivative term is electron-like in the lower half of the band, where the dispersion has a positive curvature. In this energy region the two contributions tend to cancel each other, and the cancellation is almost perfect near the bottom of the band, where the dispersion is well approximated by a parabola. As we go up to higher energies, the dispersion starts to deviate from the parabola and the second derivative changes its sign around the middle of the band. At higher energies, both contributions serve to promote the hole-like conduction. We therefore see that the Hall coefficient can only become positive when the dispersion is non-parabolic.

#### 4. Discussion

We have shown that the diamagnetic current is essential to the understanding of the sign of the Hall coefficient. It has not been fully considered so far because of two difficulties. Firstly, the previous studies rely on the original Kubo formula and one is obliged to start from a particular gauge, whereas the diamagnetic current depends on the choice of the gauge. The Peierls approximation is based upon the symmetric gauge. Although the expression (15) is apparently gauge independent, it still lacks a substantial part of the current. The second difficulty is that the contribution from the diamagnetic current to each order of perturbation is actually macroscopically large; the genuine conduction is obtained only by adding all of the infinite contributions. In the case of the tight-binding calculation, the same problem arises from the field-dependent parts of the matrix elements of the position operator, which include factors proportional to the system size. This applies to both the diagonal and the off-diagonal elements. Although the former have been treated properly in the Peierls approximation, the latter cannot be incorporated conveniently in this framework, because of their complicated dependence on the position vectors of the relevant atomic sites. We are free of the above two problems in using equation (1), since they have already been dealt with in deriving equation (1) and the cumbersome field-dependent operators are no longer required.

In the last section we attempted a  $\mathbf{k}$ -space interpretation of the result. It is interesting that the sign of the Hall coefficient is determined by a competition between the first and the second derivatives of the dispersion even in the isotropic case. This is in marked contrast to the conventional interpretation based on the Boltzmann transport theory, in which the sign is determined solely by the transport effective mass, i.e. by the first derivative, when the system is isotropic [4, 5]. In the weak-scattering limit, our result (10) is at variance with the formal solution to the Boltzmann equation in the relaxation time approximation:

$$\sigma_{xy}/H = \frac{e^3 \tau^2}{c \hbar^4} \int \frac{d\mathbf{k}}{(2\pi)^3} \left( -\frac{\partial f(\epsilon_{\mathbf{k}})}{\partial \epsilon_{\mathbf{k}}} \right) \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_x} \left\{ \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_y} \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_x \partial k_y} - \frac{\partial \epsilon_{\mathbf{k}}}{\partial k_x} \frac{\partial^2 \epsilon_{\mathbf{k}}}{\partial k_y^2} \right\} \quad (19)$$

where  $\epsilon_{\mathbf{k}}$  is a general (crystal) dispersion which allows for an anisotropy, and  $\tau$  denotes the relaxation time. As is seen in equation (10), our tight-binding calculation does not reproduce the same Lorentz-force factor as appears in equation (19), whereas the Peierls approximation (15) does. In this respect the Peierls approximation might appear to give a better result. However, we recall that in the Boltzmann theory of transport the group velocity  $\partial \epsilon_{\mathbf{k}}/\partial \mathbf{k}$  is recognized as carrying current, even under a magnetic field. Since the group velocity used there has nothing to do with the vector potential, it looks as though the effect of the diamagnetic current is neglected entirely in the Boltzmann theory of transport.

A justification of the above traditional Boltzmann theory for the Hall conduction has been given in early studies (see [18] for a comprehensive review). The analysis is based on the quantum kinetic method and has paid sufficient attention to the diamagnetic current. The argument seems plausible, yet it involves fairly delicate mathematical procedures, dealing with quantities which are in principle divergent. Equation (1) relies on linear-response theory, and the relation between the present approach and the kinetic method is not very clear at the moment. We do not encounter this kind of discrepancy when equation (1) is applied to a nearly-free-electron system. Indeed, it yields the same result as equation (16), with the dispersion  $t_{\mathbf{k}}$  being replaced by  $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m^*$  [1]. This is possibly because the band is parabolic and the first term of the Lorentz force does not contribute. Applying equation (1) to a Bloch electron would be very interesting and may resolve the puzzle.

In spite of the complications in the  $\mathbf{k}$ -space description mentioned above, the present



calculation can possibly provide a simple picture. That is, it suggests that whether a carrier is to be considered as an electron or as a hole has much to do with the filling fraction of a band, rather than with the crystalline energy band structure. Physically, this is very plausible, because the electron–hole symmetry is built into the Hamiltonian from the beginning; one can interchange the roles of the creation and annihilation operators without changing the form of the Hamiltonian. Of course, one cannot expect a complete electron–hole symmetry for a disordered system, since the effect of disorder depends on the energy relative to the atomic level. Yet it does not seem physical to have negative Hall coefficients throughout a whole tight-binding band, for which the upper band edge exists. Okamoto *et al* [19] have attempted a renormalization-group approach to a single-s-band Hamiltonian with diagonal disorder only. They have also used equation (1) and predicted positive Hall coefficients at energies higher than that of the mobility edge.

If our interpretation based on the filling fraction is sufficiently general, then we have the possibility of finding a simpler description of the Hall conduction for more complicated systems. For example, the electric conduction in liquid transition metals has been confirmed to be dominated by d electrons [20], so the sign can be critically dependent on the number of electrons in the d band. This scenario may also apply to alloy systems, and investigations of these interesting cases are now under way.

### Acknowledgment

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