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The Hall effect in the ladder approximation

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Abstract. The theory of the Hall effect of interacting electrons in the ladder approximation, formulated by Fukuyama, Ebisawa and Wada, is further investigated. The 'dispersive' contributions to the Hall conductivity, which were not given in their original paper, are calculated explicitly in order to complete the treatment. In the isotropic case the new term, as well as the old one, is shown to be related only to the electronic states at the Fermi level. The final expression thus obtained includes the effect of the damping (the finite-width effect).

1. Introduction

Microscopic theoretical treatment of the Hall effect in a weak magnetic field is known to be a difficult problem. This is particularly so for interacting electrons and not many studies have been done, although some progress has been made in the investigation of non-interacting electrons in disordered materials (Matsubara and Kaneyoshi 1968, Fukuyama *et al* 1970, Levin *et al* 1970, Niizeki and Hoshino 1976, Itoh and Watabe 1978). The earliest attempts at studying interacting electrons were made by Fukuyama *et al* (1969) (to be referred to as FEW hereafter), by using Matsubara's finite-temperature formalism and taking the ladder approximation, which is still one of very few reliable theories in the sense that it is manifestly gauge invariant and the nature of the approximation is made clear.

FEW obtained the two different types of contributions to the Hall conductivity. The first term, which they called the dissipative contribution, is dependent only on the states in the vicinity of the Fermi level. This was shown to lead to the classical result, $R_H = 1/nec$, in the limit of weak scattering†. The second term, which they called the dispersive contribution, is related to all the states below the Fermi level. Its evaluation is therefore more laborious. This contribution is, however, small in the weak scattering limit and is not calculated explicitly in the original paper.

The above result of the weak scattering calculation implies that the quantum correction cannot be evaluated without including the damping effect, i.e. the effect of the finite width of the spectral function. The calculation of the dispersive contribution is indispensable for this purpose, since it is not expected to be small when the damping is

† The result obtained by FEW was $R_H = g^{-2}/nec$, where g is the so-called Mott factor (i.e. the ratio of the electronic density of states at the Fermi level to its free electron value). In a later investigation, however, the g-factors have been shown to be cancelled out by the mass-renormalisation correction to the DC conductivity (Itoh 1984).

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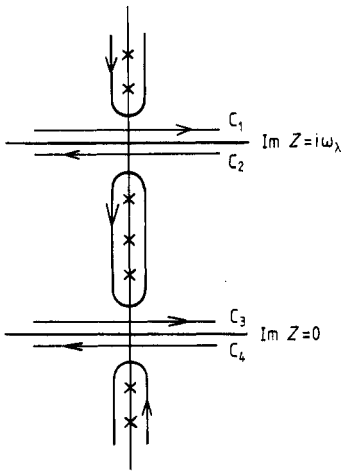

Figure 1. The contours of the integrations for the frequency summation in equation (2.1).

included. In this paper we attempt to derive an explicit expression for this contribution. This completes the quantum treatment in the ladder approximation for the first time.

According to FEW, the existence of the two different contributions appears to be an intrinsic problem. It should be recalled that, unlike in the ordinary conduction process under zero magnetic field, the states below the Fermi level make a finite contribution to the Hall conduction because the velocity operator includes the diamagnetic current term. Nevertheless, as we shall see later, this new contribution can be rewritten in a form that is dependent only on the states in the vicinity of the Fermi level if the system is isotropic. Therefore, in the ladder approximation, the Hall conductivity of an interacting system is shown to become a Fermi-surface quantity.

In section 2 we start with an introduction of FEW's result. We repeat the procedure of the frequency summation in the finite-temperature formalism in order to see how the two different contributions come out. In particular the explicit expression for the dispersive contribution is derived. At this stage the expression is apparently 'off-shell', i.e. dependent on all the states below the Fermi level. It is then rewritten in section 3 into an 'on-shell' form by assuming the isotropy of the system. The charge conservation law plays an essential role in this rewriting. The two contributions are combined into a compact form, which is expected to be useful for quantitative applications. The last section contains a discussion of the results.

2. FEW's result and frequency summation

We consider the case of a uniform magnetic field $\boldsymbol{H}$ along the z axis. The linear part of the off-diagonal conductivity tensor in H, i.e. the Hall conductivity, is given by equations (2-5) and (2-19) in FEW;

$$\sigma_{xy}/H = \frac{1}{\omega}\frac{e^3}{c\hbar} T \sum_n \mathcal{F}_{xy}(i\varepsilon_n, i\varepsilon_n - i\hbar\omega_\lambda)|_{i\omega_\lambda \to \omega + i\delta} \tag{2.1}$$

$$\mathcal{F}_{xy}(z, z') = \int \frac{d\boldsymbol{k}}{(2\pi)^3}\left(v_x(\boldsymbol{k}; z, z')\frac{\partial}{\partial k_y} v_y(\boldsymbol{k}; z, z') - v_y(\boldsymbol{k}; z, z')\frac{\partial}{\partial k_y} v_x(\boldsymbol{k}, z, z')\right)$$

$$\times \left(G(\boldsymbol{k}, z) \frac{\partial}{\partial k_x} G(\boldsymbol{k}, z') - \frac{\partial}{\partial k_x} G(\boldsymbol{k}, z) G(\boldsymbol{k}, z') \right) \tag{2.2}$$

where ω is the frequency of the applied electric field, T is the temperature, $\varepsilon_n = (2n+1)\pi T$, $G(\boldsymbol{k}, z)$ is the Green function calculated in the ladder approximation and $v_{x(y)}(\boldsymbol{k}; z, z')$ is the x (y) component of the vertex function for the operator $\hat{\boldsymbol{v}} = (1/\mathrm{i}\hbar)[\hat{\boldsymbol{r}}, \hat{H}]$ connected to the two propagators $G(\boldsymbol{k}, z)$ and $G(\boldsymbol{k}, z')$. Here we have followed the notation of Itoh (1984). The relationship to the parameters used by FEW is $\boldsymbol{k} \rightarrow \boldsymbol{p}/\hbar$ and $\boldsymbol{v}(\boldsymbol{k}; E^+, E^-) \rightarrow \boldsymbol{J}/e$. In order to obtain the explicit expression we must perform the frequency summation and the analytical continuation $\mathrm{i}\omega_\lambda \rightarrow \omega + \mathrm{i}\delta$. The frequency summation is carried out as usual by the integrations on the complex energy plane along all the circles enclosing the singularities of the Fermi–Dirac distribution function $f(z)$. These contours are seen to be transformed into C_1, C_2, C_3 and C_4 in figure 1 considering the branch cuts at Im $z = 0$ and Im $z = \omega_\lambda$. The dissipative term described in the preceding section is the one obtained from the integrations along $C_2 + C_3$. After analytical continuation it becomes

$$\int_{C_2} + \int_{C_3} = \frac{e^3}{c\hbar} \int \frac{\mathrm{d}E}{2\pi\mathrm{i}} \, f(E) \frac{1}{\omega} \left(\mathcal{F}_{xy}(E^+ + \hbar\omega, E^-) - \mathcal{F}_{xy}(E^+, E^- - \hbar\omega) \right) \tag{2.3}$$

where $E^\pm = E \pm \mathrm{i}\delta$. The contribution from $C_1 + C_4$ is calculated in the same way:

$$\int_{C_1} + \int_{C_4} = \frac{e^3}{c\hbar} \int \frac{\mathrm{d}E}{2\pi\mathrm{i}} \, f(E) \frac{1}{\omega} \left(\mathcal{F}_{xy}(E^-, E^- - \hbar\omega) - \mathcal{F}_{xy}(E^+ + \hbar\omega, E^+) \right) \tag{2.4}$$

which is the dispersive term. In the limit $\omega \rightarrow 0$, the expression (2.3) is reduced to

$$\lim_{\omega \rightarrow 0} \left(\int_{C_2} + \int_{C_3} \right) = \frac{e^3}{c} \frac{1}{2\pi\mathrm{i}} \int \mathrm{d}E \, f(E) \frac{\partial}{\partial E} \mathcal{F}_{xy}(E^+, E^-)$$

and therefore, by partial integration,

$$\lim_{\omega \rightarrow 0} \left(\int_{C_2} + \int_{C_3} \right) = \frac{e^3}{c} \frac{1}{2\pi\mathrm{i}} \int \mathrm{d}E \left(-\frac{\partial f}{\partial E} \right) \mathcal{F}_{xy}(E^+, E^-). \tag{2.5}$$

Because of the factor $(-\partial f/\partial E)$ this is seen to be a Fermi-surface quantity. The above calculation is simply a reproduction of FEW's argument; substituting (2.2) into (2.5) we obtain equation (3.7) in FEW:

$$\sigma_{xy}(C_2 + C_3)/H = \frac{e^3}{c} \int \frac{\mathrm{d}E}{2\pi\mathrm{i}} \left(-\frac{\partial f}{\partial E} \right) \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3} \left(v_{kx}^{+-} \frac{\partial}{\partial k_y} v_{ky}^{+-} - v_{ky}^{+-} \cdot \frac{\partial}{\partial k_y} v_{kx}^{+-} \right)$$

$$\times \left(G_k^+ \frac{\partial}{\partial k_x} G_k^- - \frac{\partial}{\partial k_x} G_k^+ \, G_k^- \right) \tag{2.6}$$

where we have used the abbreviated notation $\boldsymbol{v}_k^{+-} \equiv \boldsymbol{v}_k(\boldsymbol{k}; E^+, E^-)$ and $G_k^\pm \equiv G(\boldsymbol{k}, E^\pm)$, and v_{kx}^{+-} (v_{ky}^{+-}) is the x (y) component of $\boldsymbol{v}_k^{+-}$. Likewise, by noting that

$\mathcal{F}_{xy}(E^+, E^+) = \mathcal{F}_{xy}(E^-, E^-) = 0$, the expression (2.4) can be reduced in the limit of $\omega \to 0$ to

$$\lim_{\omega\to 0}\left(\int_{C_1} + \int_{C_4}\right) = -\frac{e^3}{c}\int \frac{dE}{2\pi i}\, f(E)$$
$$\times \left(\frac{\partial}{\partial z}\mathcal{F}_{xy}(z, z')|_{z=z'=E^+} + \frac{\partial}{\partial z'}\mathcal{F}_{xy}(z, z')|_{z=z'=E^-}\right) \tag{2.7}$$

and hence we obtain

$$\sigma_{xy}(C_1 + C_4)/H = -\frac{2e^3}{c}\,\mathrm{Im}\int \frac{dE}{2\pi}\, f(E)\int \frac{d\boldsymbol{k}}{(2\pi)^3}\left(v_{kx}^{++}\frac{\partial}{\partial k_y}v_{ky}^{++} - v_{ky}^{++}\frac{\partial}{\partial k_x}v_{kx}^{++}\right)$$
$$\times \left(\frac{\partial}{\partial E}G_k^+\frac{\partial}{\partial k_x}G_k^+ - \frac{\partial}{\partial k_x}\left\{\frac{\partial}{\partial E}G_k^+\right\}G_k^+\right) \tag{2.8}$$

where we have used the notation $\boldsymbol{v}_k^{++} \equiv \boldsymbol{v}(\boldsymbol{k}; E^+, E^+)$, analogous to $\boldsymbol{v}_k^{+-}$. In deriving (2.8) the terms involving the energy derivatives of the vertex functions have vanished. The second term in the large brackets on the RHS of (2.7) gives the complex conjugate of the first term. Since the above expression for $\sigma_{xy}(C_1 + C_4)$ includes $f(E)$ instead of $-\partial f/\partial E$, it is apparently dependent on all the states below the Fermi energy.

3. The contribution from C_1 and C_4

Now we show that the expressions (2.6) and (2.8) can be further simplified. In particular $\sigma_{xy}(C_1 + C_4)$ is transformed into the 'on-shell' form. The key to this transformation is to be found in the following Ward identities (see, e.g., Mahan 1981):

$$\boldsymbol{v}_k^{++} = \hbar\boldsymbol{k}/m + (1/\hbar)(\partial/\partial\boldsymbol{k})\Sigma_k^+ \tag{3.1}$$
$$\Gamma_k^{++} = 1 - (\partial/\partial E)\Sigma_k^+ \tag{3.2}$$

where Σ_k^+ is the self-energy defined by

$$G_k^+ = (E - \hbar^2k^2/2m - \Sigma_k^+)^{-1} \tag{3.3}$$

and Γ_k^{++} is the vertex function for the unit operator connected to the two propagators having the same energy E^+. From (3.1) and (3.3) we easily see that

$$(\partial/\partial E)\boldsymbol{v}_k^{++} = -(1/\hbar)(\partial/\partial\boldsymbol{k})\Gamma_k^{++} \tag{3.4}$$
$$(1/\hbar)(\partial/\partial\boldsymbol{k})G_k^+ = (G_k^+)^2\boldsymbol{v}_k^{++} \tag{3.5}$$
$$(\partial/\partial E)G_k^+ = -(G_k^+)^2\Gamma_k^{++}. \tag{3.6}$$

We also have relations similar to (3.1)–(3.6) for the energy value E^-, by defining $\boldsymbol{v}_k^{--}$, Σ_k^- and Γ_k^{--} in the same manner. It is also important to note that, if the system is isotropic, the current vertex functions are written in the form

$$\boldsymbol{v}_k^{+-} = \hat{\boldsymbol{k}}v_k^{+-} \tag{3.7}$$
$$\boldsymbol{v}_k^{++} = \hat{\boldsymbol{k}}v_k^{++}, \tag{3.8}$$

where $\hat{\boldsymbol{k}}$ is the unit vector along $\boldsymbol{k}$ and v_k^{+-} and v_k^{++} on the left hand sides are functions only of $k = |\boldsymbol{k}|$.

Using (3.5), (3.7) and (3.8), it is a straightforward task to rewrite equation (2.6) as

$$\sigma_{xy}(C_2+C_3)/H=\frac{2e^3\hbar}{3c}\int\frac{dE}{2\pi}\left(-\frac{\partial f}{\partial E}\right)\int\frac{d\boldsymbol{k}}{(2\pi)^3}\frac{1}{k}(v_k^{+-})^2\,\mathrm{Im}[(G_k^+)^2G_k^-v_k^{++}]. \tag{3.9}$$

Note that for isotropic systems the Green functions are also functions only of $k\equiv|\boldsymbol{k}|$. In order to transform (2.8), we first note that

$$\frac{\partial}{\partial E}G_k^+\frac{\partial}{\partial \boldsymbol{k}}G_k^+-\frac{\partial}{\partial \boldsymbol{k}}\left(\frac{\partial}{\partial E}G_k^+\right)G_k^+$$

$$=-\left((G_k^+)^2\frac{\partial}{\partial E}G_k^+\,\boldsymbol{v}_k^{++}+(G_k^+)^3\frac{\partial}{\partial E}\boldsymbol{v}_k^{++}\right). \tag{3.10}$$

In deriving the above relation we have used (3.4), (3.5) and (3.6). By substituting the x component of (3.10) into (2.8) and using (3.8), we then have

$$\sigma_{xy}(C_2+C_3)/H=\frac{2e^3\hbar}{3c}\,\mathrm{Im}\int\frac{dE}{2\pi}\,f(E)\int\frac{d\boldsymbol{k}}{(2\pi)^3}\,\frac{1}{k}$$

$$\times\left((G_k^+)^2\frac{\partial}{\partial E}G_k^+\,(v_k^{++})^3+(G_k^+)^3(v_k^{++})^2\frac{\partial}{\partial E}v_k^{++}\right)$$

$$=-\frac{2e^3\hbar}{3c}\,\mathrm{Im}\int\frac{dE}{2\pi}\,f(E)\int\frac{d\boldsymbol{k}}{(2\pi)^3}\,\frac{1}{3k}\,\frac{\partial}{\partial E}[(G_k^+)^3(v_k^{++})^3]. \tag{3.11}$$

Thus, by partial integration with respect to E, the expression becomes 'on-shell'. The total contribution is therefore

$$\sigma_{xy}/H=\frac{e^3\hbar}{3\pi c}\int dE\left(-\frac{\partial f}{\partial E}\right)\int\frac{d\boldsymbol{k}}{(2\pi)^3}\frac{1}{k}$$

$$\times\,\mathrm{Im}[(v_k^{+-})^2v_k^{++}\,(G_k^+)^2G_k^-\,-\tfrac{1}{3}(v_k^{++})^3(G_k^+)^3]. \tag{3.12}$$

The above result is the complete expression for the Hall conductivity in the ladder approximation, including the full damping (finite-width) effect and the vertex corrections. If we neglect the vertex corrections, v_k^{+-} and v_k^{++} are replaced by $v_k\equiv\hbar k/m$. We then obtain,

$$\sigma_{xy}/H=-\frac{4e^3\hbar}{9\pi c}\int dE\left(-\frac{\partial f}{\partial E}\right)\int\frac{d\boldsymbol{k}}{(2\pi)^3}\,\frac{1}{k}(v_k)^3\left(-\frac{1}{\pi}\,\mathrm{Im}\,G_k^+\right)^3. \tag{3.13}$$

The above expression has appeared frequently in studies of one-electron problems in disordered materials. This is because these studies have dealt with the isotropic scattering cases, for which the vertex corrections vanish.

4. Comments and discussion

Although the ladder approximation has been extensively used in various many-body problems, its application to the Hall effect was found to be extremely complicated due

to the problem of the gauge invariance (see FEW)†. Although the work by FEW was reported rather a long time ago, the evaluation of the damping effect has never been attempted because of the awkward dispersive contribution. Without considering the damping effect one cannot go beyond the classical description, as shown by Itoh (1984), apart from a small correction due to the Fermi-surface shift which cannot be caused by the interaction effect only. The treatment by the ladder approximation has been completed by the present work, and we have derived an 'on-shell' expression for the Hall conductivity including the damping effect. It must be noted that the details of the scattering mechanism are irrelevant to our conclusions and therefore they allow for many-body interactions. For non-interacting electrons, Morgan *et al* (1984) and Morgan and Howson (1985) have recently proposed a basic formula for the Hall conductivity and claimed that it should generally be an 'on-shell' expression. However, our expression (3.12) is not derived from their formula. Some degree of approximation is included in their derivation and so it is still open to question whether their conclusion is generally correct (see also Itoh 1985).

One of the most interesting observations related to the present study is the measurement made by Häussler and Baumann (1983), Häussler (1984) and by Mizutani and others (see, for a review, Mizutani 1983 and Häussler 1990). These authors have found systematic deviations of the Hall constant from its free electron value as functions of the carrier number for a number of sp metals in their glassy states. The former authors studied the noble-metal-based metallic glasses, whereas the systems investigated by the latter group of authors are based on Mg–Zn. In both cases the deviations become very small in the liquid states, as with most liquid sp metals (see Busch and Güntherodt 1974). These systems are characterised by the perfect isotropy, on average, and by the fact that the scattering is caused by disorder. The present study suggests that the damping effect is more important in the amorphous state than in the liquid state, although the short range order is expected to be stronger in the amorphous state. The d states of the noble-metal elements play no role as long as they are at a distance from the Fermi-level. Recently, Frésard *et al* (1990) calculated the spectral function and the resistivity of a model liquid system in the effective medium approximation, and found that the strong short range order can cause strong damping effects through Bragg scattering. Their conclusion is consistent with the above arguments.

It is interesting to apply the present theory to the above systems. Due to our reduction of the dispersive contribution into an 'on-shell' form, the numerical calculation including the finite-width effect has been made realistic. Some preliminary attempts to perform such calculations are now under way.

References

Busch G and Güntherodt H J 1974 *Solid State Physics* vol 29, ed F Seitz and D Turnbull (New York: Academic) p 235

Frésard R, Beck H and Itoh M 1990 *J. Phys.: Condens Matter* **2** submitted

Fukuyama H, Ebisawa H and Wada Y 1969 *Prog. Theor. Phys.* **42** 494

Fukuyama H, Saitoh M, Uemura Y and Shiba H 1970 *J. Phys. Soc. Japan* **28** 842

† The gauge invariance problem has already been solved generally by the present author (Itoh 1985), who derived a general exact formula of the Hall conductivity for interacting systems. This avoided much of the technical complication found in FEW's paper; equations (2.1) and (2.2) are easily derived by applying the ladder approximation to Itoh's formula.

Häussler P 1984 *Rapidly Quenched Metals* ed S Steeb and H Warlimont (Amsterdam: North-Holland) p 797
—— 1990 *Glassy Metals III (Springer Topics in Applied Physics)* ed H Güntherodt and H Beck (Berlin: Springer) to appear
Häussler P and Baumann F 1983 *Z. Phys.* B **49** 303
Itoh M 1984 *J. Phys. F: Met. Phys.* **14** L179
—— 1985 *J. Phys. F: Met. Phys.* **15** 1715
Itoh M and Watabe M 1978 *J. Phys. F: Met. Phys.* **8** 1725
Levin K, Velicky B and Ehrenreich H 1970 *Phys. Rev.* B **2** 1771
Mahan G D 1981 *Many Particle Physics* (New York: Plenum) ch 7
Matsubara T and Kaneyoshi T 1968 *Prog. Theor. Phys.* **40** 1257
Mizutani U 1983 *Prog. Mater. Sci.* **28** 97
Morgan G J and Howson M A 1985 *J. Phys. C: Solid State Phys.* **18** 4327
Morgan G J, Howson M A and Weir G F 1984 *J. Non-Cryst. Solids* **62** 1131
Niizeki K and Hoshino K 1976 *J. Phys. C: Solid State Phys.* **9** 3481