Electron Localization in the Quantum Hall Regime

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The theory of the insulating state discriminates between insulators and metals by means of a localization tensor, which is finite in insulators and divergent in metals. In absence of time-reversal symmetry, this same tensor acquires an off-diagonal imaginary part, proportional to the dc transverse conductivity, leading to quantization of the latter in two-dimensional systems. I provide evidence that electron localization—in the above sense—is the common *cause* for both vanishing of the dc longitudinal conductivity and quantization of the transverse one in quantum Hall fluids.

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W. Kohn showed in 1964 that the insulating state of matter reflects a peculiar organization of the electrons in their ground state: the cause for the insulating behavior is electron localization [1,2]. Such localization, however, manifests itself in a very subtle way, fully elucidated much later. In 1999 Resta and Sorella [3] defined a tensor which provides a quantitative measure of Kohn's localization, and has a common root with the modern theory of polarization [4–6]. This "localization tensor" is an intensive property characterizing the ground wave function as a whole: it is finite in any insulator and divergent in any metal. A further advance on this line was provided in 2000 by Souza, Wilkens, and Martin [7]. I am going to refer to these results altogether as to the "theory of the insulating state" (TIS) [8]: so far, it has only considered time-reversal-invariant systems. I show here that, in the absence of time-reversal symmetry, the TIS localization tensor [3,7,8] is naturally endowed with a nonvanishing imaginary part. For a two-dimensional system, the imaginary part is quantized whenever the real part is nondivergent, and is proportional to dc transverse conductivity. I show here that the theory of the quantum Hall effect (particularly in the formulation of Niu, Thouless, and Wu [9]) has a very direct—and previously unsuspected—relationship to TIS, and in fact can be regarded as a consequence of the latter. In order to predict whether the dc transverse conductivity of any two-dimensional many-electron system is quantized, it is enough to inspect electron localization in the ground state: this is the major result of the present Letter.

Phenomenologically, an insulating material is characterized by vanishing dc longitudinal conductivity. In this sense, an electron fluid in the quantum Hall regime is in fact an insulator, independently of what establishes such a regime (e.g., disorder). According to TIS the many-body wave function is then *localized*. From the present viewpoint, electron localization is the common *cause* for both vanishing of the longitudinal dc conductivity and quantization of the transverse one; the two features stem here from the same formalism. The present view may appear at odds with the established one, which in the quantum Hall regime focuses on the extended states more than on the localized ones [10]; but it is worth stressing that the TIS localization tensor is a global geometric property characterizing the ground wave function, *not* the individual one-electron states.

In the final part of this Letter I also show how TIS works for noninteracting electrons in the lowest Landau level. While disorder is obviously essential for producing a quantum Hall fluid, a flat substrate potential is used here to provide analytical results. At complete filling the (real) trace of the localization tensor is shown to be equal to the squared magnetic length, while the (imaginary) antisymmetric part of the same tensor provides the Hall conductivity; at fractional filling the real part diverges while the imaginary part is ill defined. This confirms our main message: inspecting the ground-state localization is enough to predict quantization of transverse conductivity.

The TIS localization tensor [3], also known as the second cumulant moment $\langle r_\alpha r_\beta \rangle_c$ of the electron distribution [7,8], is an intensive property having the dimensions of a squared length, and whose only ingredient is the many-body ground wave function $|\Psi_0\rangle$. In the cases dealt with so far, periodic boundary conditions were adopted; these are easily modified to accommodate a macroscopic magnetic field [9]. If $|\Psi_0\rangle$ is an N-electron wave function periodic with period L in all Cartesian coordinates $r_{j,\alpha}$ separately, we define $\boldsymbol{\kappa}_\alpha = (2\pi/L)\mathbf{e}_\alpha$, where $\mathbf{e}_\alpha$ is a unit vector along α, and

$$|\Psi_0(0)\rangle = |\Psi_0\rangle; \qquad |\Psi_0(\boldsymbol{\kappa}_\alpha)\rangle = \mathrm{e}^{i2\pi/L\sum_{j=1}^{N} r_{j,\alpha}}|\Psi_0\rangle. \quad (1)$$

According to TIS, the localization tensor is [3,7,8]

$$\langle r_\alpha r_\beta \rangle_c = \frac{L^2}{4\pi^2 N} \ln \frac{\langle \Psi_0(\boldsymbol{\kappa}_\alpha)|\Psi_0(\boldsymbol{\kappa}_\beta)\rangle}{\langle \Psi_0(\boldsymbol{\kappa}_\alpha)|\Psi_0(0)\rangle\langle \Psi_0(0)|\Psi_0(\boldsymbol{\kappa}_\beta)\rangle}, \quad (2)$$

where the thermodynamic limit is understood. In the existing literature time-reversal symmetry is assumed: the tensor is then real. When time-reversal invariance is absent, this same tensor is endowed with an off-diagonal imaginary part, which—as shown below—is particularly relevant for two-dimensional systems.

As first shown by Souza, Wilkens, and Martin [7] by means of a fluctuation-dissipation theorem, the real part of the localization tensor is related to a frequency integral of the longitudinal conductivity, which is finite in any insulator and divergent in any metal:

$$\int_0^\infty \frac{d\omega}{\omega}\,\mathrm{Re}\sigma_{\alpha\alpha}(\omega) = \frac{\pi e^2 N}{\hbar L^d}\,\mathrm{Re}\langle r_\alpha^2\rangle_c = -\frac{e^2}{4\pi\hbar L^{d-2}}\,\ln|\langle\Psi_0(0)|\Psi_0(\boldsymbol{\kappa}_\alpha)\rangle|^2. \tag{3}$$

I am going to extend this result, in order to address the off-diagonal imaginary part of the localization tensor as well, and additionally to consider cases where a macroscopic magnetic field is present. Specializing from now on to a two-dimensional system, we notice that Eq. (3) is size invariant in form.

I assume the system as isotropic in the xy plane, with a magnetic field B along z. Therefore $\sigma_{11} = \sigma_{22}$, while the off-diagonal element is purely antisymmetric: $\sigma_{12} = -\sigma_{21}$. The Kubo formula for the conductivity tensor is

$$\sigma_{\alpha\beta}(\omega) = \frac{ie^2}{\hbar\omega L^2}\lim_{\eta\to 0+}{\sum_{n\neq 0}}'\left(\frac{\langle\Psi_0|\hat{v}_\alpha|\Psi_n\rangle\langle\Psi_n|\hat{v}_\beta|\Psi_0\rangle}{\omega-\omega_{0n}+i\eta} - \frac{\langle\Psi_0|\hat{v}_\beta|\Psi_n\rangle\langle\Psi_n|\hat{v}_\alpha|\Psi_0\rangle}{\omega+\omega_{0n}+i\eta}\right), \tag{4}$$

where $\omega_{0n} = (E_n - E_0)/\hbar$ are the excitation frequencies. I then focus on the two quantities

$$\int_0^\infty \frac{d\omega}{\omega}\,\mathrm{Re}\sigma_{11}(\omega) = \frac{\pi e^2}{\hbar L^2}\,\mathrm{Re}{\sum_{n\neq 0}}\frac{\langle\Psi_0|\hat{v}_1|\Psi_n\rangle\langle\Psi_n|\hat{v}_1|\Psi_0\rangle}{\omega_{0n}^2}, \tag{5}$$

$$\mathrm{Re}\,\sigma_{12}(0) = \frac{2e^2}{\hbar L^2}\,\mathrm{Im}{\sum_{n\neq 0}}\frac{\langle\Psi_0|\hat{v}_1|\Psi_n\rangle\langle\Psi_n|\hat{v}_2|\Psi_0\rangle}{\omega_{0n}^2}, \tag{6}$$

where the right-hand side members are written as to emphasize the common structure. Notice that we have taken the limit $\eta \to 0$ at finite L. In transport theory the interest is in evaluating σ as a continuous function of ω, by smoothing the singularities in Eq. (4): this can be done by keeping the ''dissipation'' η finite while performing the thermodynamic limit first [11]. The order of the two limits is irrelevant here, since Eq. (5) is an *integrated* property, and Eq. (6) is dissipationless.

In order to transform the sum over the excited states into a ground-state property, it is expedient to consider the many-body Hamiltonian with a ''twist'' (or ''flux'')

$$\hat{H}(\mathbf{k}) = \frac{1}{2m}\sum_{i=1}^{N}\left(\mathbf{p}_i - \hbar\mathbf{k} + \frac{e}{c}\mathbf{A}\right)^2 + \hat{V}, \tag{7}$$

where $\hat{V}$ comprises the one-body substrate potential and the electron-electron interaction. We indicate the ground state of Eq. (7) as $|\Psi(\mathbf{k})\rangle$, with $|\Psi(0)\rangle = |\Psi_0\rangle$; straightforward perturbation theory yields

$$|\Psi(\mathbf{k})\rangle \simeq |\Psi_0\rangle + \mathbf{k}\cdot\sum_{n\neq 0}|\Psi_n\rangle\frac{\langle\Psi_n|\hat{\mathbf{v}}|\Psi_0\rangle}{\omega_{0n}}, \tag{8}$$

$$\langle\Psi_n|\partial_\alpha\Psi(0)\rangle = \langle\Psi_n|\hat{v}_\alpha|\Psi_0\rangle/\omega_{0n}, \qquad n\neq 0, \tag{9}$$

where the velocity operator is $\hat{\mathbf{v}} = \boldsymbol{\nabla}_{\mathbf{k}}\hat{H}(\mathbf{k})/\hbar$, and $\partial_\alpha \equiv \partial/\partial k_\alpha$. Strictly speaking, the perturbation expansion holds for a conventional insulator where the Fermi gap does not vanish in the thermodynamic limit. More generally, owing to Eq. (5), it also holds whenever $\mathrm{Re}\sigma_{\alpha\alpha}(\omega)$ goes to zero fast enough at small ω, i.e., for any insulator [7].

The sum over excited states appearing in Eqs. (5) and (6) can then be transformed into

$$\sum_{n\neq 0}\frac{\langle\Psi_0|\hat{v}_\alpha|\Psi_n\rangle\langle\Psi_n|\hat{v}_\beta|\Psi_0\rangle}{\omega_{0n}^2} = \langle\partial_\alpha\Psi(0)|\partial_\beta\Psi(0)\rangle - \langle\partial_\alpha\Psi(0)|\Psi(0)\rangle\times\langle\Psi(0)|\partial_\beta\Psi(0)\rangle. \tag{10}$$

The real part of Eq. (10) is the quantum metric tensor defined by Provost and Vallee [12], evaluated at $\mathbf{k} = 0$; the imaginary part is the corresponding curvature (divided by two).

So far, we have specified neither the magnetic gauge nor the boundary conditions. We choose the Landau gauge and the usual magnetic boundary conditions [9] for translations by L of each coordinate x_i and y_i. These require the total flux BL^2 across the system to be an integer number N_s of flux quanta $\Phi_0 = hc/e$. At filling ν the density is then

$$n_0 = \frac{\nu N_s}{L^2} = \frac{\nu}{2\pi l^2}, \tag{11}$$

where $l = (\hbar c/eB)^{1/2}$ is the magnetic length.

If the insulating ground state is nondegenerate at any $\mathbf{k}$, the eigenstate $|\Psi(\mathbf{k})\rangle$ assumes a simple form whenever the $\mathbf{k}$ coordinates are integer multiples of $2\pi/L$. For instance, if $\mathbf{k}$ coincides with one of the $\boldsymbol{\kappa}_\alpha$ vectors defined above, then $|\Psi(\mathbf{k})\rangle$ coincides with Eq. (1) apart from a phase factor which is irrelevant here: in fact the two wave functions obey the same Schrödinger equation and the same magnetic boundary conditions. The case of degenerate ground states has been considered as well [13]. We then discretize the derivatives in Eq. (10) using the special $\boldsymbol{\kappa}_\alpha$ vectors of Eq. (1) and replacing $\langle\Psi_0(\boldsymbol{\kappa}_\alpha)|\Psi_0(0)\rangle \simeq 1 + \ln\langle\Psi_0(\boldsymbol{\kappa}_\alpha)|\Psi_0(0)\rangle$, as usual when dealing with Berry phases [14]. The result is

$$\langle\partial_\alpha\Psi(0)|\partial_\beta\Psi(0)\rangle - \langle\partial_\alpha\Psi(0)|\Psi(0)\rangle\langle\Psi(0)|\partial_\beta\Psi(0)\rangle \simeq \frac{L^2}{4\pi^2}\ln\frac{\langle\Psi_0(\boldsymbol{\kappa}_\alpha)|\Psi_0(\boldsymbol{\kappa}_\beta)\rangle}{\langle\Psi_0(\boldsymbol{\kappa}_\alpha)|\Psi_0(0)\rangle\langle\Psi_0(0)|\Psi_0(\boldsymbol{\kappa}_\beta)\rangle} = N\langle r_\alpha r_\beta\rangle_c. \tag{12}$$

Replacing the real part of Eq. (12) into Eqs. (5) and (10) one recovers the Souza-Wilkens-Martin sum rule, Eq. (3), which is nondivergent in the insulating case.

The imaginary part of Eq. (12) shares the same convergence properties as the real one, after Eq. (10); in the insulating case it takes the form of a discrete Berry phase [14] over the three-point path in $\mathbf{k}$ space from 0 to $\boldsymbol{\kappa}_1$ to $\boldsymbol{\kappa}_2$ to 0. However, since Berry phases are defined modulo 2π, this expression does not provide a unique value. The ambiguity is removed by replacing the Berry phase, i.e., the loop integral of the Berry connection, with the surface integral of the Berry curvature. We therefore evaluate the imaginary part of Eq. (10) as

$$\mathrm{Im}\langle\partial_1\Psi(0)|\partial_2\Psi(0)\rangle = \frac{L^2}{4\pi^2}\,\mathrm{Im}\int_0^{2\pi/L} dk_1 \times \int_0^{2\pi/L} dk_2\langle\partial_1\Psi(\mathbf{k})|\partial_2\Psi(\mathbf{k})\rangle, \tag{13}$$

in the limit of large L. The dimensionless integral equals $-\pi C_1$, where C_1, known as the first Chern number, is a topological integer [9,15,16] characterizing the electron distribution. The imaginary part of the localization tensor is then

$$\mathrm{Im}\,\langle xy\rangle_c = \frac{1}{N}\,\mathrm{Im}\langle\partial_1\Psi(0)|\partial_2\Psi(0)\rangle = -\frac{1}{4\pi}\,\frac{L^2}{N}\,C_1 = -\frac{l^2}{2\nu}\,C_1. \tag{14}$$

Upon replacement of the previous expressions into Eq. (6) we retrieve the seminal result of Niu, Thouless, and Wu [9]:

$$\mathrm{Re}\,\sigma_{12}(0) = -\frac{e^2}{h}\,C_1. \tag{15}$$

This was originally obtained by an analysis of the Green function, under the hypothesis that the system has a Fermi gap; in the present approach the presence of a Fermi gap—possibly in the weak sense outlined above—is a necessary and sufficient condition for the convergence of Eq. (10) in the thermodynamic limit. But this property, belonging to the *excitations* of the system, is transformed here into a pure *ground-state* property, owing to a fluctuation-dissipation theorem. As far as the longitudinal conductivity is concerned, a quantum Hall fluid is no different from any other insulator, and its wave function is localized in the sense of TIS [3,7,8]. I have shown that, owing to such localization, any two-dimensional insulator may display a quantized transverse conductance in the absence of time-reversal symmetry (even in the absence of a macroscopic B field [17]).

Equation (15) seems to legislate integer quantization of the Hall conductance in all circumstances, contrary to experimental evidence. For fractional fillings, Ref. [9] assumes then a degenerate ground state, whose different components are uncoupled and macroscopically separated. The degeneracy problem has been thoroughly discussed in the literature (for a review, see Ref. [18]); the present Letter has nothing to add.

In the metallic case both sums in Eqs. (5) and (6) do not converge: the former is positively divergent while the latter is indeterminate. Therefore TIS formally defines the diagonal elements of the localization tensor as infinite [3,7,8] (delocalized ground wave function). The off-diagonal element $\langle xy\rangle_c$ however, remains ill defined, and the Kubo formula, Eq. (6) is invalid. The transverse dc conductivity is therefore not quantized as in Eq. (15) and has to be evaluated by different means, e.g., classically [10].

In the final part of this Letter we specialize to noninteracting electrons and to the integer quantum Hall effect. In the noninteracting case (and *only* in this case) the real part of the localization tensor, Eq. (2), has a meaningful expression in terms of the one-body reduced density matrix [8,19]:

$$\mathrm{Re}\,\langle r_\alpha r_\beta\rangle_c = \frac{1}{2N}\int d\mathbf{r}d\mathbf{r}'(\mathbf{r}-\mathbf{r}')_\alpha(\mathbf{r}-\mathbf{r}')_\beta|\rho^{(1)}(\mathbf{r},\mathbf{r}')|^2, \tag{16}$$

where single occupancy is assumed. The integral converges whenever the density matrix vanishes fast enough at large $|\mathbf{r}-\mathbf{r}'|$: therefore the localization tensor discriminates between insulators and metals by measuring via Eq. (16) the "nearsightedness" [20] of the electron distribution. Our major, very general, result implies that the finiteness of Eq. (16) warrants quantization of dc transverse conductivity.

Noninteracting electrons are kept in the quantum Hall regime by disorder, and an analytical implementation of the present formalism is obviously not possible. In order to demonstrate how the theory works, I consider the academic case of a flat substrate potential, with noninteracting electrons in the lowest Landau level. I show explicitly that the system is insulating, in the sense of TIS, at complete filling, and metallic otherwise.

For complete filling ($\nu = 1$) the system is uniform with density n_0, Eq. (11); the modulus of the density matrix is gauge invariant and equals $n_0\exp-[(\mathbf{r}-\mathbf{r}')^2/(4l^2)]$. The trace of the localization tensor $\langle r^2\rangle_c = \langle x^2\rangle_c + \langle y^2\rangle_c$ is

$$\langle r^2\rangle_c = \frac{1}{2n_0}\int d\mathbf{r}r^2|\rho^{(1)}(0,\mathbf{r})|^2 = \pi n_0\int_0^\infty dr r^3 e^{-r^2/(2l^2)} = l^2, \tag{17}$$

and therefore it equals precisely the squared magnetic length.

The case of $B = 0$ is qualitatively different: the density matrix is polynomial (instead of exponential) in $|\mathbf{r}-\mathbf{r}'|$, and not nearsighted enough to make the integral in Eq. (16) convergent. Therefore, the real part of the localization tensor is formally infinite, as expected, while its imaginary

part vanishes owing to time-reversal symmetry. At finite B values, instead, the convergence of the real part of the tensor (hence the insulating nature of the system) can be regarded as the cause for quantization of the transverse conductivity.

Any single-determinant wave function is invariant by unitary transformations of the occupied orbitals among themselves, and, in particular, by transformations which localize the orbitals; in the general case the localized orbitals are not eigenstates of the single-particle Hamiltonian. The real part of the localization tensor, Eq. (16), provides an important bound for such transformations [8,19]. Suppose one looks for orbitals which are optimally localized in one Cartesian direction, say x, and delocalized along y. These orbitals have been called ''hermaphrodite'' orbitals in Ref. [19]: their quadratic spread in the x direction is minimum and equals the tensor element $\langle x^2 \rangle_c$.

For electrons in the lowest Landau level at complete filling, any unitary transformation of the occupied orbitals among themselves leads to Hamiltonian eigenstates, owing to energy degeneracy. In this case the hermaphrodite orbitals are easily identified with the Landau-gauge orbitals [10]:

$$\psi_k(\mathbf{r}) \propto e^{ik_y y} e^{-(x+k_y l^2)^2/(2l^2)}. \tag{18}$$

In fact these orbitals are plane-wave-like in the y direction, while their quadratic spread in the x direction equals precisely $\langle x^2 \rangle_c = l^2/2$.

Next, we consider a single case study at fractional ν where the longitudinal conductivity does not vanish and therefore—according to TIS—the ground state is delocalized. It is expedient to switch to the central gauge, where the single-particle orbitals are

$$\psi_m(z) = \frac{1}{\sqrt{2\pi 2^m m! l}} z^m e^{-|z|^2/4}, \tag{19}$$

where $z = (x - iy)/l$. Any state with fractional filling is nonuniform. A possible state with $\nu = 1/2$ is built by occupying the odd-m orbitals only, i.e.,

$$\begin{aligned} \rho^{(1)}(z, z') &= \sum_{m=0}^{\infty} \psi_{2m+1}(z) \psi^*_{2m+1}(z') \\ &= \frac{1}{2\pi l^2} e^{-|z|^2/4} e^{-|z'|^2/4} \sinh(z z'^*/2). \end{aligned} \tag{20}$$

This density matrix is *not* nearsighted: taking for instance $z' = -z$ we have

$$\rho^{(1)}(z, -z) = -\frac{1}{2\pi l^2} e^{-|z|^2/2} \sinh(|z|^2/2), \tag{21}$$

which clearly does not vanish at large $|z|$. The integral in Eq. (16) is positively divergent, providing a formally infinite real part of the localization tensor, as expected. Because of the above general considerations, the corresponding imaginary part is ill-defined and the transverse conductivity is not quantized.

In conclusion, I have shown quite generally that the TIS localization tensor [3,7,8]—besides discriminating between insulators and metals on the basis of longitudinal conductivity—also yields very directly the transverse dissipationless dc conductivity in the insulating case, as, e.g., in a quantum Hall fluid. It is enough to inspect electron localization in order to predict whether the dc transverse conductivity is quantized. The localization tensor is a pure ground-state property and has a geometric nature: it coincides in fact with the quantum metric-and-curvature tensor of Provost and Vallee [12] (divided by N), Eqs. (10) and (12). Both the real and the imaginary parts of the TIS localization tensor carry an outstanding physical meaning.

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