

Hall effect of noninteracting electrons as a Fermi-surface property: A rigorously derived gauge-independent formula in the on-shell form

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(Received 21 June 1991)

A rigorously derived formula for the Hall conductivity of a one-electron Hamiltonian is obtained. The formula is written in terms of the correlation functions with *four* vertices. For degenerate electrons, the only relevant energy parameter is found to be the Fermi energy, which shows clearly that the Hall coefficient for independent electrons in a weak magnetic field is in general, determined only by states on the Fermi surface. When this formula is evaluated in the ladder approximation, we recover the result previously derived by Fukuyama *et al.* and by Itoh.

I. INTRODUCTION

Prior to the advent of the quantum Hall effect under a strong magnetic field, the study of the nonquantized Hall effect in a weak uniform field continued to be one of the most important probes for solid-state physicists and its importance is by no means diminished even nowadays.¹ Of course the quantum-mechanical treatment is essential even for understanding the nonquantized Hall effect, which is known to be a difficult problem. In most cases the analysis of the data has been made based on the purely classical result, $R_H = 1/nec$, or its suitable generalizations to the multicarrier systems. A better treatment is to use the "semiclassical" Boltzmann equation, which can incorporate the band-structure effect. However, it is known that the latter adds nothing new to the former when the band is isotropic.

Full quantum-mechanical treatments are required particularly for disordered materials and for interacting systems. A number of modern theoretical calculations have indeed been attempted for the former cases in connection with impurity band conduction in semiconductors,² solid disordered alloys,^{3,4} and with liquid or amorphous metals.⁵⁻⁷ Although these calculations are based on the general Kubo formula, their applicability is more or less limited because of the speciality of the models; only the tight-binding Hamiltonians or the zero-range potentials have been treated so far. As for the latter case the only legitimate theory seems to be the ladder approximation, formulated by Fukuyama, Ebisawa, and Wada.⁸ In this formalism arbitrary types of scatterings, including many-body interactions, can be treated in a manifestly gauge-invariant way. However, the technical complexity involved in these calculations appears enormous. This seems to be the price for the general applicability of the formalism.

The purpose of the present paper is not to introduce another successful example of approximation but to provide a rigorously derived formula, from which one can start full quantum calculations of the Hall effect with any suitable approximation. The source of the difficulty underlying the problem, which has restricted the applicabil-

ity or reduced the mathematical simplicity of the above theories, is the gauge-invariance condition and the related divergence of the perturbation expansion. In all of the above theories the calculations are separated into two stages. In the first stage the off-diagonal part of the conductivity tensor is calculated by using the Kubo formula for a system in a magnetic field. In the second stage the calculated conductivity tensor, given as a function of the field \mathbf{H} , is expanded in powers of \mathbf{H} to obtain the expression for the linear term. The difficulty in this procedure is that the vector potential representing the field, which comes into the Hamiltonian, is in general macroscopically large for a uniform field. To be more precise, it is proportional to the system size and so are all its contributions to the conductivity. Therefore we must sum up the divergent terms and find a suitable partial resummation to give a finite and gauge-invariant answer. In order to circumvent the above problem, we seek a *rigorously* derived expression for the linear part of the off-diagonal conductivity (Hall conductivity), which is sufficient for the calculation of the Hall coefficient.

The only limitation in the treatment here is that we start with a one-electron Hamiltonian assumed to be of the form

$$\mathcal{H} = \frac{p^2}{2m} + \sum_i \omega(\mathbf{r} - \mathbf{R}_i) \quad (1.1)$$

in which many-body interactions will be neglected. The present author has already derived a general formula for interacting Hamiltonians.⁹ In the present paper, however, we will make the most of the above limitation to simplify the expression in the noninteracting case. It is indeed shown to be simplified to a great extent, into the form of the correlation function of the unperturbed system, and the calculation of the Hall effect is thus reduced to the level of, say, the dc conductivity. We also find a very important fact; *the Hall conductivity of independent electrons is determined solely by states at the Fermi level.* The result is important both physically and in practice, showing that the Hall effect of independent electrons is a Fermi-surface property, just like the dc conductivity.

We will not start from Itoh's formula for interacting

Hamiltonians. Instead we follow a similar argument to that adopted in his paper, starting from the Kubo formula for the one-electron Hamiltonian (1.1) in the presence of a uniform magnetic field. This is presented in the next section. We actually sum up all the contributions without recourse to any approximation and obtain the finite and gauge-invariant expression for the Hall conductivity. It is represented by an energy integration of a four-vertex correlation function, multiplied by the energy derivative of the Fermi-Dirac distribution function, so that the above statements are manifestly shown. The derivation also shows how the gauge invariance is ensured. In Sec. IV an approximate evaluation of the for-

mula is attempted. The ladder approximation is employed as an example and we recover the one-electron version of the result obtained for interacting Hamiltonians.^{8,10} Also, a comparison is made to a formula proposed by Morgan and Howson,¹¹ who adopted different approaches to the problem. Our formula is shown to disagree with theirs.

II. DERIVATION OF THE FORMULA

We start from the following variation of the Kubo formula for the conductivity tensor¹² of independent electrons

$$\sigma_{\mu\nu} = ie^2 \hbar \int dE f(E) \left\langle \text{Tr} \left[(\nu_H)_\mu \frac{dG_H^+}{dE} (\nu_H)_\nu \delta(E - \mathcal{H}) - (\nu_H)_\mu \delta(E - \mathcal{H}) (\nu_H)_\nu \frac{dG_H^-}{dE} \right] \right\rangle, \quad (2.1)$$

where ν_H and G_H^\pm (G_H^\pm) are the velocity operator and the retarded (advanced) Green function for an electron under a magnetic field, i.e.,

$$\nu_H = \nu - \frac{e}{mc} \mathbf{A}(\mathbf{r}), \quad (2.2)$$

$$G_H^\pm = (E \pm i\delta - \mathcal{H})^{-1}, \quad (2.3)$$

and $\langle \dots \rangle$ denotes an ensemble average over the distribution of the scatterers. The one-electron Hamiltonian \mathcal{H} in G_H^\pm and $\delta(E - \mathcal{H})$ includes the perturbation due to the magnetic field

$$H_{\text{ex}} = -\frac{e}{2mc} [\mathbf{p} \cdot \mathbf{A}(\mathbf{r}) + \mathbf{A}(\mathbf{r}) \cdot \mathbf{p}] \quad (2.4)$$

so that, to the first order in the magnetic field,

$$G_H^\pm = G^\pm - \frac{e}{2mc} G^\pm [\mathbf{p} \cdot \mathbf{A}(\mathbf{r}) + \mathbf{A}(\mathbf{r}) \cdot \mathbf{p}] G^\pm. \quad (2.5)$$

In the above equation $\mathbf{A}(\mathbf{r})$ is the vector potential and the symbols without the subscript H are to denote the field-independent quantities. We have retained only the terms up to the first order in the magnetic field; the same procedure will be followed hereafter. The second term of (2.2) is sometimes called the diamagnetic current. The δ functions in (2.1) can be eliminated by using the relation

$$\delta(E - \mathcal{H}) = \frac{i}{2\pi} (G_H^+ - G_H^-). \quad (2.6)$$

We can then gather up all the contributions to (2.1), which are linear in $\mathbf{A}(\mathbf{r})$, by substituting (2.2) and (2.4) into (2.1). It must be noted that each term is dependent on the choice of the gauge although the totality of the linear contributions is gauge invariant. It is also noted that, in the case of a uniform magnetic field, the vector potential becomes macroscopically large, as is seen from the forms of the symmetric gauge or of the Landau gauge. Under these particular choices of the gauge, each of the contributions obtained above becomes not only macroscopically large but also dependent on the sample shape. Therefore special care must be paid to obtain a

physically meaningful result, namely the correct thermodynamic limit in finite and gauge-invariant form.

We shall follow the procedure invented by Fukuyama, Ebisawa, and Wada⁸ to handle the above problem. This is described as follows. First the vector potential is assumed to have the periodic form

$$\mathbf{A}(\mathbf{r}) = \mathbf{A}_q e^{i\mathbf{q} \cdot \mathbf{r}} \quad (2.7)$$

characterized by a wave number \mathbf{q} . The magnetic field is then given by

$$\mathbf{H} = i(\mathbf{q} \times \mathbf{A}_q) e^{i\mathbf{q} \cdot \mathbf{r}} \quad (2.8)$$

and the uniform magnetic field is described as a limit of $q \equiv |\mathbf{q}| \rightarrow 0$. It is important to note that \mathbf{A}_q diverges as $1/q$ in this limit. The wave number is therefore kept finite throughout the calculation, so that the periodicity is much less than the sample size. We then sum up all the contributions. If we carefully combine the terms we obtain a gauge-invariant and divergence-free expression, and the thermodynamic limit is taken naturally. Finally, the magnitude of the wave number $q \equiv |\mathbf{q}|$ is set equal to zero at the end of the calculation.

The procedure described above was followed by Fukuyama, Ebisawa, and Wada in the ladder approximation in the case of interacting Hamiltonians. The argument was extended later to all orders by Itoh,⁹ without recourse to any approximation. In principle, the latter result includes the case of independent electrons as a special case (some discussion is given in his paper about this problem). Instead of deriving a formula for this special case starting from Itoh's expression, here we deal with the noninteracting electrons from the beginning. We first note that the following expansion is sufficient for our purpose:

$$\mathbf{A}(\mathbf{r}) \cong \mathbf{A}_q + \mathbf{A}_q(i\mathbf{q} \cdot \mathbf{r}); \quad (2.9)$$

the higher-order terms do not survive in the limit of $q \rightarrow 0$. We now gather up all the contributions to (2.1), which are linear in \mathbf{A}_q , by following the procedure described earlier. The result is

$$\sigma_{\mu\nu} = -(e^2\hbar/2) \int \frac{dE}{2\pi} f(E) \zeta^{\mu\nu}(E), \quad (2.10)$$

$$\zeta^{\mu\nu}(E) = \zeta_d^{\mu\nu}(E) + \zeta_c^{\mu\nu}(E), \quad (2.11)$$

$$\begin{aligned} \zeta_d^{\mu\nu}(E) = & \frac{2e}{mc} A_q^\alpha \{ -\delta_{\alpha\mu} \langle \text{Tr}[(G^+)'\epsilon_\nu G^+] \rangle - \delta_{\alpha\nu} \langle \text{Tr}[\epsilon_\mu(G^+)G^+] \rangle + \delta_{\alpha\mu} \langle \text{Tr}[(G^+)'\epsilon_\nu G^-] \rangle + \delta_{\alpha\nu} \langle \text{Tr}[\epsilon_\mu(G^+)G^-] \rangle \\ & + \delta_{\alpha\mu} \langle \text{Tr}[G^+\epsilon_\nu(G^-)'] \rangle + \delta_{\alpha\nu} \langle \text{Tr}[\epsilon_\mu G^+(G^-)'] \rangle - \delta_{\alpha\mu} \langle \text{Tr}[G^-\epsilon_\nu(G^-)'] \rangle - \delta_{\alpha\nu} \langle \text{Tr}[\epsilon_\mu G^-(G^-)'] \rangle \} \\ & + \frac{2e}{c} A_q^\alpha \{ -\langle \text{Tr}[\epsilon_\mu(G^+\epsilon_\alpha G^+)'\epsilon_\nu G^+] \rangle + \langle \text{Tr}[\epsilon_\mu(G^+\epsilon_\alpha G^+)'\epsilon_\nu G] \rangle \\ & + \langle \text{Tr}[\epsilon_\mu G^+\epsilon_\nu(G^-\epsilon_\alpha G^-)'] \rangle - \langle \text{Tr}[\epsilon_\mu G^-\epsilon_\nu(G^-\epsilon_\alpha G^-)'] \rangle \\ & - \langle \text{Tr}[\epsilon_\mu(G^+)'\epsilon_\nu G^+\epsilon_\alpha G^+] \rangle + \langle \text{Tr}[\epsilon_\mu(G^+)'\epsilon_\nu G^-\epsilon_\alpha G^-] \rangle \\ & + \langle \text{Tr}[\epsilon_\mu G^+\epsilon_\alpha G^+\epsilon_\nu(G^-)'] \rangle - \langle \text{Tr}[\epsilon_\mu G^-\epsilon_\alpha G^-\epsilon_\nu(G^-)'] \rangle \}, \end{aligned} \quad (2.12)$$

$$\begin{aligned} \zeta_c^{\mu\nu}(E) = & i \frac{2e}{mc} A_q^\alpha q_\beta \{ -\delta_{\alpha\mu} \langle \text{Tr}[r_\beta(G^+)'\epsilon_\nu G^+] \rangle - \delta_{\alpha\nu} \langle \text{Tr}[\epsilon_\mu(G^+)r_\beta G^+] \rangle \\ & + \delta_{\alpha\mu} \langle \text{Tr}[r_\beta(G^+)'\epsilon_\nu G^-] \rangle + \delta_{\alpha\nu} \langle \text{Tr}[\epsilon_\mu(G^+)r_\beta G^-] \rangle \\ & + \delta_{\alpha\mu} \langle \text{Tr}[r_\beta G^+\epsilon_\nu(G^-)'] \rangle + \delta_{\alpha\nu} \langle \text{Tr}[\epsilon_\mu G^+ r_\beta(G^-)'] \rangle \\ & - \delta_{\alpha\mu} \langle \text{Tr}[r_\beta G^-\epsilon_\nu(G^-)'] \rangle - \delta_{\alpha\nu} \langle \text{Tr}[\epsilon_\mu G^- r_\beta(G^-)'] \rangle \} \\ & + i \frac{e}{mc} A_q^\alpha q_\beta \{ -\langle \text{Tr}[\epsilon_\mu(G^+ r_\beta p_\alpha G^+)'\epsilon_\nu G^+] \rangle - \langle \text{Tr}[\epsilon_\mu(G^+ p_\alpha r_\beta G^+)'\epsilon_\nu G^+] \rangle \\ & + \langle \text{Tr}[\epsilon_\mu(G^+ r_\beta p_\alpha G^+)'\epsilon_\nu G^-] \rangle + \langle \text{Tr}[\epsilon_\mu(G^+ p_\alpha r_\beta G^+)'\epsilon_\nu G^-] \rangle \\ & + \langle \text{Tr}[\epsilon_\mu G^+\epsilon_\nu(G^- r_\beta p_\alpha G^-)'] \rangle + \langle \text{Tr}[\epsilon_\mu G^+\epsilon_\nu(G^- p_\alpha r_\beta G^-)'] \rangle \\ & - \langle \text{Tr}[\epsilon_\mu G^-\epsilon_\nu(G^- r_\beta p_\alpha G^-)'] \rangle - \langle \text{Tr}[\epsilon_\mu G^-\epsilon_\nu(G^- p_\alpha r_\beta G^-)'] \rangle \\ & - \langle \text{Tr}[\epsilon_\mu(G^+)'\epsilon_\nu G^+ r_\beta p_\alpha G^+] \rangle - \langle \text{Tr}[\epsilon_\mu(G^+)'\epsilon_\nu G^+ p_\alpha r_\beta G^+] \rangle \\ & + \langle \text{Tr}[\epsilon_\mu(G^+)'\epsilon_\nu G^- r_\beta p_\alpha G^-] \rangle + \langle \text{Tr}[\epsilon_\mu(G^+)'\epsilon_\nu G^- p_\alpha r_\beta G^-] \rangle \\ & + \langle \text{Tr}[\epsilon_\mu G^+ r_\beta p_\alpha G^+\epsilon_\nu(G^-)'] \rangle + \langle \text{Tr}[\epsilon_\mu G^+ p_\alpha r_\beta G^+\epsilon_\nu(G^-)'] \rangle \\ & - \langle \text{Tr}[\epsilon_\mu G^- r_\beta p_\alpha G^-\epsilon_\nu(G^-)'] \rangle - \langle \text{Tr}[\epsilon_\mu G^- p_\alpha r_\beta G^-\epsilon_\nu(G^-)'] \rangle \}, \end{aligned} \quad (2.13)$$

where $\zeta_d^{\mu\nu}(E)$ and $\zeta_c^{\mu\nu}(E)$ denote the contributions from the first and the second terms of (2.9), respectively. The summation over α and β is assumed in (2.12) and (2.13), and $(\cdot \cdot \cdot)'$ denotes the differentiation with respect to E . The terms in (2.12) are proportional to A_q^α and divergent, but we will shortly see that they are canceled out. Those in (2.13) are finite and expected to be combined in a gauge-invariant form. The latter are further classified into three groups. The first one includes only the retarded Green functions G^+ . We denote this by $\zeta_c^{\mu\nu}(++)$. Likewise we define $\zeta_c^{\mu\nu}(--)$ by the sum of all the terms with G^- only. The rest of the terms involve both G^+ and G^- , and we denote the contribution from them by $\zeta_c^{\mu\nu}(+-)$. Each of these contributions will be seen to be gauge invariant. In the following we discuss $\zeta_d^{\mu\nu}(E)$, $\zeta_c^{\mu\nu}(++) = \zeta_c^{\mu\nu}(--)^*$, and $\zeta_c^{\mu\nu}(+-)$ separately.

A. Proof of $\zeta_d^{\mu\nu}(E) = 0$

We rewrite Eq. (2.12) by using the identities

$$(G)' = -G^2 \quad (2.14)$$

and

$$G\epsilon_\alpha G = \frac{1}{i\hbar} [r_\alpha, G], \quad (2.15)$$

The first identity is trivial, and the second is readily proved from $\epsilon_\alpha = -(1/i\hbar)[r_\alpha, G^{-1}]$. In both cases G denotes either G^+ or G^- . Then we obtain

$$\begin{aligned}
\xi_d^{\mu\nu}(E) = & \frac{2e}{mc} A_q^\alpha \langle \text{Tr} \{ \delta_{\alpha\mu} [(G^+)^3 \epsilon_\nu - (G^+)^2 \epsilon_\nu G^- - G^+ \epsilon_\nu (G^-)^2 + \epsilon_\nu (G^-)^3] \\
& + \delta_{\alpha\nu} [\epsilon_\mu (G^+)^3 - G^- \epsilon_\mu (G^+)^2 - (G^-)^2 \epsilon_\mu G^+ + (G^-)^3 \epsilon_\mu] \} \rangle \\
& + \frac{2e}{i\hbar c} A_q^\alpha \langle \text{Tr} \{ \epsilon_\mu [r_\alpha, (G^+)^2] \epsilon_\nu G^+ - \epsilon_\mu [r_\alpha, (G^+)^2] \epsilon_\nu G^- \\
& - \epsilon_\mu G^+ \epsilon_\nu [r_\alpha, (G^-)^2] + \epsilon_\mu G^- \epsilon_\nu [r_\alpha, (G^-)^2] + \epsilon_\mu (G^+)^2 \epsilon_\nu [r_\alpha, G^+] - \epsilon_\mu (G^+)^2 \epsilon_\nu [r_\alpha, G^-] \\
& - \epsilon_\mu [r_\alpha, G^+] \epsilon_\nu (G^-)^2 + \epsilon_\mu [r_\alpha, G^-] \epsilon_\nu (G^-)^2 \} \rangle . \tag{2.16}
\end{aligned}$$

The first term in the above equation is the contributions from the diamagnetic current. The second term is simplified by recombining the terms in the curly brackets. For example, the combination of the first and the fifth terms yields

$$\begin{aligned}
& \frac{2e}{i\hbar c} A_q^\alpha \langle \text{Tr} \{ \epsilon_\mu [r_\alpha, (G^+)^2] \epsilon_\nu G^+ + \epsilon_\mu (G^+)^2 \epsilon_\nu [r_\alpha, G^+] \} \rangle \\
& = \frac{2e}{i\hbar c} A_q^\alpha \langle \text{Tr} \{ -\epsilon_\mu (G^+)^2 [r_\alpha, \epsilon_\nu] G^+ - [r_\alpha, \epsilon_\mu] (G^+)^2 \epsilon_\nu G^+ \} \rangle \\
& = \frac{2e}{mc} A_q^\alpha \langle \text{Tr} [-\delta_{\alpha\nu} \epsilon_\mu (G^+)^3 - \delta_{\alpha\mu} (G^+)^3 \epsilon_\nu] \rangle , \tag{2.17}
\end{aligned}$$

where we have used the cyclic rotations of the operators in the trace operation and also the commutation relation

$$[r_\alpha, \epsilon_\beta] = (i\hbar/m) \delta_{\alpha\beta} . \tag{2.18}$$

Equation (2.17) is seen to cancel two of the diamagnetic-current contributions in (2.16). Likewise we can combine the second, third, and fourth terms with the sixth, seventh, and eighth terms, respectively, and the cancellation is readily proved.

B. Expressions for $\xi_c^{\mu\nu}(++)$ and $\xi_c^{\mu\nu}(--)$

By collecting all those contributions to (2.13) with G^+ only, we obtain

$$\begin{aligned}
\xi_c^{\mu\nu}(++) = & \frac{ie}{c} q_\beta A_q^\alpha \{ (2/m) \delta_{\alpha\mu} \langle \text{Tr} [r_\beta (G^+)^2 \epsilon_\nu G^+] \rangle_{(a)} + (2/m) \delta_{\alpha\nu} \langle \text{Tr} [\epsilon_\mu (G^+)^2 r_\beta G^+] \rangle_{(b)} \\
& + \langle \text{Tr} [\epsilon_\mu (G^+)^2 \epsilon_\nu G^+ (r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta) G^+] \rangle_{(c)} \\
& + \langle \text{Tr} [\epsilon_\mu (G^+)^2 (r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta) G^+ \epsilon_\nu G^+] \rangle_{(d)} \\
& + \langle \text{Tr} [\epsilon_\mu G^+ (r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta) (G^+)^2 \epsilon_\nu G^+] \rangle_{(e)} \} , \tag{2.19}
\end{aligned}$$

where we have already used (2.14), and each term has been labeled as $\eta_{(a)}, \dots, \eta_{(e)}$ for later use. A similar expression is also obtained for $\xi_c^{\mu\nu}(--)$. After some manipulations (see the Appendix) we can transform (2.19) into the following form:

$$\begin{aligned}
\xi_c^{\mu\nu}(++) = & -\frac{e}{2c\hbar} q_\beta A_q^\alpha \frac{\partial}{\partial E} \{ (2/m) \delta_{\alpha\nu} \langle \text{Tr} (r_\beta r_\mu G^+) \rangle_{(f)} - (2/m) \delta_{\alpha\mu} \langle \text{Tr} (r_\beta r_\nu G^+) \rangle_{(g)} \\
& + \langle \text{Tr} [G^+ (r_\mu v_\nu - r_\nu v_\mu) G^+ (r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta)] \rangle_{(h)} \} . \tag{2.20}
\end{aligned}$$

Therefore, by a partial integration with respect to E , the contribution of $\xi_c^{\mu\nu}(++)$ to $\sigma_{\mu\nu}$ is seen to be on shell. The gauge invariance of $\xi_c^{\mu\nu}(++)$ however, is, not explicitly shown by (2.20). We need further manipulations for its manifestation. For this purpose we use the following identity:

$$\begin{aligned}
G(r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta) G & = \frac{1}{i\hbar} [r_\alpha r_\beta, G] + G(\epsilon_\alpha r_\beta - \epsilon_\beta r_\alpha) G \\
& = \frac{1}{i\hbar} [r_\alpha r_\beta, G] + (\delta_{\alpha\mu} \delta_{\beta\nu} - \delta_{\alpha\nu} \delta_{\beta\mu}) G(\epsilon_\mu r_\nu - \epsilon_\nu r_\mu) G , \tag{2.21}
\end{aligned}$$

where G denotes either G^+ or G^- . The first line of the above relation is readily proved by using $v_\alpha = -(1/i\hbar)[r_\alpha, G^{-1}]$ and Eq. (2.15). The second line is obtained if we recall that μ and ν directions are perpendicular to the magnetic field \mathbf{H} , and that, from Eq. (2.8), the vectors \mathbf{A}_q and \mathbf{q} are also perpendicular to \mathbf{H} . In other words, we can assume that the indices α and β are either μ or ν . By using (2.21) the expression (2.20) is transformed to (see the Appendix)

$$\zeta_c^{\mu\nu}(++) = \left[\frac{ie}{2c} \right] q_\beta (\delta_{\alpha\mu} \delta_{\beta\nu} - \delta_{\alpha\nu} \delta_{\beta\mu}) A_q^\alpha \frac{\partial}{\partial E} \{ \langle \text{Tr}[\epsilon_\nu G^+ \epsilon_\mu G^+ (r_\mu \epsilon_\nu - r_\nu \epsilon_\mu) G^+] \rangle - \langle \text{Tr}[\epsilon_\mu G^+ \epsilon_\nu G^+ (r_\mu \epsilon_\nu - r_\nu \epsilon_\mu) G^+] \rangle \} . \quad (2.22)$$

By noting that

$$H = -iq_\beta (\delta_{\alpha\mu} \delta_{\beta\nu} - \delta_{\alpha\nu} \delta_{\beta\mu}) A_q^\alpha , \quad (2.23)$$

the vector potential is eliminated from (2.21) and the expression is manifestly gauge invariant. It is interesting to note that the angular momentum operator appears in (2.21). The calculation of the contribution from $\zeta_c^{\mu\nu}(++)$ is therefore reduced to that of the correlation functions with three vertices, one of which corresponds to the angular momentum operator. This corresponds to the expression obtained by Itoh [Ref. 9, Eq. (3.7)].

In many cases it is practical to avoid the angular momentum operator. This is possible at the cost of introducing one more vertex (see the Appendix) and we obtain a very simple expression

$$\zeta_c^{\mu\nu}(++) = -\frac{ie\hbar}{2c} H \frac{\partial}{\partial E} \langle \text{Tr}(\epsilon_\mu G^+ \epsilon_\nu G^+ \epsilon_\mu G^+ \epsilon_\nu G^+) \rangle . \quad (2.24)$$

The expression for $\zeta_c^{\mu\nu}(--)$ is also obtained by replacing μ by ν and G^+ by G^- in (2.24),

$$\zeta_c^{\mu\nu}(--) = +\frac{ie\hbar}{2c} H \frac{\partial}{\partial E} \langle \text{Tr}(\epsilon_\mu G^- \epsilon_\nu G^- \epsilon_\mu G^- \epsilon_\nu G^-) \rangle . \quad (2.25)$$

C. Expression for $\zeta_c^{\mu\nu}(+-)$

The rest of the contributions to (2.13), involving both G^+ and G^- , gives the expression for $\zeta_c^{\mu\nu}(+-)$. By noting (2.14), it is obviously written in the following form of the energy derivatives:

$$\begin{aligned} \zeta_c^{\mu\nu}(+-) = & +\frac{ie}{2c} q_\beta A_q^\alpha \frac{\partial}{\partial E} \{ (2/m) \delta_{\alpha\mu} \langle \text{Tr}(r_\beta G^+ \epsilon_\nu G^-) \rangle_{(i)} + (2/m) \delta_{\alpha\nu} \langle \text{Tr}(r_\beta G^- \epsilon_\mu G^+) \rangle_{(j)} \\ & + \langle \text{Tr}[\epsilon_\mu G^+ (r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta) G^+ \epsilon_\nu G^+] \rangle_{(k)} + \langle \text{Tr}[\epsilon_\nu G^- (r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta) G^- \epsilon_\mu G^+] \rangle_{(l)} \} , \end{aligned} \quad (2.26)$$

where, again, the terms have been labeled. After similar manipulations to those used for $\zeta_c^{\mu\nu}(++)$, Eq. (2.26) is transformed into a gauge-invariant form (see the Appendix):

$$\begin{aligned} \zeta_c^{\mu\nu}(+-) = & +\frac{eH}{2c} \frac{\partial}{\partial E} \{ (1/m) \langle \text{Tr}(\epsilon_\mu G^+ r_\mu G^-) \rangle - (1/m) \langle \text{Tr}(\epsilon_\nu G^- r_\nu G^+) \rangle \\ & + \langle \text{Tr}[\epsilon_\mu G^+ \epsilon_\nu G^- (r_\mu \epsilon_\nu - r_\nu \epsilon_\mu) G^-] \rangle + \langle \text{Tr}[\epsilon_\nu G^- \epsilon_\mu G^+ (r_\mu \epsilon_\nu - r_\nu \epsilon_\mu) G^+] \rangle \} . \end{aligned} \quad (2.27)$$

We can further eliminate the angular momentum components from the above expressions (see the Appendix)

$$\zeta_c^{\mu\nu}(+-) = -\frac{ie\hbar}{c} H \frac{\partial}{\partial E} [\langle \text{Tr}(\epsilon_\mu G^+ \epsilon_\nu G^- \epsilon_\mu G^- \epsilon_\nu G^-) \rangle_{(m)} - \langle \text{Tr}(\epsilon_\nu G^- \epsilon_\mu G^+ \epsilon_\nu G^+ \epsilon_\mu G^+) \rangle_{(n)}] , \quad (2.28)$$

which is quite analogous to (2.24) and (2.25).

From Eqs. (2.10), (2.24), (2.25), and (2.28) we finally obtain the gauge-invariant and rigorous expression for the Hall conductivity in the on-shell form

$$\sigma_{\mu\nu}/H = -\frac{e^3 \hbar^2}{2c} \int \frac{dE}{2\pi} \left[-\frac{\partial f}{\partial E} \right] \text{Im} [2 \langle \text{Tr}(\epsilon_\mu G^+ \epsilon_\nu G^- \epsilon_\mu G^- \epsilon_\nu G^-) \rangle + \langle \text{Tr}(\epsilon_\mu G^+ \epsilon_\nu G^+ \epsilon_\mu G^+ \epsilon_\nu G^+) \rangle] . \quad (2.29)$$

The calculation of the Hall effect is thus reduced to that of the four-vertex correlation function. It is further transformed into a compact form

$$\sigma_{\mu\nu}/H = -\frac{\pi e^3 \hbar^2}{c} \int \frac{dE}{2\pi} \left[-\frac{\partial f}{\partial E} \right] \text{Im} \langle \text{Tr}[\epsilon_\mu G^+ \epsilon_\nu \delta(E - \mathcal{H}) \epsilon_\mu G^+ \epsilon_\nu \delta(E - \mathcal{H})] \rangle , \quad (2.30)$$

where \mathcal{H} is the Hamiltonian (1.1) without magnetic field. The second expression, (2.30), is obtained from (2.29) by inserting into the curly brackets the term

$$+ \langle \text{Tr}(\epsilon_\mu G^+ \epsilon_\nu G^- \epsilon_\mu G^+ \epsilon_\nu G^-) \rangle ,$$

which is a real quantity and so contributes nothing, and also replacing half of the first term by the negative of its complex conjugate.

III. APPLICATIONS
TO DISORDERED SYSTEMS

Our formula (2.29) is particularly useful for disordered systems if the one-electron picture holds. Since it is written in terms of the Green-function operators, the diagrammatic expansion can be used to evaluate it. When the resistance is caused by the random array of rather weak scattering potentials, the nearly-free-electron representation is a suitable starting point. Interesting examples are liquid or amorphous simple metals, in which only *sp* electrons are considered to be relevant to the conduction. The Edwards theory¹³ for the resistivity calculation, which is the first to discuss the electron transport by combining the Green-function technique and the Kubo formula, is still one of the few reliable theories for these systems.¹⁴ This is the ideal test case for our formula and we attempt to evaluate Eq. (2.30) by using the approximation adopted in his theory.

The scattering between the two states **k** and **k'** is given

in the Edwards theory by the (averaged) matrix element $|\langle \mathbf{k} | w | \mathbf{k}' \rangle|^2 a(\mathbf{k} - \mathbf{k}')$, where *w* is the scattering (pseudo)potential and *a*(**k** - **k'**) is the atomic structure factor. The two-vertex Kubo-Greenwood formula for the dc conductivity is then evaluated by summing up the ladder diagrams for a current vertex. The procedure is readily extended to our four-vertex formula (2.29) as shown in Figs. 1 and 2. In these figures the hatched corners represent the current vertex functions calculated in the ladder approximation. There exist three possible cases, $v^{++}(\mathbf{k})$, $v^{--}(\mathbf{k})$, and $v^{+-}(\mathbf{k})$, and also there appear two components (μ or ν) for each. The bold lines are the renormalized Green functions G_k^+ and G_k^- and the hatched belts in the figures represent the scattering kernels in the ladder approximation, for the particle-particle, hole-hole, and particle-hole pairs. The diagrams (D) and (H) in Fig. 1 are seen to cancel each other; they have been introduced artificially in order to make the calculation easier. The contributions from these diagrams are

$$I^{(A)+(E)} = 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \sigma_{\mu}^{+-}(\mathbf{k}) \sigma_{\nu}^{+-}(\mathbf{k}) \{ G_{\mathbf{k}}^+ (G_{\mathbf{k}}^-)^3 \sigma_{\mu}^{--}(\mathbf{k}) \sigma_{\nu}^{--}(\mathbf{k}) - (G_{\mathbf{k}}^+)^3 G_{\mathbf{k}}^- \sigma_{\mu}^{++}(\mathbf{k}) \sigma_{\nu}^{++}(\mathbf{k}) \}, \quad (3.1)$$

$$I^{(B)+(F)} = \int \frac{d\mathbf{k}}{(2\pi)^3} \sigma_{\mu}^{+-}(\mathbf{k}) \sigma_{\nu}^{+-}(\mathbf{k}) \left[G_{\mathbf{k}}^+ (G_{\mathbf{k}}^-)^2 \frac{1}{\hbar} \frac{\partial}{\partial k_{\nu}} \sigma_{\mu}^{--}(\mathbf{k}) - (G_{\mathbf{k}}^+)^2 G_{\mathbf{k}}^- \frac{1}{\hbar} \frac{\partial}{\partial k_{\mu}} \sigma_{\nu}^{++}(\mathbf{k}) \right], \quad (3.2)$$

$$I^{(C)+(D)} = 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \sigma_{\nu}^{+-}(\mathbf{k}) G_{\mathbf{k}}^+ \frac{1}{\hbar} \frac{\partial}{\partial k_{\mu}} G_{\mathbf{k}}^- \frac{1}{\hbar} \frac{\partial}{\partial k_{\nu}} \sigma_{\mu}^{+-}(\mathbf{k}), \quad (3.3)$$

$$I^{(G)+(H)} = -2 \int \frac{d\mathbf{k}}{(2\pi)^3} \sigma_{\mu}^{+-}(\mathbf{k}) \frac{1}{\hbar} \frac{\partial}{\partial k_{\mu}} G_{\mathbf{k}}^+ G_{\mathbf{k}}^- \frac{1}{\hbar} \frac{\partial}{\partial k_{\mu}} \sigma_{\nu}^{+-}(\mathbf{k}). \quad (3.4)$$

$$2i \text{Im} \langle \text{Tr } v_{\mu} G_{\nu}^+ G_{\nu}^- v_{\mu} G_{\nu}^+ G_{\nu}^- \rangle$$

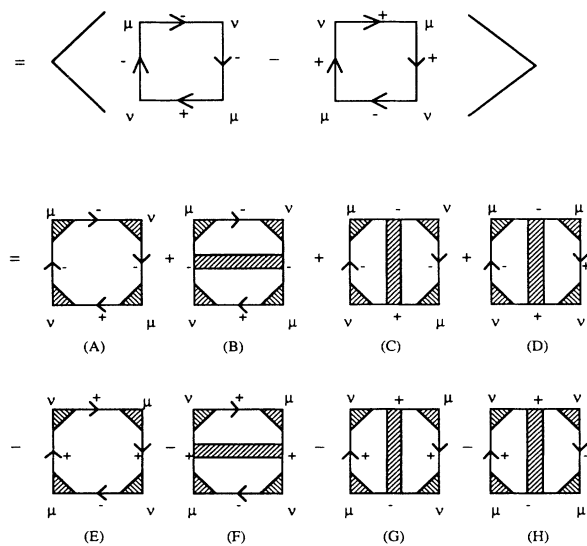


FIG. 1. The diagram representations of the first term of Eq. (2.29). The diagrams (D) and (H) are introduced artificially, and cancel each other.

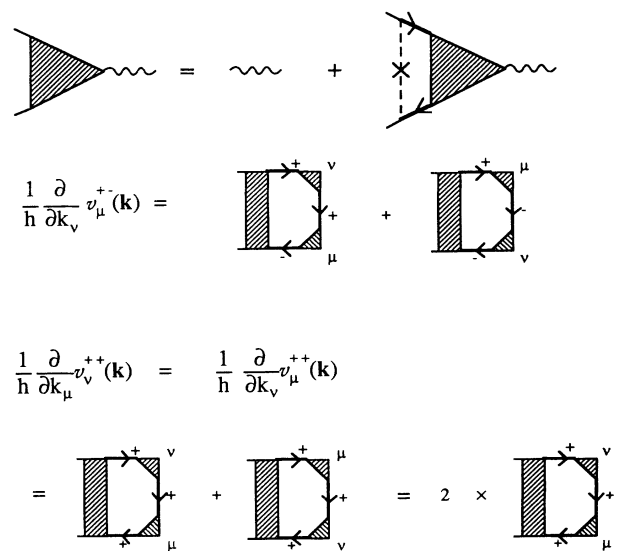


FIG. 2. The diagram equations for the current vertices in Edwards theory (the first line). The expressions for their momentum derivatives (the second and the third lines) are obtained by differentiating the first line for the particle-hole and the hole-hole pairs. The identity for the particle-particle pair is the same as the second line.

Equation (3.1) is trivial. In deriving Eqs. (3.2)–(3.4) we have used the relations shown in Fig. 2. By noting the Ward identities

$$\frac{1}{\hbar} \frac{\partial}{\partial \mathbf{k}} G_{\mathbf{k}}^+ = (G_{\mathbf{k}}^+)^2 \sigma^{++}(\mathbf{k}) \quad (3.5a)$$

and

$$\frac{1}{\hbar} \frac{\partial}{\partial \mathbf{k}} G_{\mathbf{k}}^- = (G_{\mathbf{k}}^-)^2 \sigma^{--}(\mathbf{k}), \quad (3.5b)$$

Eqs. (3.1) and (3.2) are combined as

$$I^{(A)+(E)+(B)+(F)} = \frac{1}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} \sigma_{\mu}^{+-}(\mathbf{k}) \sigma_{\nu}^{+-}(\mathbf{k}) \left[G_{\mathbf{k}}^+ \frac{\partial}{\partial k_{\nu}} [(G_{\mathbf{k}}^-)^2 \sigma_{\mu}^{--}(\mathbf{k})] - \frac{\partial}{\partial k_{\mu}} [(G_{\mathbf{k}}^+)^2 \sigma_{\nu}^{++}(\mathbf{k})] G_{\mathbf{k}}^- \right]. \quad (3.6)$$

It is then easy to show by partial integrations that the summation over (A)–(H) amounts to

$$I^{(A)+(B)+\dots+(H)} = \frac{1}{\hbar^2} \int \frac{d\mathbf{k}}{(2\pi)^3} \left[\left[\sigma_{\nu}^{+-}(\mathbf{k}) \frac{\partial}{\partial k_{\mu}} \sigma_{\mu}^{+-}(\mathbf{k}) - \sigma_{\mu}^{+-}(\mathbf{k}) \frac{\partial}{\partial k_{\mu}} \sigma_{\nu}^{+-}(\mathbf{k}) \right] \frac{\partial}{\partial k_{\nu}} G_{\mathbf{k}}^+ G_{\mathbf{k}}^- \right. \\ \left. - \left[\sigma_{\mu}^{+-}(\mathbf{k}) \frac{\partial}{\partial k_{\nu}} \sigma_{\nu}^{+-}(\mathbf{k}) - \sigma_{\nu}^{+-}(\mathbf{k}) \frac{\partial}{\partial k_{\nu}} \sigma_{\mu}^{+-}(\mathbf{k}) \right] G_{\mathbf{k}}^+ \frac{\partial}{\partial k_{\mu}} G_{\mathbf{k}}^- \right]. \quad (3.7)$$

As for the second term of (2.29), we only need to sum up three diagrams with the topological structures of (A), (B), and (C) in Fig. 1. The result is

$$\langle \text{Tr}(\sigma_{\mu} G^+ \sigma_{\nu} G^+ \sigma_{\mu} G^+ \sigma_{\nu} G^+) \rangle = 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \left[[\sigma_{\mu}^{++}(\mathbf{k}) \sigma_{\nu}^{++}(\mathbf{k})]^2 (G_{\mathbf{k}}^+)^4 + \sigma_{\mu}^{++}(\mathbf{k}) \sigma_{\nu}^{++}(\mathbf{k}) \frac{1}{\hbar} \frac{\partial}{\partial k_{\nu}} \sigma_{\mu}^{++}(\mathbf{k}) (G_{\mathbf{k}}^+)^3 \right]. \quad (3.8)$$

Again, by noting (3.5b) and using partial integration, the first term is seen to be written as

$$-\frac{2}{3} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\hbar} \frac{\partial}{\partial k_{\nu}} \{ [\sigma_{\mu}^{++}(\mathbf{k})]^2 \sigma_{\nu}^{++}(\mathbf{k}) \} (G_{\mathbf{k}}^+)^3, \quad (3.9)$$

so that it becomes

$$\langle \text{Tr}(\sigma_{\mu} G^+ \sigma_{\nu} G^+ \sigma_{\mu} G^+ \sigma_{\nu} G^+) \rangle = \frac{2}{3} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{\hbar} \left[\frac{\partial}{\partial k_{\nu}} \sigma_{\mu}^{++}(\mathbf{k}) \sigma_{\mu}^{++}(\mathbf{k}) \sigma_{\nu}^{++}(\mathbf{k}) - \frac{\partial}{\partial k_{\nu}} \sigma_{\nu}^{++}(\mathbf{k}) [\sigma_{\mu}^{++}(\mathbf{k})]^2 \right] (G_{\mathbf{k}}^+)^3. \quad (3.10)$$

Finally, we make use of the isotropy of the system; namely we write the vertex functions in the following forms,

$$\sigma^{+-}(\mathbf{k}) = \hat{\mathbf{k}} \cdot \sigma_{\mathbf{k}}^{+-} \quad (3.11a)$$

and

$$\sigma^{++}(\mathbf{k}) = \hat{\mathbf{k}} \cdot \sigma_{\mathbf{k}}^{++}, \quad (3.11b)$$

where $\sigma_{\mathbf{k}}^{+-}$ and $\sigma_{\mathbf{k}}^{++}$ are functions of $k = |\mathbf{k}|$ only, and $\hat{\mathbf{k}} = \mathbf{k}/k$. From (2.29), (3.7), and (3.10) we obtain, after some manipulations using (3.11a) and (3.11b),

$$\sigma_{xy}/H = \frac{e^3 \hbar}{3\pi c} \int dE \left[-\frac{\partial f}{\partial E} \right] \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{k} \text{Im}[(\sigma_{\mathbf{k}}^{+-})^2 \sigma_{\mathbf{k}}^{++} (G_{\mathbf{k}}^+)^2 G_{\mathbf{k}}^- - \frac{1}{3} (\sigma_{\mathbf{k}}^{++})^3 (G_{\mathbf{k}}^+)^3]. \quad (3.12)$$

The above expression is different from the one obtained by Fukuyama *et al.*,⁸ who adopted the same approximation to the interacting electrons in evaluating the on-shell contributions. The off-shell contributions have been evaluated explicitly by the present author¹⁰ and their inclusion is shown to lead exactly to the above form, as it should be. Once we know the exact formula (2.29), the derivation becomes simple for noninteracting electrons. Equation (3.12) has been applied to liquid and amorphous metals recently.¹⁵

When the vertex corrections are neglected, Eq. (3.12) is reduced to the following form:

$$\sigma_{xy}/H = -\frac{4\pi^2 e^3 \hbar}{9c} \int dE \left[-\frac{\partial f}{\partial E} \right] \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{k} (\sigma_{\mathbf{k}})^3 \left[-\frac{1}{\pi} \text{Im} G_{\mathbf{k}}^+ \right]^3, \quad (3.13)$$

where $\sigma_{\mathbf{k}} = \hbar \mathbf{k}/m$. The above expression is known to be a typical form of the Hall conductivity when the vertex correction does not exist.^{2-4,6,16}

IV. DISCUSSION

It is a well-known fact that the dc conductivity is determined solely by the electronic states at the Fermi level. This conclusion is valid both for the noninteracting and the interacting electrons. In particular, it is explicitly shown by the Kubo-Greenwood formula that

$$\sigma_{\mu\mu} = \pi e^2 \hbar \int dE \left[-\frac{\partial f}{\partial E} \right] \langle \text{Tr}[\epsilon_{\mu} \delta(E - \mathcal{H}) \epsilon_{\mu} \delta(E - \mathcal{H})] \rangle \quad (4.1)$$

for the noninteracting case (for interacting electrons, see Mahan¹⁷). The present study has shown that the same can be said for the Hall conductivity of noninteracting electrons. In this respect it is interesting to note that the second form (2.30) of our formula is somewhat similar to (4.1). The present author¹⁰ has also shown, under some approximation, that the situation is the same for interacting electrons. He indeed obtained the same expression as (3.12) in the ladder approximation, allowing for any kind of many-body interaction. It is therefore strongly suggested that our theorem is possibly generalized to interacting electrons.

A simple physical explanation is possible for the dc conductivity. When the system is under an electric field the distribution of electrons in \mathbf{k} space is distorted by an

infinitesimal amount. However, the states inside the Fermi surface do not cause any change to the total current because they cancel out, so that there should arise no net current in the zero electric field. We therefore need to calculate only the distortion of the distribution function, which has finite amplitude only in the vicinity of the Fermi surface. When a magnetic field is applied, the cancellation occurs in a very complicated way. The current component associated with each electronic state acquires an additional term, i.e., the diamagnetic current, as is shown in Eq. (2.2), so the states inside the Fermi surface do have the contribution to the conduction. It is therefore surprising that the total contribution has been written in the on-shell form. Also, the final expression is surprisingly simple, considering the rather enormous calculations involved in its derivation.

In this connection it should be worth noting the similarity of the present work to that of Baranger and Stone,¹⁸ who claimed that, in the case of two-dimensional noninteracting electrons, the *conductance* of any multiprobe structure of finite size under an arbitrary magnetic field is determined solely by the states at the Fermi level. These authors have also derived rigorous expressions for the conductances in terms of the exact Green functions under a magnetic field. The starting point of Baranger and Stone is the inhomogeneous version of the following expression for the conductivity tensor:

$$\sigma_{\mu\nu} = \frac{e^2 \hbar}{2\pi} \int dE \left[-\frac{\partial f(E)}{\partial E} \right] \langle \text{Tr}[(\epsilon_H)_{\mu} G_H^+ (\epsilon_H)_{\nu} G_H^-] \rangle - \frac{e^2 \hbar}{2\pi} \int dE f(E) \left\langle \text{Tr} \left[(\epsilon_H)_{\mu} \frac{dG_H^+}{dE} (\epsilon_H)_{\nu} G_H^+ + (\epsilon_H)_{\mu} G_H^- (\epsilon_H)_{\nu} \frac{dG_H^-}{dE} \right] \right\rangle, \quad (4.2)$$

which is obtained from (2.1) by integrating by parts with respect to energy [cf. Eq. (52) in their paper]. They then show that the off-shell contributions, which correspond to the second term of the above equation, do not contribute to the *conductance of any finite multiprobe structure*. Several points should be borne in mind in making comparison between the two theories.

In spite of the close resemblance between the two works, there seems to be a fundamental difference. First, it is obvious that the off-shell contribution definitely has a finite contribution to the *conductivity of a macroscopic sample* [for example, without this term we would not recover the correct expression for the longitudinal conductivity (4.1)]. Second, the boundary condition of the problem treated in their paper is different from ours. In particular, they have adopted the Landau gauge to examine the asymptotic behavior of the Green functions, a procedure which cannot be applied to the present case of a macroscopic system under a uniform magnetic field, which involves intrinsically the divergence, as we have often emphasized. The physical meanings of the two similar assertions are therefore different. No gauge-invariant (and finite) expression would have been ob-

tained for the conductivity if we had omitted the off-shell term in (4.2). In the actual Hall constant measurement the Hall field is exerted upon electrons in the system to cancel the Lorentz force. Our calculation is therefore a determination of the macroscopic conductivity tensor which makes the net current flow in the infinite system along the direction of the applied electric field when the total field is exerted upon electrons.

A similar formula to Eq. (2.30) has also been proposed rather recently by Morgan and Howson,¹¹ the validity of which was then questioned by the present author from the viewpoint of the gauge invariance and the associated divergence problem.^{9,10} In their expression all G 's in Eq. (2.30) are replaced by $\delta(E - \mathcal{H})$ and the operation to take the imaginary part is not required. In their derivation the contributions from the principal part integrations are set equal to zero and this is probably the major source of the error. Also, they have omitted from symmetry considerations the macroscopic integrations including the vector potential in a particular choice of the gauge. As we have seen, it is essential to take the proper macroscopic limit when we deal with the system under a uniform magnetic field, so their symmetry consideration will not

be justified.

In any case, the Hall effect has been rigorously shown to be attributed to the states at the Fermi level, and this fact has important physical implications. It explains, for example, why the measured Hall constants of liquid noble metals are so close to the free-electron value, despite the fact that the d -resonance states are very close to the Fermi level. As an example of more recent experiments, we note the measurements by Häussler and Baumann,¹⁹ who discovered systematic changes of the Hall constant, as well as of other transport properties of the noble-metal-based amorphous alloys, as functions of the carrier number. We can now confirm that their data on the Hall constant have depicted the change of the scattering strength at the Fermi level associated with the structural changes.

Besides its fundamental importance, the formula is also useful for practical purposes; we have already seen in the preceding section that the analytic calculation is

simplified to a great extent compared to the earlier treatments. It is generally useful for disordered materials, and more sophisticated approximations can be used to evaluate the formula. Among others the effective medium approximation (EMA) is most interesting,²⁰ in connection with the positive Hall coefficients observed in many liquid and amorphous metals including the transition-metal or rare-earth elements, and the author hopes to deal with this problem in future publications.

APPENDIX

The details of the proofs of the equations are given in this appendix.

Equation (2.20)

First we show that the terms $\eta_{(a)}, \dots, \eta_{(e)}$ in Eq. (2.19) are rewritten as

$$\eta_{(a)} + \eta_{(b)} = \frac{1}{(i\hbar)^2} \{ (2/m) \delta_{\alpha\mu} \langle \text{tr}(r_\beta G^+ [r_\nu, G^+]) \rangle + (2/m) \delta_{\alpha\nu} \langle \text{Tr}([r_\mu, G^+] G^+ r_\beta) \rangle \}, \quad (\text{A1})$$

$$\eta_{(c)} = \frac{1}{(i\hbar)^2} \langle \text{Tr}([r_\mu, G^+] [r_\nu, G^+] (r_\beta v_\alpha + v_\alpha r_\beta)) \rangle, \quad (\text{A2})$$

$$\begin{aligned} \eta_{(d)} = & \frac{1}{2i\hbar} \langle \text{Tr}[G^+ (r_\mu v_\nu - r_\nu v_\mu) (G^+)^2 (r_\beta v_\alpha + v_\alpha r_\beta)] \rangle \\ & + \frac{1}{2(i\hbar)^2} \langle \text{Tr}((r_\nu [r_\mu, G^+] - [r_\nu, G^+] r_\mu) G^+ (r_\beta v_\alpha + v_\alpha r_\beta)) \rangle, \end{aligned} \quad (\text{A3})$$

$$\begin{aligned} \eta_{(e)} = & \frac{1}{2i\hbar} \langle \text{Tr}[G^+ (r_\beta v_\alpha + v_\alpha r_\beta) (G^+)^2 (r_\mu v_\nu - r_\nu v_\mu)] \rangle \\ & + \frac{1}{2(i\hbar)^2} \langle \text{Tr}((r_\beta v_\alpha + v_\alpha r_\beta) G^+ (r_\nu [r_\mu, G^+] - [r_\nu, G^+] r_\mu)) \rangle. \end{aligned} \quad (\text{A4})$$

Equations (A1) and (A2) are readily obtained by using (2.15). As for (A3), we first note that the two alternative forms for (d) are obtained by using (2.15) in different ways:

$$\eta_{(d)} = \frac{1}{i\hbar} \langle \text{Tr}\{[r_\nu, G^+] v_\mu (G^+)^2 (r_\beta v_\alpha + v_\alpha r_\beta)\} \rangle \quad (\text{A5})$$

or

$$= \frac{1}{i\hbar} \langle \text{tr}\{G^+ v_\nu [r_\mu, G^+] G^+ (r_\beta v_\alpha + v_\alpha r_\beta)\} \rangle.$$

Each of the above expressions are further transformed by using (2.15) again:

$$\eta_{(d)} = -\frac{1}{i\hbar} \langle \text{Tr}[G^+ r_\nu v_\mu (G^+)^2 (r_\beta v_\alpha + v_\alpha r_\beta)] \rangle + \frac{1}{(i\hbar)^2} \langle \text{Tr}\{r_\nu [r_\mu, G^+] G^+ (r_\beta v_\alpha + v_\alpha r_\beta)\} \rangle \quad (\text{A6})$$

or

$$= \frac{1}{i\hbar} \langle \text{Tr}[G^+ v_\nu r_\mu (G^+)^2 (r_\beta v_\alpha + v_\alpha r_\beta)] \rangle - \frac{1}{(i\hbar)^2} \langle \text{Tr}\{[r_\nu, G^+] r_\mu G^+ (r_\beta v_\alpha + v_\alpha r_\beta)\} \rangle.$$

Equation (A3) is then obtained by adding the above two expressions and dividing by 2. Equation (A4) is derived in exactly the same way.

Now the terms in (A2)–(A4) are seen to be proportional either to $(i\hbar)^{-1}$ or $(i\hbar)^{-2}$. We can combine the terms in the latter group and, after some rearrangement by using the cyclic rotations of the operators in the trace operation, we have

$$\begin{aligned}
\eta_{(c)} + \eta_{(d)} + \eta_{(e)} = & \frac{1}{2i\hbar} \{ \langle \text{Tr}[G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)(G^+)^2(r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta)] \rangle + \langle \text{Tr}[(G^+)^2(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+(r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta)] \rangle \} \\
& + \frac{1}{(i\hbar)^2} \{ \langle \text{Tr}(G^+ r_\mu G^+[r_\nu, r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta]) \rangle - \langle \text{Tr}(G^+ r_\nu G^+[r_\mu, r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta]) \rangle \} \\
& + \frac{1}{2(i\hbar)^2} (- \langle \text{Tr}\{r_\mu (G^+)^2[r_\nu, r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta]\} \rangle + \langle \text{Tr}\{(G^+)^2 r_\nu [r_\mu, r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta]\} \rangle). \tag{A7}
\end{aligned}$$

The commutators appearing in the above equation can be simplified by using (2.18). The resultant terms are partly canceled by the contributions from $\eta_{(a)} + \eta_{(b)}$ of Eq. (A1). Equation (2.19) then becomes

$$\begin{aligned}
\xi_c^{\mu\nu}(++) = & \frac{e}{2c\hbar} q_\beta A_q^\alpha \{ (2/m)\delta_{\alpha\nu} \langle \text{Tr}[r_\beta r_\mu (G^+)^2] \rangle - (2/m)\delta_{\alpha\mu} \langle \text{Tr}[r_\beta r_\nu (G^+)^2] \rangle \} \\
& + \langle \text{Tr}[G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)(G^+)^2(r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta)] \rangle \\
& + \langle \text{Tr}[(G^+)^2(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+(r_\beta \epsilon_\alpha + \epsilon_\alpha r_\beta)] \rangle. \tag{A8}
\end{aligned}$$

Thus, from (2.14), the terms $\eta_{(f)}$, $\eta_{(g)}$, and $\eta_{(h)}$ in (2.20) are obtained.

Equation (2.22)

The term $\eta_{(h)}$ in Eq. (2.20) is rewritten by using (2.21) as

$$\eta_{(h)} = -\frac{1}{i\hbar} \langle \text{Tr}([r_\alpha r_\beta, r_\mu \epsilon_\nu - r_\nu \epsilon_\mu]G^+) \rangle - (\delta_{\alpha\mu}\delta_{\beta\nu} - \delta_{\alpha\nu}\delta_{\beta\mu}) \langle \text{Tr}[(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle \tag{A9}$$

where the cyclic rotation has been used to deal with the commutator $[r_\alpha r_\beta, G^+]$ to obtain the first term. The second term is transformed by using (2.15):

$$\begin{aligned}
& \langle \text{Tr}[(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle \\
& = \langle \text{Tr}[\epsilon_\nu (i\hbar G^+ \epsilon_\mu G^+ + G^+ r_\mu)(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle + \langle \text{Tr}[(i\hbar G^+ \epsilon_\nu G^+ - r_\nu G^+) \epsilon_\mu G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)] \rangle.
\end{aligned}$$

By using (2.15) again, it becomes

$$\begin{aligned}
& = 2i\hbar \langle \text{Tr}[\epsilon_\nu G^+ \epsilon_\mu G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle \\
& \quad + \frac{1}{i\hbar} \langle \text{Tr}\{[r_\nu, G^+]r_\mu(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)\} \rangle - \frac{1}{i\hbar} \langle \text{Tr}\{r_\nu[r_\mu, G^+](r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)\} \rangle.
\end{aligned}$$

The second and the third terms can be simplified by using the cyclic rotations and applying (2.18). We thus have

$$\begin{aligned}
& \langle \text{Tr}[(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle \\
& = 2i\hbar \langle \text{Tr}[\epsilon_\nu G^+ \epsilon_\mu G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle - (1/m)[\langle \text{Tr}(G^+ r_\mu r_\mu) \rangle + \langle \text{Tr}(G^+ r_\nu r_\nu) \rangle]. \tag{A10}
\end{aligned}$$

The left-hand side of the above equation is seen to be symmetric with respect to μ and ν . Therefore we can symmetrize the right-hand side:

$$\begin{aligned}
& \langle \text{Tr}[(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle \\
& = i\hbar \{ \langle \text{Tr}[\epsilon_\nu G^+ \epsilon_\mu G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle - \langle \text{Tr}[\epsilon_\mu G^+ \epsilon_\nu G^+(r_\mu \epsilon_\nu - r_\nu \epsilon_\mu)G^+] \rangle \} \\
& \quad - (1/m)[\langle \text{Tr}(G^+ r_\mu r_\mu) \rangle + \langle \text{Tr}(G^+ r_\nu r_\nu) \rangle]. \tag{A11}
\end{aligned}$$

Now we substitute (A11) into (A9). Together with the factor $(\delta_{\alpha\mu}\delta_{\beta\nu} - \delta_{\alpha\nu}\delta_{\beta\mu})$ in (A9), the second term of (A11) yields the terms which just cancels $\eta_{(f)}$ and $\eta_{(g)}$ in (2.20), and we finally arrive at (2.22).

Equation (2.24)

It is easier to show that Eq. (2.24) is reduced to (2.22). By using (2.15) differently we obtain the following alternative forms:

$$\begin{aligned}
& \langle \text{Tr}(\epsilon_\mu G^+ \epsilon_\nu G^+ \epsilon_\mu G^+ \epsilon_\nu G^+) \rangle \\
& = \frac{1}{i\hbar} \langle \text{Tr}(\epsilon_\mu G^+ \epsilon_\nu G^+ \epsilon_\mu [r_\nu, G^+]) \rangle \\
& \text{or} \\
& = \frac{1}{i\hbar} \langle \text{Tr}(\epsilon_\nu G^+ \epsilon_\mu G^+ \epsilon_\nu [r_\mu, G^+]) \rangle. \tag{A12}
\end{aligned}$$

By adding the above two and then dividing by 2, we obtain

$$= \frac{1}{2i\hbar} \{ \langle \text{Tr}[\sigma_v G^+ \sigma_\mu G^+ (r_\mu \sigma_v - r_v \sigma_\mu) G^+] \rangle - \langle \text{Tr}[\sigma_\mu G^+ \sigma_v G^+ (r_\mu \sigma_v - r_v \sigma_\mu) G^+] \rangle \}$$

$$\eta_{(k)} + \eta_{(l)} = \frac{1}{i\hbar} \langle \text{Tr}(\sigma_\mu [r_\alpha r_\beta, G^+] \sigma_v G^-) \rangle_{(p)} + \frac{1}{i\hbar} \langle \text{Tr}(\sigma_v [r_\alpha r_\beta, G^-] \sigma_\mu G^+) \rangle_{(q)} - (\delta_{\alpha\mu} \delta_{\beta\nu} - \delta_{\alpha\nu} \delta_{\beta\mu}) \{ \langle \text{Tr}[\sigma_\mu G^+ (r_\mu \sigma_v - r_v \sigma_\mu) G^+ \sigma_v G^-] \rangle + \langle \text{Tr}[\sigma_v G^- (r_\mu \sigma_v - r_v \sigma_\mu) G^- \sigma_\mu G^+] \rangle \}. \quad (\text{A13})$$

The third term in the above equation has the desired gauge invariance, due to the factor $(\delta_{\alpha\mu} \delta_{\beta\nu} - \delta_{\alpha\nu} \delta_{\beta\mu})$. The first and second terms, labeled as $\eta_{(p)}$ and $\eta_{(q)}$, are recombined by using the cyclic rotations as

$$\eta_{(p)} + \eta_{(q)} = -\frac{1}{i\hbar} \langle \text{Tr}([r_\alpha r_\beta, \sigma_\mu] G^+ \sigma_v G^-) \rangle - \frac{1}{i\hbar} \langle \text{Tr}([r_\alpha r_\beta, \sigma_v] G^- \sigma_\mu G^+) \rangle. \quad (\text{A14})$$

The commutators in the above equation are simplified by using (2.18). The resulting terms are partly canceled by $\eta_{(i)}$ and $\eta_{(j)}$, leaving just the gauge-invariant contributions proportional to $(\delta_{\alpha\mu} \delta_{\beta\nu} - \delta_{\alpha\nu} \delta_{\beta\mu})$. We thus obtain (2.27).

Equation (2.28)

The proof of (2.28) is somewhat similar to that of (2.24). We shall derive (2.27) from (2.28) to show their equivalence. By using (2.18) we rewrite the term $\eta_{(m)}$ in (2.28) as

$$\eta_{(m)} = +\frac{1}{2i\hbar} \{ \langle \text{Tr}(\sigma_\mu G^+ \sigma_v [r_\mu, G^-] \sigma_v G^-) \rangle + \langle \text{Tr}(\sigma_\mu G^+ \sigma_v G^- \sigma_\mu [r_v, G^-]) \rangle \},$$

$$\eta_{(m)} + \eta_{(n)} = -\frac{1}{2i\hbar} \{ \langle \text{Tr}[\sigma_\mu G^+ \sigma_v G^- (r_\mu \sigma_v - r_v \sigma_\mu) G^-] \rangle + \langle \text{Tr}[\sigma_v G^- \sigma_\mu G^+ (r_\mu \sigma_v - r_v \sigma_\mu) G^+] \rangle \} + \frac{1}{2(i\hbar)^2} \{ \langle \text{Tr}(G^+ \sigma_v G^- [r_\mu r_\nu, \sigma_\mu]) \rangle - \langle \text{Tr}(G^- \sigma_\mu G^+ [r_\mu r_\nu, \sigma_v]) \rangle \}, \quad (\text{A17})$$

where we have used the cyclic rotations to compose the commutators. The second term of (A17) is further simplified by using (2.18) and the equivalence of (2.28) to (2.27) is then trivial.

and the equivalence between (2.24) and (2.22) has thus been proved.

Equation (2.27)

The terms $\eta_{(k)}$ and $\eta_{(l)}$ in (2.26) can be transformed by using (2.21), as in the case of $\eta_{(h)}$:

where we have summed up two different expressions for $\eta_{(m)}$ and divided by 2. We decompose the commutators and obtain

$$\eta_{(m)} = -\frac{1}{2i\hbar} \langle \text{Tr}[\sigma_\mu G^+ \sigma_v G^- (r_\mu \sigma_v - r_v \sigma_\mu) G^-] \rangle + \frac{1}{2(i\hbar)^2} \{ \langle \text{Tr}(\sigma_\mu G^+ \sigma_v r_\mu [r_\nu, G^-]) \rangle - \langle \text{Tr}(r_\nu \sigma_\mu G^+ \sigma_v [r_\mu, G^-]) \rangle \}, \quad (\text{A15})$$

where we have again used (2.18) to derive the second term. In the same way we also obtain the expression for the term $\eta_{(n)}$ in (2.28):

$$\eta_{(n)} = -\frac{1}{2i\hbar} \langle \text{Tr}[\sigma_v G^- \sigma_\mu G^+ (r_\mu \sigma_v - r_v \sigma_\mu) G^+] \rangle - \frac{1}{2(i\hbar)^2} \{ \langle \text{Tr}(\sigma_v G^- \sigma_\mu r_\nu [r_\mu, G^+]) \rangle - \langle \text{Tr}(r_\mu \sigma_v G^- \sigma_\mu [r_\nu, G^+]) \rangle \} \quad (\text{A16})$$

and therefore,

¹See, for a review, *The Hall Effect and its Applications* edited by H. U. Kunzi and H. J. Güntherodt (Plenum, New York, 1980).

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