Universality of Quantum Hall Effect: Topological Invariant and Observable

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We show a universality in the quantum Hall effect in that the flux-averaged Hall conductivity in any two- or three-dimensional system with or without disorder is given by a topological invariant quantized in units of e^2/h at $T=0$ for every energy level in a finite system. Relevance to the observable Hall conductivity over the whole energy spectrum is presented together with numerical results for lattice systems.

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The current interest in the quantum Hall effect[1] leads naturally to the question of how this remarkable quantization is universal. This query comprises two stages: (i) Exactly what property of the wave function specific to systems in a magnetic field gives rise to the quantized Hall effect? (ii) Given an exact proof for the quantization, what is the actual relevance to the observable quantities? In this Letter we first show that the quantum Hall effect is indeed universal. Namely, the Hall conductivity for any single sample in finite magnetic fields in any two- or three-dimensional system with or without disorder is quantized in units of e^2/h at $T=0$ for every energy level in a finite system. The ubiquitous quantization comes from the fact that the Hall conductivity can be expressed as a topological invariant in a mapping from the gauge field to the complex wave function. Second, we proceed to show that, although the topological invariant varies from one eigenstate to another, its value has a definite distribution for a given system size and degree of randomness in the system resulting in the averaged Hall conductivity as a continuous function of energy. Thus the observable Hall conductivity over the whole energy spectrum is worked out from the somewhat esoteric topological invariant. The original theory[2,3] showing that the quantized Hall plateau is a consequence of the localization is also confirmed. The close relation of the quantum Hall effect with the gauge transformation was already anticipated by Laughlin[3] from the very early stage of the theoretical study. The topological aspect of the Hall conductivity has been studied by Avron, Seiler, and Simon[4] and Simon[5] for systems with external periodic potential first studied by Thouless *et al.*[6] A similar argument has also been employed by Niu, Thouless, and Wu[7] in a discussion of the quantum Hall effect in many-body systems. However, these studies assume translational invariance of the system with Bloch wave numbers, or E_F being in a gap. In contrast, we work on the Hall conductivity in a general case to give the properties of σ_{xy} over the energy spectrum with both extended and localized regimes. The analysis also opens up a natural way to relate σ_{xy} with the diagonal conductivity, σ_{xx}, a direct probe of localization.

In a magnetic field, the Hamiltonian $\mathcal{H}$ of a system contains the vector potential, $\mathbf{A}_0$ with $\mathrm{rot}(\mathbf{A}_0)=\mathbf{H}$. In the presence of external Aharonov-Bohm (AB) magnetic fluxes, $\mathbf{A}_0$ is replaced by $\mathbf{A}_0+\mathbf{A}$ with an extra vector potential, $\mathbf{A}=(A_x,A_y)$.[8] In the Laughlin geometry with the system wound into a cylinder, a magnetic flux Φ_x penetrates the opening of the cylinder. The full vector potential, $\mathbf{A}$, introduced here may be thought of as two magnetic fluxes, $(\Phi_x,\Phi_y)=(A_xL,A_yL)$, which penetrate respectively inside and through the opening of a torus when we impose periodic boundary conditions in both x and y directions for the system of size L. According to the Byers-Yang theorem,[9] the physical system assumes its original state every time A_x or A_y increases by ϕ_0/L, with $\phi_0=hc/e$ being the magnetic-flux quantum. The Hall conductivity at absolute zero temperature is generally given by the Kubo formula as[2,10]

$$\sigma_{xy}=\frac{\hbar}{i\pi L^2}\int dE\, f(E)\,\mathrm{Tr}\left[j_x\frac{\partial}{\partial E}\mathrm{Re}\,G(E+i0)j_y\,\mathrm{Im}\,G(E+i0)-(x\leftrightarrow y)\right],$$

where $G=(z-\mathcal{H})^{-1}$ is the Green's function. Since the current operator is expressed as $\mathbf{j}=c\,\partial\mathcal{H}/\partial\mathbf{A}$, the Hall conductivity averaged over A_x and A_y, which we shall denote $\langle\sigma_{xy}\rangle$, can be written as

$$\frac{\langle\sigma_{xy}\rangle}{e^2/h}=\frac{1}{8\pi^2}\int_C dz\int\int_0^{\phi_0/L}dA_x\,dA_y\,\mathrm{Tr}\left[G\frac{\partial G^{-1}}{\partial A_x}G\frac{\partial G^{-1}}{\partial A_y}G\frac{\partial G^{-1}}{\partial z}-(x\leftrightarrow y)\right].\qquad(1)$$

The path C for the energy in the complex plane may be taken as an infinite line parallel to the imaginary axis, since, when the states at E_F are localized, the matrix elements of the current vanish there. C may be regarded as a closed contour in the z plane with $G(\mathrm{Im}(z)=\infty) = G(\mathrm{Im}(z)=-\infty)$. We immediately recognize Eq. (1) as an expression for the topological invariant (Pontrjagin number)[11] n, which gives the winding number of the mapping from the space of $(\mathbf{A},z)$ to the space of G. A similar expression for the winding number appears in the gauge-field theory[12,13] in a different context. Thus we end up with $\langle\sigma_{xy}\rangle = ne^2/h$ for the flux average. For infinite systems σ_{xy} is independent of $\mathbf{A}$, so that the average over $\mathbf{A}$ is trivial. For small systems σ_{xy} does depend on $\mathbf{A}$, a feature which is discussed below.

To explore the physical meaning, we can reduce Eq. (1) to another form. If we integrate the formula over z and make use of

$$\frac{\partial u^\alpha}{\partial \mathbf{A}} = \sum_\beta{}' \frac{\langle\beta\,|\,\partial\mathcal{H}/\partial\mathbf{A}\,|\,\alpha\rangle}{(E_\alpha - E_\beta)} u^\beta,$$

then by first-order perturbation, where u^α is the αth orthonormal eigenstate of the Hamiltonian, we can rewrite $\langle\sigma_{xy}\rangle$ for a fixed number of electrons as

$$\frac{\langle\sigma_{xy}\rangle}{e^2/h} = \frac{1}{2\pi i}\sum_\alpha^{\mathrm{occ}}\int\!\!\int\left[\left\langle\frac{\partial u^\alpha}{\partial A_x}\middle|\frac{\partial u^\alpha}{\partial A_y}\right\rangle - \left\langle\frac{\partial u^\alpha}{\partial A_y}\middle|\frac{\partial u^\alpha}{\partial A_x}\right\rangle\right] dA_x\, dA_y, \tag{2}$$

where $\langle u\,|\,v\rangle$ stands for an inner product of two vectors. The integral exactly gives the Euler's index (equal to the first Chern class in 2D). We may note that, in abovementioned gauge theory, Euler's index (equal to the second Chern class in 4D) integrated over space-time gives the topological charge. Equation (2) shows that nonzero Hall conductivity arises because each wave function when the flux is changed as $A_x \to A_x + \Delta A_x$ followed by $A_y \to A_y + \Delta A_y$ can be essentially different from the wave function when we first let $A_y \to A_y + \Delta A_y$ followed by $A_x \to A_x + \Delta A_x$ (i.e., $\partial/\partial A_x$ and $\partial/\partial A_y$ do not commute). Note that this is not the Peierls phase factor, but we are talking of the essential (internal) phase of the (complex) vector bundle in the Hilbert space. In fact, Eq. (2) is of the same form as that discussed by Simon,[5] who identifies the extra phase as Berry's phase, and by Niu, Thouless, and Wu.[7] The structure of Eq. (2) is made more explicit by our defining (nondiagonal) matrices $\{B_x\}_{\alpha\beta} \equiv \langle\alpha\,|\,\partial/\partial A_x\,|\,\beta\rangle$, $\{B_y\}_{\alpha\beta} \equiv \langle\alpha\,|\,\partial/\partial A_y\,|\,\beta\rangle$. The integrand in the equation then becomes a diagonal element of a matrix given, with shorthand $u^\alpha \equiv \alpha$, $A_x \equiv x$, etc., as

$$\begin{aligned} F_{\alpha\beta} &\equiv \left\langle\frac{\partial\alpha}{\partial x}\middle|\frac{\partial\beta}{\partial y}\right\rangle - \left\langle\frac{\partial\alpha}{\partial y}\middle|\frac{\partial\beta}{\partial x}\right\rangle \\ &= \left\langle\alpha\middle|\frac{\partial^2}{\partial y\partial x} - \frac{\partial^2}{\partial x\partial y}\middle|\beta\right\rangle + \left\{\frac{\partial B_y}{\partial x} - \frac{\partial B_x}{\partial y}\right\}_{\alpha\beta} \\ &= \{B_y B_x - B_x B_y\}_{\alpha\beta}, \end{aligned}$$

which is just the commutator of matrices representing $\partial/\partial A_x$ and $\partial/\partial A_y$.

Here it is very illuminating to look at the numerical result. We have employed a lattice system of finite size, since the AB effect in the quantum Hall effect was studied for the first time[14] for this system, and the characteristic quantum Hall effect[6] in periodic systems is of intrinsic interest. We employ the tight-binding Hamiltonian with disorder in site energies in torus boundary conditions. Figure 1 shows the result for $\langle\sigma_{xy}\rangle$ [Eq. (2)] for an 8×8 lattice with $\tilde{H} = \frac{1}{8}$ and $W=2$, where $\tilde{H}$ is the magnetic flux in a unit cell of the lattice divided by ϕ_0, and W is the distribution width of site energies relative to the nearest-neighbor transfer. The quantization of $\langle\sigma_{xy}\rangle$ for *every* level is excellently exhibited. The flux average is accurately obtained from the numerical integration of σ_{xy} calculated from the Kubo formula at 60×60 mesh points in the (A_x,A_y) unit cell.

More importantly, we can actually look at the structure of ψ. The winding number for the mapping from $\mathbf{A}$ to ψ is nonzero when ψ as a function of $\mathbf{A}$ has a nontrivial global topology. Figure 2 shows an example of the dependence of a wave function on $\mathbf{A}$. We plot the relative phase of one coefficient, c_i/c_l, in $u^\alpha = \sum_i c_i^\alpha \psi_i$ with the Wannier basis ψ_i. Every wave function has turned out to be a continuous function of $\mathbf{A}$ except for a number

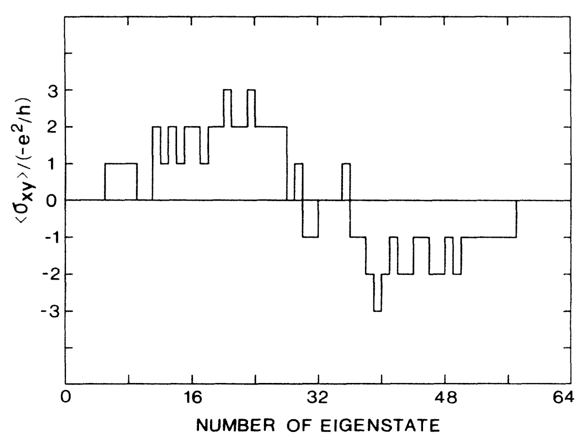

FIG. 1. The Hall conductivity σ_{xy} averaged over A_x and A_y is plotted for all the eigenstates in an 8×8 lattice with $\tilde{H} = \frac{1}{8}$ and $W=2$.

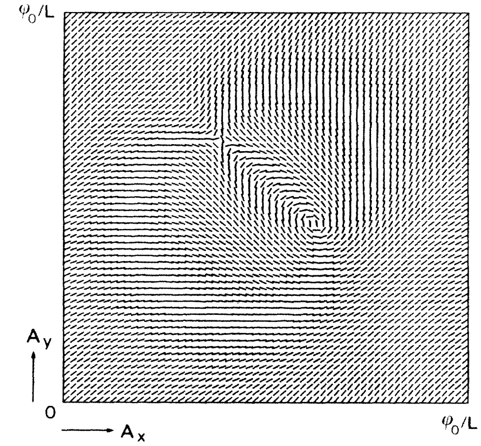

FIG. 2. The phase of a component of an eivenvector (the eighth in energy) for the same sample as in Fig. 1 is shown as a function of (A_x, A_y).

of phase vortices and antivortices.[15]

Here we should mention that, although we consider the geometry with magnetic flux, our approach is completely different from Laughlin's. The latter approach considers the system with electrodes attached to both edges to look at the net number of electrons which are transferred across the electrodes with a potential drop when the flux is changed from 0 to ϕ_0. The occupation of electrons changes in the system including electrodes, in which the transferred electrons actually correspond to the Hall current. By contrast, we consider systems with no edges, so that there is no electron transfer. We calculate the Hall conductivity at $T=0$ for each value of (Φ_x, Φ_y), and look at the average of $\sigma_{xy}(\Phi_x, \Phi_y)$. This may also be regarded as an average when Φ is changed adiabatically for a sample, since the occupation of electrons always remains in the ground state. Note that no two energy levels versus Φ can cross in the presence of disorder in finite systems. If a pair of levels accidentally cross in a disorder-free crystal, these levels repel each other upon the introduction of random potentials.

Another essential point is that, in the formulation above, no assumptions have been made on the details of the system, so that the formulation applies to any system in a continuous space or on a lattice with or without disorder. The Fermi energy is also arbitrary, so that $\langle \sigma_{xy} \rangle$ is quantized for every energy in the localized regime in infinite systems, or for every energy level for finite systems with fixed number of electrons. The system is not restricted to two-dimensional systems, either. In higher-d dimensions, with a change in the prefactor in the Kubo formula, we have quantization of Hall *conductance*, $R_{xy}^{-1} = L^{d-2} \langle \sigma_{xy} \rangle = ne^2/h$.[16] The formulation also applies to many-body systems. In the fractional quantum Hall effect, the discussion is similar except that the system returns to the original state when the magnetic

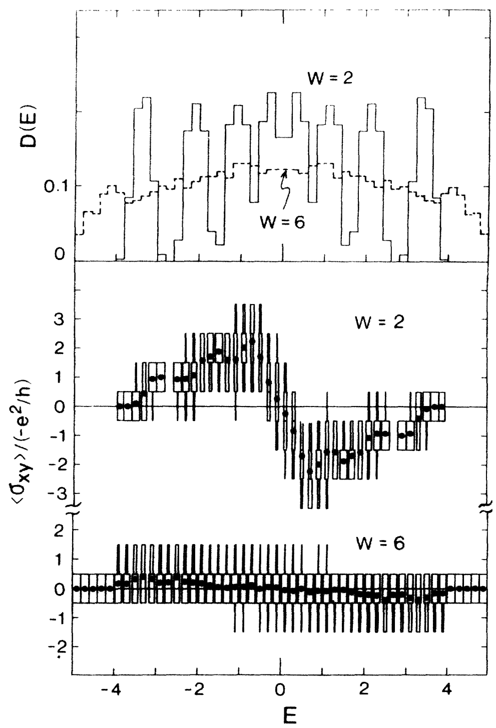

FIG. 3. The distribution (histogram) and the average (circles) of the winding number are plotted for each energy bin together with the density of states for $\tilde{H} = \frac{1}{8}$ with two values of W for 8×8 lattice systems with ensemble average over 36 samples.

flux is increased by $M\phi_0$, with M being the degeneracy, in which case $\langle \sigma_{xy} \rangle/(e^2/h)$ is given by an integer divided by M.

Now we elucidate the behavior of $\langle \sigma_{xy} \rangle$. Localized states, which are independent of **A**, do not contribute to σ_{xy} and give plateaus. Contribution from states delocalized within the sample makes $\langle \sigma_{xy} \rangle$ a sequence of step

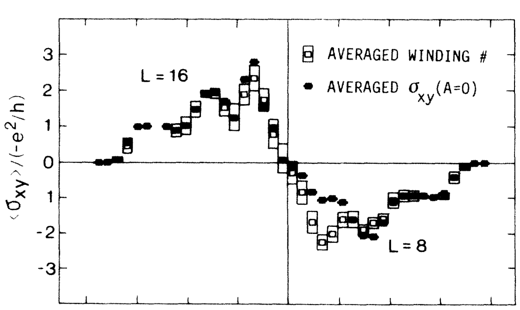

FIG. 4. Ensemble-averaged winding number (open squares) is compared with ensemble-averaged σ_{xy} for $\mathbf{A}=0$ (closed squares) for $\tilde{H} = \frac{1}{8}$ and $W=2$ for 8×8 and 16×16 lattice systems. Error bars are also indicated.

functions as E_F is swept. How do we get a physical Hall conductivity as a continuous function of energy? We consider the probability distribution of the $\langle \sigma_{xy} \rangle$ for each energy bin averaegd over ensembles (Fig. 3). The distribution is well behaved as a function of energy, and the ensemble-averaged $\langle \sigma_{xy} \rangle$ for small disorder exhibits a number of plateaus with dips in between due to mixing of Landau levels,[10] while the averaged $\langle \sigma_{xy} \rangle$ is suppressed for large disorder because of small $\omega_c \tau$.

Let us now discuss the relation of the flux average and the usual ensemble average. The ensemble-averaged $\langle \sigma_{xy} \rangle$ should coincide, for sufficiently large systems, with ensemble-averaged σ_{xy} for fixed **A**, which is the observable. Figure 4 compares the averaged $\langle \sigma_{xy} \rangle$ with the averaged σ_{xy} for $\mathbf{A}=0$. Despite exceedingly small sample sizes here, the two quantities are seen to have virtually the same energy dependence. The result shows that the difference between the two quantities, which diminishes with increasing size, comes from the strong **A** dependence of eigenfunctions for small systems, especially for regions of energy with strong lattice effects, in exact agreement with Aoki's study.[14]

The behavior of σ_{xy} naturally depends on the sample size and the localization length. The diagonal conductivity, σ_{xx}, which directly measures the localization, is also related to the **A** dependence of the system via the Thouless number derived from the **A**-dependent energy levels.[17,18] From this line of approach we can in fact discuss the scaling properties[19] of the relation of σ_{xx} vs σ_{xy}.

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