Sum Rule for the Optical Hall Angle

H. D. Drew[1] and P. Coleman[2,3]
[1]Department of Physics, University of Maryland, College Park, Maryland 20742
[2]Serin Laboratory, Rutgers University, P.O. Box 849, Piscataway, New Jersey 08855-0849
[3]Institute for Theoretical Physics, UCSB, Santa Barbara, California 93106-4030
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We consider the optical Hall conductivity of a general electronic medium and prove that the optical Hall angle obeys a new sum rule. This sum rule governs the response of an electronic fluid to a Lorentz force and can be thought of as a counterpart to the f-sum rule in optical conductivity. The physical meaning of this sum rule is discussed, giving a number of examples of its application to a variety of electronic media. [S0031-9007(97)02494-0]

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The optical Hall conductivity is a new experimental probe [1,2]. Like the optical conductivity, by extending Hall conductivity measurements into the microwave and far infrared, it should be possible to extract a host of new information about the properties of electronic systems in a magnetic field [3]. Electronic systems where this probe might prove particularly important are the cuprate metals [2], type II superconductors [4,5], and the integer and fractional quantum Hall systems [6].

A powerful tool in the analysis of the optical conductivity is the f-sum rule [7]

$$2\int_0^\infty \frac{d\omega}{\pi}\,\sigma'_{xx}(\omega) = \epsilon_0\omega_p^2\,, \tag{1}$$

where $\sigma\prime_{xx}(\omega)$ is the real part of the conductivity and ω_p is the plasma frequency. The distribution of optical spectral weight in an electronic medium gives us important information about the underlying physics. In this paper, we introduce a corresponding sum rule for the analysis of the optical Hall angle. The optical Hall angle,

$$t_H(\omega) \equiv \tan\theta_H(\omega) = \frac{\sigma_{xy}(\omega)}{\sigma_{xx}(\omega)}\,, \tag{2}$$

where σ_{xx} and σ_{xy} are the optical and Hall conductivities, respectively, and can be measured directly in optical transmission experiments [1,2].

We shall show that this response function obeys the sum rule

$$2\int_0^\infty \frac{d\omega}{\pi}\,t'_H(\omega) = \omega_H\,, \tag{3}$$

where the Hall frequency ω_H is unaffected by interactions, and in the absence of a lattice corresponds to the bare cyclotron frequency $\omega_c = eB/m$. This sum rule governs the retarded response to a Lorentz force. The way in which the corresponding spectral weight redistributes enables us to make some important qualitative distinctions between normal metals, superconductors, cuprate metals, and quantum Hall systems.

Sum rules are a statement about the asymptotic properties of a response function. A key element in the proof of a sum rule is the existence of a Kramers-Krönig relation that links the real and imaginary parts of a response function to a spectral function. Normally, an explicit spectral decomposition of the response function is used to show that a Kramers-Krönig relation exists. Unfortunately, this is not possible for the ac Hall angle, which determines the response to an injected current rather than an applied field. If an injected current, $j_y(\omega) = \sigma_{xx}(\omega)E_y(\omega)$, is applied to a material, the transverse Hall current is given by (Fig. 1)

$$j_x(\omega) = \sigma_{xy}(\omega)E_y(\omega) = t_H(\omega)j_y(\omega)\,. \tag{4}$$

To prove the existence of a spectral representation of the optical Hall angle, we shall appeal to its analyticity. Sufficient conditions for $t_H(\omega)$ to satisfy a Kramers-Krönig relation are (i) that it is analytic in the upper-half complex plane and (ii) that it vanishes at least as fast as $1/\omega$ at high frequencies [8]. Since $t_H(\omega)$ is a quotient, its analyticity requires that $\sigma_{xx}(\omega)$ has no zeros in the upper-half complex plane. This follows from a general theorem [8] that a generalized susceptibility $\sigma(\omega)$ can only take on real values along the imaginary axis $\omega = iy$, where it varies monotonically from its value at $\omega = i\delta$ to zero at $\omega = i\infty$. It follows that causal

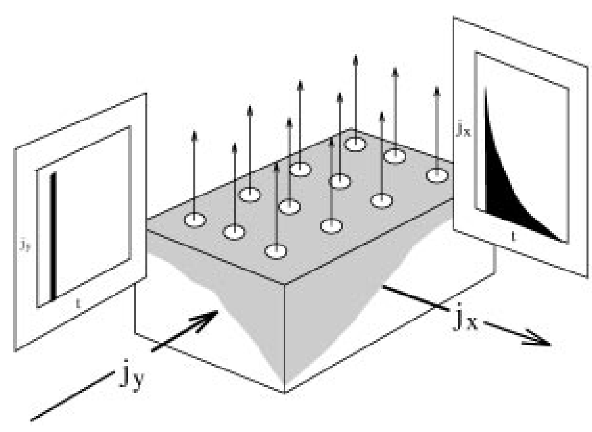

FIG. 1. Illustrating the Hall response $j_y(\omega) = t_H(\omega)j_x(\omega)$ to an input current pulse.

response functions have neither poles *nor* zeros in the upper-half complex plane. The ratio of conductivities $t_H(\omega) = \sigma_{xy}(\omega)/\sigma_{xx}(\omega)$ is consequently analytic (with no zeros) in the upper-half complex plane. We shall shortly use microscopic considerations to show at high frequencies

$$\lim_{|\omega|\to\infty}[-i\omega t_H(\omega)] = \omega_H\,, \tag{5}$$

where ω_H will be given an explicit form. Using the Kramers-Krönig relation, it then follows that [8]

$$t_H(\omega) = \frac{1}{\pi i}\, P\int_{-\infty}^{\infty} dx\, \frac{1}{(x-\omega)}\, t_H(x)\,. \tag{6}$$

Multiplying (6) by $-i\omega$ and taking $\omega \to \infty$, we obtain

$$\omega_H = \frac{1}{\pi}\int_{-\infty}^{\infty} dx t_H(x)\,. \tag{7}$$

The sum rule follows with the additional information that the real and imaginary parts of $t_H(x)$ are even and odd functions of x, respectively.

To complete our proof, we now derive an expression for ω_H. Consider a system of interacting electrons described by the Hamiltonian

$$H[A] = \sum_{\vec p} \epsilon_{\vec p - e\vec A}\hat n_{\vec p} + \dots\,, \tag{8}$$

where $\hat n_{\vec p} = \psi^\dagger_{\vec p}\psi_{\vec p}$ is the number operator at momentum $\vec p$, $\vec A$ is the coarse-grained vector potential, and $\epsilon(\vec p)$ is the electron kinetic energy. $H[A]$ may contain any additional interaction terms or impurity scattering terms as long as these terms do not involve the vector potential and thus do not modify the current operator. Let us take the magnetic field to lie along the z direction, assuming the conductivity to be isotropic about this axis. Using the Kubo formula, the conductivity tensor in the basal plane can be written in the form $\sigma_{ab}(\omega) = Q_{ab}(\omega)/(-i\omega)$, where

$$Q_{ab}(\omega) = \epsilon_0\omega_p^2\delta_{ab} - i\langle[\hat j_a(\omega), \hat j_b(-\omega)]\rangle\,. \tag{9}$$

The first term describes the instantaneous diamagnetic response. The second term involves the current operator $\vec j = e\sum_{\vec p}\psi^\dagger_{\vec p}\vec v_{\vec p - e\vec A}\psi_{\vec p}$, where $\vec v_{\vec p} = \nabla_{\vec p}\epsilon_{\vec p}$ defines the velocity operator. Carrying out a spectral decomposition of the current-current correlation function, one obtains [3]

$$i\langle[\hat j_a(\omega), \hat j_b(-\omega)]\rangle = \int \frac{dx}{\pi}\,\frac{1}{\omega - x}\, Q''_{ab}(x)\,,$$

$$\begin{aligned} Q''_{ab}(x) = \pi(1 - e^{-\beta x})\sum_{\zeta\lambda} e^{-\beta(E_\zeta - \Omega)} \\ \times \langle\zeta|j_a|\lambda\rangle\langle\lambda|j_b|\zeta\rangle \\ \times \delta(x - E_\zeta + E_\lambda)\,. \end{aligned} \tag{10}$$

It follows that the asymptotic high-frequency behavior is given by [3]

$$Q_{ab}(z) = \epsilon_0\omega_p^2\delta_{ab} + \langle[\hat j_a, \hat j_b]\rangle/z\,, \quad (|z|\to\infty)\,, \tag{11}$$

so that, at high frequencies, $t_H(\omega) = Q_{xy}(\omega)/Q_{xx}(\omega) \to \omega_H/(-i\omega)$, where

$$i\omega_H = \lim_{|z|\to\infty}\frac{zQ_{xy}(z)}{Q_{xx}(z)} = \frac{\langle[\hat j_x, \hat j_y]\rangle}{\epsilon_0\omega_p^2}\,. \tag{12}$$

The plasma frequency of the medium is given by

$$\epsilon_0\omega_p^2 = \langle\nabla^2_{\vec A_x}H[A]\rangle = (e^2/2)\sum_{\vec p}\mathrm{Tr}(\underline{m}^{-1}_{\vec p})\langle\hat n_{\vec p}\rangle\,, \tag{13}$$

where $[\underline{m}^{-1}_{\vec p}]_{ab} = \nabla^2_{ab}\epsilon_{\vec p}$ is the effective mass tensor. Provided that the magnetic flux per unit cell is far less than a flux quantum h/e, we may use a weak field approximation to $[\hat j_x, \hat j_y]$, obtained by linearizing the velocity operator

$$\vec v_{\vec p - e\vec A} = \vec v_{\vec p_0} + \underline{m}^{-1}_{\vec p}(\vec{\not p} - \vec p_0)\,, \tag{14}$$

where $\vec{\not p} = \vec p - e\vec A$. Since $[\not p_x, \not p_y] = -ieB_z$, it follows that $-i[\vec v_x, \vec v_y] = (eB)\det(\underline{m}^{-1}_{\vec p})$. Writing $\hat j = e\sum\times \psi^\dagger_{\vec p}\vec v_{\vec{\not p}}\psi_{\vec p}$, we obtain the operator identity

$$-i[\hat j_x, \hat j_y] = \sum_{\vec p}[e^3B\det(\underline{m}^{-1}_{\vec p})]\hat n_{\vec p} + O(B^3)\,. \tag{15}$$

Combining (13) and (15),

$$\omega_H = eB\frac{\sum_{\vec p}\det[\underline{m}^{-1}_{\vec p}]\langle\hat n_{\vec p}\rangle}{\frac{1}{2}\sum_{\vec p}\mathrm{Tr}[\underline{m}^{-1}_{\vec p}]\langle\hat n_{\vec p}\rangle}\,. \tag{16}$$

For a parabolic band, (16) reverts to the free cyclotron frequency $\omega_c = eB/m$. Since all electronic systems are ultimately derived from a system with a quadratic dispersion, this is an exact result, but recovery of the full spectral weight requires an integration over all interband transitions. The usefulness of the sum rule derives from the fact that, when the bands are well separated, an effective sum rule applies to the lowest band.

Physically, the Hall sum rule is closely related to the short-time response of Hall currents. To see this, one should suppose that a small pulse of current $j_t(t)$ is injected into a material. The induced Hall current is given by (Fig. 1)

$$j_x(t) = \int_{-\infty}^{t} dt' t_H(t - t')j_y(t')\,, \tag{17}$$

where $t_H(t - t')$ is the Fourier transform of $t_H(\omega)$. Since $t_H(\omega) \sim \omega_H/-i\omega$ at high frequencies, it follows that $t_H(t - t') \sim \omega_H\Theta(t - t')$ at short times. In other words, during a short current pulse,

$$d\vec j/dt = -\omega_H\hat z\times\vec j\,. \tag{18}$$

This is nothing more than the precession of the current in the magnetic field. ω_H is thus identified as the effective cyclotron frequency for the electron fluid. Reflecting this conclusion, the general expression for ω_H is dominated by contributions far from the Fermi surface, and we expect it to be only weakly temperature dependent. Suppose the system possesses a Fermi surface where $n_p = 1$ far inside and $n_p = 0$ far outside. To extract the dominant contribution to ω_H, we restrict the integrals within each Fermi surface sheet and set $n_{\vec{p}} = 1$. Both integrands are total derivatives,

$$\det[\underline{m}_{\vec{p}}^{-1}] = \frac{1}{2}\nabla \times [(\vec{u} \times \nabla)\vec{u}],$$
$$\mathrm{Tr}[\underline{m}_{\vec{p}}^{-1}] = \nabla \cdot \vec{u}, \quad (19)$$

where $\vec{a} \times \vec{b} = \epsilon_{\alpha\beta} a_\alpha b_\beta$ denotes the two-dimensional cross product, $\vec{u}$ denotes the component of the group velocity in the x-y plane, and $(\nabla\vec{u})_{ab} = \underline{m}_{ab}^{-1}$. This enables us to rewrite the Hall sum rule as a ratio of Fermi surface integrals,

$$\omega_H = eB \frac{\int dp_z \int_{\mathrm{FS}} \vec{u} \times d\vec{u}}{\int dp_z \int_{\mathrm{FS}} d\vec{S} \cdot \vec{u}} + O(\delta\epsilon^2/\epsilon_F^2). \quad (20)$$

Here, FS denotes a line integral around all sheets of the Fermi surface at constant p_z, $d\vec{S}$ denotes the surface increment that lies perpendicular to this line, $d\vec{u} = dk$. $\nabla\vec{u}$ is the change in $\vec{u}$ along the line, and $\delta\epsilon/\epsilon_F$ is the ratio of the smearing of the Fermi surface to the Fermi energy. The numerator is readily identified as twice the area swept out by the Fermi velocity vector $\vec{u}$ in passing around the Fermi surface. A variant of this expression has been obtained by Ong [9] using the Boltzmann transport theory.

We now illustrate the qualitative implications of the Hall sum rule using a few physical examples. In the case of a simple metal, the transverse optical conductivity in a magnetic field is given by

$$\sigma_\pm = \sigma_{xx} \pm i\sigma_{xy} = \frac{ne^2}{m} \frac{1}{\Gamma_{\mathrm{tr}} - i(\omega \mp \omega_c)} \quad (21)$$

so that the optical conductivity is peaked at the cyclotron frequency. Remarkably, these poles do not enter the Hall response,

$$t_H(\omega) = \frac{\omega_c}{\Gamma_{\mathrm{tr}} - i\omega}, \quad (22)$$

which has the same form as the zero field optical conductivity [Fig. 2(a)]. The Hall spectral weight is peaked at zero frequency and is independent of carrier density. In this case, the Hall constant $R_H(\omega) = t_H(\omega)/\sigma_{xx}(\omega)$ is frequency independent.

An intriguing exception to this behavior is found in the normal state of the cuprate metals. Unlike conventional metals, transport measurements indicate that $\Gamma_{\mathrm{tr}} \sim 2T$, but dc Hall measurements show that $[\cot\theta_H] \sim T^2$ is a quadratic function of temperature [10]. Since the dc Hall angle scales as $1/T^2$, the sum rule tells us that the Hall relaxation rate Γ_H is a quadratic function of temperature $\Gamma_H = T^2/W$ and that, furthermore, $\sigma_{xy} \sim 1/(\Gamma_{\mathrm{tr}}\Gamma_H)$. This multiplicative combination of relaxation rates is unprecedented and does not fit into a conventional picture of normal metals. Based on this observation, Anderson has conjectured that the Hall currents are subject to an autonomous decay process that depends quadratically on temperature $\Gamma_H \propto T^2$ [11]. This controversial interpretation follows naturally from a Hall sum rule, in a fashion that is independent of the microscopic physics. A definitive measurement of the quadratic temperature dependence of the Hall decay rate would constitute a striking confirmation of the power of the Hall sum rule [Fig. 2(b)].

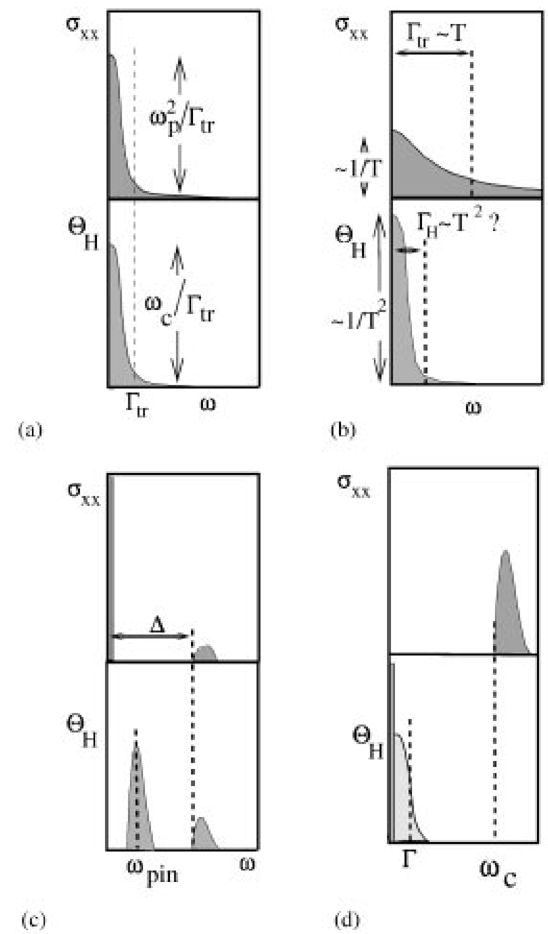

FIG. 2. Contrasting the optical conductivity and the optical Hall angle in (a) a simple metal, (b) a cuprate metal, (c) a superconductor, and (d) a quantum Hall fluid. The superconductor displays condensation in the dynamical conductivity; the quantum Hall fluid displays a condensation in the optical Hall angle at a Hall plateau which periodically broadens into a Drude peak between plateaus.

As a second application, consider a type II superconductor with a pinned vortex lattice. In a superconductor, the optical conductivity condenses into a zero-frequency delta function peak. However, the same condensation does not take place in the Hall angle because, unlike conventional currents, super currents cannot precess in a magnetic field: The deflection of a supercurrent requires a sideways movement of the flux lattice. Hsu [12] has computed the Hall response of a pinned flux lattice and has shown that it is shifted to the flux lattice pinning frequency [Fig. 2(c)], as observed in recent experiments on YBCO [13]. Perhaps the most important property of the sum rule in this respect, however, is that it does not depend on temperature or the thermodynamic state of the system. Despite the radically different physics of the vortex lattice and the normal state, the Hall sum is identical.

As a final example, we consider the Hall response of a two-dimensional electron gas in a high magnetic field. When the quantized, or fractionally quantized Hall ground state develops, the conductivity (21) is qualitatively modified, leading to the quantum Hall effect in the dc response: $\sigma_{xx} = 0$, $\sigma_{xy} = \nu e^2/h$, where $\nu = p/q$ is a rational number with an odd denominator. However, the oscillator strength sum rule is still dominated by the poles at ω_c. What happens to the Hall angle? Like an insulating dielectric, the optical conductivity at a Hall plateau vanishes linearly with frequency $\sigma_{xx}(\omega) = \alpha(-i\omega)$ at $T = 0$ [14]. This implies that the ac Hall angle has the form

$$t_H(\omega) = \frac{1}{-i\omega}\left(\frac{\nu e^2}{h\alpha}\right), \tag{23}$$

i.e., the Hall angle response has condensed into a delta function. Assuming all the Drude weight condenses, then $t_H(\omega) = \omega_c/(-i\omega)$, and α takes its minimum value $\alpha = \nu e^2/h\omega_c$. From this qualitative reasoning, we clearly see how a quantum Hall system at $T = 0$ is the transverse counterpart to a superconductor. In a superconductor, the longitudinal current accelerates in response to an electric field, but there is no Hall response. In a quantum Hall system, the Hall current exhibits a superfluid response to a Lorentz force, but there is no longitudinal response. Between Hall steps, we expect the delta function to broaden into a Drude form of width $\sim\Gamma_{\text{tr}}$. At $T = 0$ this occurs abruptly as a function of electron density or magnetic field, corresponding to a quantum phase transition. Therefore, we again see the analogy between the Hall angle in this system and the change in the conductivity at a superconducting phase transition. At finite temperatures, $\sigma'_{xx} \sim \frac{e^2}{\hbar} e^{-E_g/k_BT}$, where E_g is the gap in the density of states, so we expect the delta function to broaden into a Lorentzian of width $\delta\omega \sim \nu\omega_c e^{-E_g/k_BT}$. The Hall angle sum rule should prove very useful in studies of the conductivity of quantum Hall systems, since it gives a spectral sum rule that may saturate at frequencies $\omega \sim \Gamma_{\text{tr}} \ll \omega_c$, which is the physically interesting range of frequencies.

In conclusion, we have considered the optical Hall angle as a dynamical response function, and showed that it obeys a sum rule that governs the evolution of transverse Hall currents. From our discussion of its qualitative application to metals, cuprate metals, BCS superconductors, and quantized Hall systems, we see that the optical Hall angle may be thought of as the transverse analog to the optical conductivity. Like the f-sum rule of the optical conductivity, the corresponding Hall sum rule is independent of detailed microscopic physics, making it of great utility in the qualitative analysis of the magneto-optic response of electronic systems.

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