Zero-Temperature Hall Coefficient of an Insulator

Shou-Cheng Zhang
IBM Research Division, Almaden Research Center, San Jose, California 95120-6099

Steven Kivelson
Department of Physics, University of California at Los Angeles, Los Angeles, California 90024

Dung-Hai Lee
IBM Research Division, Thomas J. Watson Research Center, Yorktown Heights, New York 10598
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We prove that for noninteracting electrons at zero temperature, an insulator exhibits finite Hall resistivity in the dc limit. More generally, we present simple macroscopic arguments that this behavior is generic for all insulators. We therefore conclude that the zero-temperature Hall coefficient is *not* a measure of the number of mobile carriers.

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An insulator is characterized by a vanishing conductivity tensor at zero temperature. For noninteracting electrons, there are two realizations of such behavior—an Anderson insulator and a band insulator. It is well established that in any dimension (with or without external magnetic field) *sufficient disorder* renders a system insulating. In particular, when enough disorder is introduced to an otherwise free-electron gas, all occupied one-particle states become localized, and the conductivity tensor vanishes at zero temperature. In this state, there is no electrical condition; however, the compressibility is, as in a metal, finite. This *compressible* insulating state is called an Anderson insulator. While disorder is essential in producing an Anderson insulator, a band insulator can arise from noninteracting electrons propagating in a perfect periodic potential. In this case when the number of electrons per unit cell is even, an energy gap separates the filled valence bands and the empty conduction bands. This state, like an Anderson insulator, has no electrical conduction at zero temperature. What distinguishes it from an Anderson insulator is that it is also *incompressible*.

While it is by definition true that $\lim_{\omega\to 0}\sigma_{xx}(\omega)=\lim_{\omega\to 0}\sigma_{xy}(\omega)=0$, and $\lim_{\omega\to 0}\rho_{xx}(\omega)=\infty$ in an insulating state, the value of $\lim_{\omega\to 0}\rho_{xy}(\omega)$ remains ambiguous. For example, if σ_{xx} and σ_{xy} vanish in such a way that the ratio $\sigma_{xy}/\sigma_{xx}^2$ stays finite, the Hall resistivity computed from

$$\rho_{xy}=\sigma_{yx}/(\sigma_{xx}^2+\sigma_{xy}^2) \tag{1}$$

would be finite. In a previous paper we dubbed this peculiar insulating state a "Hall insulator" [1]. Experimentally, Hall insulating behavior has been found in the strong-magnetic-field limit in doped 3D semiconductors [2] and 2D quantum Hall devices [3]. For example, in Ref. [3], in a search for the $\nu=\frac{1}{7}$ quantum Hall liquid, Goldman, Shayegan, and Tsui found that around $\nu=\frac{1}{7}$ ρ_{xx} diverges with decreasing temperature but ρ_{xy} stays approximately B/nec. This behavior is in fact a *prototype result* of any magnetotransport measurement on quantum Hall devices.

Theoretically, based on the Chern-Simons-Ginzburg-Landau theory of the quantum Hall effect [4], the present authors suggested that the entire insulating phase surrounding the quantum Hall liquids is a Hall insulator [1]. One of the central points of this paper is that the Hall insulating behavior is not a unique strong-field phenomenon. The Hall resistivity in the weak-field and weak-localization regime was first calculated by Fukuyama [5]. In Ref. [5] it was shown that to leading order in $1/k_F l$ the Hall coefficient $R_H\equiv\sigma_{xy}/\sigma_{xx}^2$ is *not* affected by localization. Recently, in an interesting paper, Wang *et al.* [6] performed a renormalization-group analysis and claimed that localization *does* affect R_H such that the latter diverges at the metal-insulator transition. This result was then regarded by the authors of Ref. [6] as support for the notion that R_H is a measure of the density of mobile carriers. Extrapolating this notion to the insulating side, one might then conclude that ρ_{xy} is infinite in an Anderson insulator. Since the analyses in Ref. [6] are performed on the metallic side, we feel that in order to address the issue of the Hall insulating behavior a direct investigation of the insulating regime is needed.

In the following, we study the *zero-temperature* frequency-dependent conductivities $\sigma_{xx}(\omega)$ and $\sigma_{xy}(\omega)$ of localized noninteracting electrons. For such systems it is well known [7] that

$$\sigma_{xx}(\omega)=iK_1\omega+K_2\omega^2\ln^{\nu}(1/\omega^2)\,, \tag{2}$$

where $K_{1,2}$ are real, frequency-independent constants. The exponent ν is equal to $D+1$ (D is the dimensionality of space) in the absence of a magnetic field [7], and is equal to 1 in the $D=2$ strong-magnetic-field limit [8]. The first term in Eq. (2) is *generally present* for all insulators. This follows from the fact that an insulator has a nonzero electric polarizability in the low-frequency limit.

In fact, as will be discussed later, K_1 is the real part of the dc polarizability. The second term in Eq. (2) results from quantum tunneling between two localized states with an energy difference $\sim\omega$. Given Eqs. (1) and (2) we conclude that Hall insulating behavior occurs if

$$\lim_{\omega\to 0}[\sigma_{xy}(\omega)/\omega^2] = \text{a finite positive constant}. \tag{3}$$

In a recent paper [9], Viehweger and Efetov addressed the issue of the Hall resistivity in the high-field insulating state. In that work, after *assuming* the existence of a Taylor series expansion of $\sigma_{xy}(\omega)$ in ω, the authors argued that the ω^1 term vanishes by symmetry and calculated the coefficient of the ω^2 term in the one-instanton approximation. We find that the assumption concerning the existence of Taylor expansion is generally invalid for an Anderson insulator. In fact, we shall prove below that for an Anderson insulator where the density of states at the Fermi energy is finite, there is no region surrounding the origin in the complex ω plane in which a Taylor expansion is convergent. However, we will prove a weaker form of their result [Eq. (3)] for the Hall insulating behavior of noninteracting electrons in all dimensions.

We start from the Kubo formula for σ_{xy}, defined at the Matsubara frequencies $i\omega_n = i2\pi n/\beta$ ($\beta = 1/k_B T$),

$$\sigma_{xy}(i\omega_n) = [i(i\omega_n)]^{-1}\pi_{xy}(i\omega_n), \tag{4a}$$

where

$$\pi_{xy}(i\omega_n) = \frac{e^2(i\omega_n)^2}{2V}\int dr\,dr'\,xy'\left\{\frac{1}{\beta}\sum_{iv_n}\langle G(r,r';iv_n)G(r',r;iv_n+i\omega_n)\rangle - (r\to r')\right\}. \tag{4b}$$

In Eqs. (4) $\langle\cdots\rangle$ denotes the impurity configurational averaging, V is the total volume, π_{xy} is the current-current correlation function, and $G(r,r';iv_n)$ is the one-particle Green's function. In obtaining Eqs. (4) we have used the Heisenberg equation of motion

$$\frac{d\mathbf{r}}{dt} = i[H,\mathbf{r}] = \frac{1}{m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)$$

to express the matrix elements of the current operator in terms of those of the position operator. The physical conductivity is obtained by taking the thermodynamic ($V\to\infty$) limit and analytically continuing the result from $i\omega_n$ to $\omega - i\delta$ (where δ is a positive infinitesimal). Here, we have assumed that rotational invariance is recovered after the configuration averaging [i.e., $\sigma_{xy}(\omega) = -\sigma_{yx}(\omega)$], and this accounts for the term $-(r\to r')$ in (4b).

In order to perform the analytic continuation, we express the sum over the Matsubara frequencies as a contour integral enclosing the poles of the Fermi function $f(z)$ and deform the contour so that it encloses the poles or the branch cut of the Green's function on the real axis. Thus we obtain

$$\sigma_{xy}(i\omega_n) = \frac{1}{i(i\omega_n)}\pi_{xy}(i\omega_n) \equiv e^2(i\omega_n)^2\tilde{\pi}_{xy}(i\omega_n), \tag{5a}$$

where

$$\tilde{\pi}_{xy}(i\omega_n) = \frac{1}{i(i\omega_n)}\frac{1}{2V}\int dr\,dr'\,xy'\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi i}f(\varepsilon)\{\langle\Delta G(r,r';\varepsilon)G(r',r;\varepsilon+i\omega_n)\rangle + \langle G(r,r';\varepsilon-i\omega_n)\Delta G(r',r;\varepsilon)\rangle - (r\to r')\} \tag{5b}$$

and $\Delta G(r,r';\varepsilon) = G(r,r';\varepsilon-i\delta) - G(r,r';\varepsilon+i\delta)$. For an insulating phase with finite electric polarizability the thermodynamic limit of (5b) converges. We are then ready to analytically continue $\tilde{\pi}_{xy}(i\omega_n)$ to the real axis from the lower half of the complex ω plane. It is straightforward to prove that $\tilde{\pi}_{xy}$ has the following properties.

(i) From the analytic structure of G, one can show that $\tilde{\pi}_{xy}(z)$ is analytic everywhere in the complex ω plane except a (possible) branch cut on the real axis.

(ii) The discontinuity of $\tilde{\pi}_{xy}(z)$ across this branch cut, $\Delta\tilde{\pi}_{xy}(\omega,\delta) \equiv \tilde{\pi}_{xy}(\omega+i\delta) - \tilde{\pi}_{xy}(\omega-i\delta)$, satisfies $\Delta\tilde{\pi}_{xy}(\omega,\delta) = -\Delta\tilde{\pi}_{xy}(-\omega,\delta)$. This crucial property follows from the rotational invariance, i.e., the term $-(r\to r')$ in (4b).

(iii) From (i) and (ii) it follows that $\lim_{\omega\to 0}\Delta\tilde{\pi}_{xy}(\omega,\delta) = 0$ for all $\delta\neq 0$. In view of the fact that $\Delta\tilde{\pi}_{xy}(z)$ is analytic in the lower and upper half planes, we conclude that $\lim_{z\to 0}\Delta\tilde{\pi}_{xy}(z) = 0$ independent of the direction in which the limit is taken except for along the real axis. Therefore, the discontinuity of $\tilde{\pi}_{xy}(z)$ vanishes at $z = 0$. However, for an Anderson insulator, due to the branch cut on the real axis there is *no region* surrounding $z = 0$ in which the $\tilde{\pi}_{xy}(z)$ is analytic. As a result, the assumption of Viehweger and Efetov that there exists a Taylor expansion about the origin is not valid.

(iv) Since $G^*(r,r';\varepsilon+i\delta) = G(r',r;\varepsilon-i\delta)$, $\mathrm{Im}\tilde{\pi}_{xy}(\omega - i\delta) = \frac{1}{2}i\Delta\tilde{\pi}_{xy}(\omega,\delta)$. Therefore (iii) implies that

$$\lim_{z\to 0}\mathrm{Im}\tilde{\pi}_{xy}(z) = 0, \tag{6}$$

where the $z\to 0$ limit is taken in the same sense as specified in (iii).

(v) Because of (i), we can use Cauchy's theorem to write

$$\tilde{\pi}_{xy}(z=\omega-i\delta)=\oint_C \frac{dz'}{2\pi i}\frac{\tilde{\pi}_{xy}(z')}{z'-z}, \tag{7}$$

where C is any contour in the lower-half plane which encloses z.

(vi) From a general sum rule it follows that $\sigma_{xy}\to A/iz$ and therefore $\tilde{\pi}_{xy}\to A'/iz^3$ for large $|z|$, where A and A' are real, frequency-independent numbers. Therefore if we choose C to be the contour along, and infinitesimally below, the real axis closed by an infinite semicircle in the lower half plane, we obtain the following dispersion relation for $\tilde{\pi}_{xy}$:

$$\mathrm{Re}\tilde{\pi}_{xy}(\omega)=\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\tilde{\pi}_{xy}(\varepsilon)}{\varepsilon-\omega}d\varepsilon. \tag{8}$$

(vii) From Eq. (6) and the sum rule, it follows that the integral in Eq. (8) is both infrared and ultraviolet convergent; hence

$$\lim_{\omega\to 0}\mathrm{Re}\tilde{\pi}_{xy}(\omega)=\text{finite}. \tag{9}$$

Combining Eqs. (5a) and (9), we conclude that Eq. (3) is proven.

To reiterate, the above proof is valid in *all* dimensions and it is based on the assumptions that (i) the electrons are noninteracting, (ii) impurity averaging recovers rotational invariance, and (iii) the infinite volume limit of $\tilde{\pi}_{xy}$ exists.

Although the proof presented above is limited to noninteracting electrons, we shall now provide physical arguments suggesting that the same conclusion can be drawn for interacting systems. We first recall the earlier discussion that at zero temperature, an insulator has a *nonzero* electric polarizability in the dc limit. Let us imagine applying an ac electric field E in the x direction and a dc magnetic field B in the z direction. Because of the Lorentz force law we may write the following equations for the steady-state electric polarizations in a *homogeneous* isotropic insulator:

$$\mathbf{J}(\mathbf{r},\omega)=\dot{\mathbf{P}}(\mathbf{r},\omega),\quad \mathbf{P}(\mathbf{r},\omega)=[\alpha(\omega)/e]\mathbf{F}(\mathbf{r},\omega),$$
$$\mathbf{F}(\mathbf{r},\omega)=e\mathbf{E}(\omega)+\frac{1}{nc}\mathbf{J}(\mathbf{r},\omega)\times\mathbf{B}, \tag{10}$$

where $\alpha(\omega)$ is the frequency-dependent polarizability, and ne, an effective charge density, is determined by the total density of charges that contribute to the polarizability. From Eq. (10) the conductivity tensor can be computed and the result, in the low-frequency limit, is

$$\sigma_{xx}(\omega)=i\omega\alpha(\omega),$$
$$\sigma_{xy}(\omega)=(B/nec)[\omega\alpha(\omega)]^2, \tag{11}$$

which in turn gives $\rho_{xy}=B/nec$. Therefore we conclude that the *at zero temperature the Hall coefficient is not a measure of the density of mobile carriers.*

So far, we have been concentrating on the zero-temperature $\omega\to 0$ Hall resistivity in a localized phase. It is important to realize that the *experimentally* determined resistivities are typically obtained by first setting $\omega\to 0$ and then taking the $T\to 0$ limit. In the following we shall provide examples where these two limits *do not commute.* Therefore one must be extremely careful in extending our zero-temperature results to finite temperatures.

Let us consider a n-type-doped semiconductor. The general arguments presented above imply that at $T=0$, $\lim_{\omega\to 0}\rho_{xy}=$a finite constant. At finite temperature, however, the dc conductivities are dominated by the thermally activated conduction. In the Drude approximation the dc conductivity tensor is given by

$$\sigma_{xx}(T)=\frac{n(T)e^2\tau}{m}\frac{1}{1+(\omega_c\tau)^2},$$
$$\sigma_{xy}(T)=\omega_c\tau\sigma_{xx}(T), \tag{12}$$

where τ is the transport lifetime, $\omega_c=eB/m^*c$ is the cyclotron frequency, and $n(T)=n_0e^{-\Delta/k_BT}$ is the thermally activated conduction-band carrier density. As a result, at *finite temperatures* $\rho_{xy}=B/n(T)ec$ measures the density of mobile carriers. Transport experiments are carried out at a finite temperature, and in most cases at a finite but small observation frequency ω_0, in order to lock into the signal. The analysis carried out above indicates that the temperature-frequency plane can be divided into two regions where different behavior for the Hall resistivity is to be expected. For every ω_0, there is a crossover temperature $T^*(\omega_0)$, estimated from the relation $\mathrm{Im}\sigma_{xx}(\omega_0,T=0)=\mathrm{Re}\sigma_{xx}(\omega=0,T^*)$. For T much less than $T^*(\omega_0)$, one should take the $T\to 0$ limit before taking the $\omega\to 0$ limit in calculating ρ_{xy}, since the ac conductivity is much greater than the dc conductivity. In this limit, one obtains a Hall coefficient which is independent of the mobile carriers. On the other hand, for T much greater than $T^*(\omega_0)$ one should take the $\omega\to 0$ limit before taking the $T\to 0$ limit in calculating ρ_{xy}, and obtain in this case a Hall coefficient which is determined by the density of mobile carriers. At $\omega_0=1$ Hz, $\mathrm{Im}\sigma_{xx}=1.2\times10^{-12}(\varepsilon-1)/4\pi\ (\Omega^{-1}\mathrm{cm}^{-1})$, whereas the dc conductivity for a typical semiconductor, antimony-doped germanium with a donor concentration of 5.3×10^{14} cm^{-3}, is about $10^{-12}\ \Omega^{-1}\mathrm{cm}^{-1}$ at $T=3$ K. Therefore, below this temperature, the Hall coefficient would be essentially temperature independent.

It is a more subtle question whether the order of limits commutes in an Anderson insulator. It is now commonly accepted that for a localized phase where $\xi_0>l_{\mathrm{in}}$ (where ξ_0 is the localization length and l_{in} is the inelastic scattering length), the effects of inelastic scattering can be summarized by introducing an effective finite size L_{eff} given by the Thouless length [10]. In this regime, it is quite plausible that by replacing ω with $1/\tau_{\mathrm{ph}}$ (where τ_{ph}, the

phase breaking time, is given by $\tau_{ph}=L_{eff}^2/D$, where D is the diffusion constant) in the expressions for the *zero temperature* ac transport coefficients, we obtain the corresponding dc quantities at *finite* temperature. If this is true, the results we discussed above imply that Anderson insulators at temperatures such that $\xi_0 > l_{in}(T)$ are also Hall insulators. In the deep insulating phase, however, this is not true. In that case $\xi_0 < l_{in}$, and the low-temperature transport on length scales greater than ξ_0 is governed by classical variable-range hopping. The results we discussed above are not directly applicable in this regime.

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