Diophantine Equation for the Hall Conductance of Interacting Electrons on a Torus

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(Received 22 January 1986)

We derive a Diophantine equation for the Hall conductance of N interacting electrons moving on a torus. The equation holds for general background fields, including inhomogeneous magnetic fields, and random substrates, but is effective when combined with symmetries. For example, together with translation invariance in one direction it determines the Hall conductance uniquely and constrains the degeneracy and crossings of eigenvalues.

PACS numbers: 72.20.My, 03.65.−w

In a profound paper, Thouless *et al.*[1] made two discoveries about the Hall conductance of noninteracting electrons in an infinitely extended periodic potential and homogeneous magnetic field (with rational flux through the unit cell). The first is that when E_F lies in a gap, the Hall conductance has a differential geometric meaning, which accounts for why it is quantized to be an integer.[2] The second is that the Hall conductance satisfies a certain Diophantine equation.[3] This equation constrains the allowed integers. More precisely, for rational magnetic fields, with flux m/q through the unit cell,[4] the Hall conductance of N full bands, $\sigma(N)$, is the integer satisfying

$$m\sigma(N) - N = qk, \tag{1}$$

with k an integer. This Diophantine equation determines $\sigma(N)$ modulo q. Related results have been described by Streda,[5] MacDonald,[6] Thouless,[7] and Dana, Avron, and Zak.[8] Equation (1) can be understood to be a consequence of the magnetic translational symmetry.[8]

It is natural to ask to what extent these two results generalize to a wider class of models and in particular to models where electrons interact.

The first result of Thouless *et al.* has indeed a generalization to a wide class of multiparticle Hamiltonians[9–12]: The Hall conductance, when appropriately defined, is a topological invariant with a precise meaning within the theory of characteristic classes[13,14] and is quantized to be an integer whenever the ground state of the multiparticle Hamiltonian is nondegenerate.[15] This gives a mathematically satisfactory theory of Laughlin's argument[16] for the integer quantization of the conductance in finite systems at zero temperatures.

The purpose of the present work is to present an analog generalization of the Diophantine equation. The method we shall use is general enough to recover all the Diophantine equations in quantum mechanics we are familiar with. In particular, it can be used to give Eq. (1), and the Wannier-Johnson-Moser-Bellissard-Lima-Testard gap-labeling equations[7] in almost-periodic Schrödinger equations.

We consider N interacting electrons moving on the two-dimensional torus, with a general background potential and a magnetic field in the perpendicular direction. The magnetic field may, but need not be, homogeneous. It is constrained to have total flux of m units,[17] as it must. This geometry has been used for the studies[18,19] of degeneracies in the spectrum, and in various numerical studies; see references in Ref. 19. We shall recover the results in Refs. 18 and 19 as a by-product of the Diophantine equation when applied to the translation-invariant situation.

We have chosen the same letters, N and m, to denote different things here and in Eq. (1) for reasons that shall become clear presently.

Formally, the system is described by the Hamiltonian given in Eq. (5) below and the boundary conditions given in Eqs. (6) and (7). More precisely, $H(\boldsymbol{\phi})$ of (5) is a family of Hamiltonians, depending parametrically on $\boldsymbol{\phi}$. $\boldsymbol{\phi}$ is a vector in the two-dimensional plane. The physical significance of its first component is related to the flux that drives the emf in one direction and that of the second component to a second flux, originally introduced by Laughlin,[16] which serves to determine the charge transport. See Ref. 10 for more details.

There is some ambiguity in what is meant by the Hall conductance which is *a priori* $\boldsymbol{\phi}$ dependent. The natural choice, also made originally by Laughlin,[16] in Refs. 9–12, and by Halperin,[20] is to average. σ then acquires geometric content. There is no such ambiguity for noninteracting electrons in an infinitely extended crystal because the thermodynamic limit makes σ independent of $\boldsymbol{\phi}$.[9]

We shall first describe the main result, Eq. (2) below, then show how symmetries combine to give useful information on σ and the degeneracy and crossings of eigenvalues. The derivation of Eq. (2) and its concomitants, Eqs. (3) and (4), are deferred to the end of the paper.

Fix $\boldsymbol{\phi}$. Since $H(\boldsymbol{\phi})$ describes a finite system, its spectrum is discrete and bounded below. Let $E_j(\boldsymbol{\phi})$ be the jth point in the spectrum, counted from below, and assume no crossings, i.e., $E_j(\boldsymbol{\phi}) > E_k(\boldsymbol{\phi})$ if $j > k$ for all $\boldsymbol{\phi}$.[15] Let $P_j(\boldsymbol{\phi})$ denote the associated projection. $d_j = \mathrm{Tr}[P_j(\boldsymbol{\phi})]$ is its degeneracy. The Diophantine equation is

$$(m\sigma_j - N)\, d_j = k_j, \tag{2}$$

where k_j and $d_j\sigma_j$ are integers associated to $P_j(\boldsymbol{\phi})$. We shall give below explicit formulas for them [Eqs. (13) and (17)]. In the general case of crossings, d_j is the dimension of the space of crossing eigenvalues. Equation (2) is independent of statistics, and holds for fermions as well as bosons. Given N and m, Eq. (2) alone does not give useful information on the σ_j. But, as we shall see, if $H(\boldsymbol{\phi})$ has symmetries, Eq. (2) becomes quite useful and it yields information on σ_j and the d_j.

Suppose that $H(\boldsymbol{\phi})$ is translation invariant in one direction. This is the case if the magnetic field and the background potential are functions of one coordinate only. As we shall show below, this implies that $k_j = 0$ for all j. Now Eq. (2) actually determines σ_j:

$$\sigma_j = N/m. \tag{3}$$

This result is known for noninteracting electrons, and interacting electrons in a constant background potential in infinite geometries. It is also apparently known for the geometry of the torus with full translation invariance although we are not aware of a formal derivation.

We can now recover, and extend, the results of Refs. 18 and 19. Since $\sigma_j d_j$ is an integer, it follows from Eq. (3) that d_j must be a multiple of m if N and m are relatively prime, and in general must be a multiple of $m/(N,m)$ where (N,m) is the largest common divisor of N and m. This is the analog of Landau degeneracy and it has been known for interacting electrons in the infinite geometry with translation-invariant fields.[21] Maksym[18] and more recently Haldane[19] derived this result for the torus with translation invariant fields.

The second application we consider is for the case of discrete translation invariance: Suppose that the background fields have a unit cell so that q such cells cover the torus. q and m are assumed to be relatively prime. Then, as we shall show, k_j is a multiple of q and Eq. (2) reads

$$(m\sigma_j - N)\, d_j = q k_j'. \tag{4}$$

Note that in the case $d_j = 1$, which is the generic situation in the absence of symmetries,[15] Eq. (4) is formally identical with Eq. (1). In particular, it determines σ_j modulo q. In the general case, Eq. (4) determines $\sigma_j d_j$ to be a multiple of (N,q). There are more complicated results when q and m are not relatively prime.

We shall now outline the derivation of the above results. The Hamiltonians are given formally by[22]

$$H(\boldsymbol{\phi}) = \sum_j \tfrac{1}{2}[(\mathbf{v}_j - \boldsymbol{\phi})^2 + V(\mathbf{x}_j)] + \sum_{j<k} W(\mathbf{x}_j - \mathbf{x}_k), \quad \mathbf{v}_j = -i\nabla_j - e\mathbf{A}(\mathbf{x}_j), \tag{5}$$

where $\mathbf{x}_j$ is a point on the two-torus and $\mathbf{x}_j - \mathbf{x}_k$ is the natural distance on it. e is the electric charge. It is convenient to regard $\mathbf{x}$ as a point in the plane or in the rectangle $\Omega = [\mathbf{t}_1 \times \mathbf{t}_2]$ where $\mathbf{t}_\alpha$, $\alpha = 1,2$, are the period vectors of the torus. $V(\mathbf{x})$, $W(\mathbf{x})$, and $\mathbf{B}(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x})$ must then be periodic functions of their arguments with period t_α. The vector potential need not be periodic in $\mathbf{x}$ but it can be decomposed into a periodic piece, $A_p(\mathbf{x})$, and a piece which is linear in $\mathbf{x}$, $A_1(\mathbf{x})$, which is absent if and only if the total flux vanishes.

The boundary conditions for $H(\boldsymbol{\phi})$ are somewhat subtle and although the answer is known, it may be useful to describe the reasoning behind it. Consider the $\mathbf{x}_i$ to be in the rectangle Ω. The question is, what boundary conditions on $\psi(\mathbf{x}_1, \ldots, \mathbf{x}_N)$ describe the dynamics on a torus? The point is that parallel transport of the state ψ—translation without affecting the observable properties—is subtle when a gauge field is present and "periodic boundary conditions" involve a certain twist. More precisely, parallel transport is generated by the velocity, $-i\nabla - e\mathbf{A}(\mathbf{x})$, and not by the canonical momentum $-i\nabla$. Parallel transport of ψ from $\mathbf{x}$ to $\mathbf{x} + \mathbf{t}_\alpha$ along a path in the $\mathbf{t}_\alpha$ direction is given by

$$\psi(\mathbf{x}) \Rightarrow \psi(\mathbf{x} + \mathbf{t}_\alpha)\exp\{-ie[\int_0^1 \mathbf{A}(\mathbf{x} + \tau\mathbf{t}_\alpha)\cdot\mathbf{t}_\alpha\, d\tau]\}.$$

The appropriate boundary conditions are therefore

$$\psi(\ldots, \mathbf{x}_j, \ldots) = \exp[-ie\Lambda_\alpha(\mathbf{x}_j)]\psi(\ldots, \mathbf{x}_j + \mathbf{t}_\alpha, \ldots), \tag{6}$$

where

$$\Lambda_\alpha(\mathbf{x}) = \int_0^1 \mathbf{A}(\mathbf{x} + \tau\mathbf{t}_\alpha)\cdot\mathbf{t}_\alpha\, d\tau. \tag{7}$$

Parallel transport is path dependent if $B \neq 0$: The magnetic field plays the role of curvature. A consequence of this is that the boundary conditions constrain the flux to be quantized. This can be seen by comparing $\psi(\ldots, \mathbf{t}_1 + \mathbf{t}_2, \ldots)$ with $\psi(\ldots, 0 \ldots)$ using Eq. (6) twice: once for the path $\mathbf{t}_1 + \mathbf{t}_2 \Rightarrow \mathbf{t}_1 \Rightarrow 0$ and once for $\mathbf{t}_1 + \mathbf{t}_2 \Rightarrow \mathbf{t}_2 \Rightarrow 0$. Consistency requires

$$[\Lambda_2(\mathbf{t}_1) - \Lambda_2(0)] - [\Lambda_1(\mathbf{t}_2) - \Lambda_1(0)] = 2\pi m/e, \tag{8}$$

with m an integer. But

$$\int \mathbf{B}\cdot d\mathbf{x} = \oint \mathbf{A}\cdot d\mathbf{l} = [\Lambda_1(0) - \Lambda_1(\mathbf{e}_2)] - [\Lambda_2(0) - \Lambda_2(\mathbf{e}_1)], \tag{9}$$

giving the flux quantization.

This type of argument is also used for the quantization of the Hall conductance; compare, e.g., Ref. 1. The difference is that flux quantization is related to the transport in coordinate space while Hall quantization is related to transport in the parameter space of $\boldsymbol{\phi}$ where the adiabatic evolution provides a natural parallel transport.[23–26]

The following is known about periodic, parameter-dependent projections: Suppose that $P(\boldsymbol{\phi})$ is an orthogonal projection, smooth and periodic in $\boldsymbol{\phi}$, and let BZ denote the unit cell in the $\boldsymbol{\phi}$ parameter space. Then[10,27]

$$n(P) = (i/2\pi)\int_{BZ} \mathrm{Tr}[dP\,P\,dP] \tag{10}$$

is an integer. d is the exterior derivative with respect to $\boldsymbol{\phi}$. We shall apply Eq. (10) for the spectral projection, $P(\boldsymbol{\phi})$, of periodic, parameter-dependent, Hamiltonians.

Equation (10) is not directly applicable to $H(\boldsymbol{\phi})$ becasue $H(\boldsymbol{\phi})$ is not periodic in $\boldsymbol{\phi}$, and neither are its projections. However, there are unitary transformations that make $H(\boldsymbol{\phi})$ periodic. Indeed, we shall introduce two such transformations; one gives k_j and one $\sigma_j d_j$. To this end, we need a technical tool that describes how Eq. (10) is modified under unitary transformations.

Let $Q(\phi) = U(\phi)P(\phi)U^\dagger(\phi)$ (where the dagger denotes the adjoint), then

$$\mathrm{Tr}(dP\,P\,dP) = \mathrm{Tr}(dQ\,Q\,dQ) + d\,\mathrm{Tr}(Q\,dU\,U^\dagger). \tag{11}$$

In deriving (11) we used the facts that $Q^2(\boldsymbol{\phi}) = Q(\boldsymbol{\phi})$, $Q\,dQ\,Q = 0$, and $(dU^\dagger)U + U^\dagger dU = 0$; the cyclicity of the trace; and the anticommutativity of one-forms.

Now take $U_1(\boldsymbol{\phi}) = \exp - i\mathbf{x}\cdot\boldsymbol{\phi}$ with $\mathbf{x} = \sum \mathbf{x}_j$. Then $H_1(\boldsymbol{\phi}) = U_1(\boldsymbol{\phi})H(\boldsymbol{\phi})U_1^\dagger(\boldsymbol{\phi})$ is formally $\boldsymbol{\phi}$ independent and, in particular, is periodic in $\boldsymbol{\phi}$. The period is determined by the boundary conditions: Since $\psi_1 = U_1(\boldsymbol{\phi})\psi$, then

$$\psi_1(\ldots, \mathbf{x}_j, \ldots) = \exp\{-i[e\Lambda_\alpha(\mathbf{x}) + \boldsymbol{\phi}\cdot\mathbf{t}_\alpha]\}\psi_1(\ldots, \mathbf{x}_j + \mathbf{t}_\alpha, \ldots). \tag{12}$$

[$H(\boldsymbol{\phi})$ has $\boldsymbol{\phi}$-independent boundary conditions.] The period of (12) is $BZ = {}^*\mathbf{t}_1 \times {}^*\mathbf{t}_2$, where ${}^*\mathbf{t}_\alpha$ are the duals of $\mathbf{t}_\alpha$, i.e., ${}^*\mathbf{t}_\alpha\cdot\mathbf{t}_\beta = 2\pi\delta_{\alpha,\beta}$. This is the period of the spectral projections $P_1(\boldsymbol{\phi})$, which is smooth if it projects on an energy band bordered by gaps. Now $dU_i^\dagger U_1 = i\mathbf{x}\cdot d\boldsymbol{\phi}$ is $\boldsymbol{\phi}$ independent and so the boundary term in (11) drops out and

$$\int_{BZ} \mathrm{Tr}(dP_1 P_1 dP_1) = \int_{BZ} \mathrm{Tr}(dP\,P\,dP).$$

The relation between $P(\boldsymbol{\phi})$, $P_1(\boldsymbol{\phi})$, and the Hall conductance is given by

$$\sigma_j = (i/2\pi d_j)\int_{BZ} \mathrm{Tr}(dP\,P\,dP). \tag{13}$$

Here, the two factors of dP are associated with the external emf and the response, and the P reflects the underlying expectation value. When the jth level is degenerate we assume that the system is described by the density matrix P/d_j. This relation has been discussed (for rank-one projection) in Ref. 10. When levels cross we take Eq. (13) to be the definition of σ_j. Combined with Eq. (10), it implies that $\sigma_j d_j$ is an integer. Thus, σ_j is a fraction with a denominator related to the ground-state degeneracy.[9–11,28]

The same mechanism produces a second integer by choice of another unitary transformation $U_2(\boldsymbol{\phi})$. The Diophantine equation will come from a relation between these two integers.

Let $\mathbf{u} = -i\nabla - e\mathbf{A}_1(\mathbf{x})$. One verifies the following relations:

$$\exp[-i(\boldsymbol{\beta}\cdot\mathbf{u})f(\mathbf{x})]\exp[i(\boldsymbol{\beta}\cdot\mathbf{u})] = f(\mathbf{x}-\boldsymbol{\beta}), \tag{14}$$

$$\exp[-i(\boldsymbol{\beta}\cdot\mathbf{u})f(\mathbf{v})]\exp[i(\boldsymbol{\beta}\cdot\mathbf{u})] = f(\mathbf{v} - e\boldsymbol{\beta}\times\mathbf{B}_0 - e\mathbf{A}_p(\mathbf{x}+\boldsymbol{\beta}) + e\mathbf{A}_p(\mathbf{x}+\boldsymbol{\beta}) + e\mathbf{A}_p(\mathbf{x})),$$

where $\mathbf{B}_0 = \nabla\times\mathbf{A}_1$ is a constant. Now let $\mathbf{u} = \sum \mathbf{u}_j$ and $\mathbf{b} = \mathbf{B}/\mathbf{B}\cdot\mathbf{B}$, and take

$$U_2(\boldsymbol{\phi}) = \exp(i\mathbf{u}\cdot\boldsymbol{\phi}\times\mathbf{b}).$$

From Eq. (14)

$$H_2(\boldsymbol{\phi}) = U_2(\boldsymbol{\phi})H(\boldsymbol{\phi})U_2^\dagger(\boldsymbol{\phi}) = \tfrac{1}{2}\sum_j[\mathbf{v}_j - e\mathbf{A}_p(\mathbf{x}-\boldsymbol{\phi}\times\mathbf{b}) + e\mathbf{A}_p(\mathbf{x})]^2 + \sum_j V(\mathbf{x}_j - \boldsymbol{\phi}\times\mathbf{b}) + \sum_{j<k} W(\mathbf{x}_j - \mathbf{x}_k). \tag{15}$$

The wave function, $\psi_2 = U_2(\boldsymbol{\phi})\psi$, satisfies the boundary conditions

$$\psi_2(\ldots,\mathbf{x}_j,\ldots) = \exp[-ie\Lambda_\alpha(\mathbf{x}_j)]\exp\{-i[\mathbf{t}_\alpha\cdot\mathbf{A}_1(\boldsymbol{\phi}\times\mathbf{b}) + \mathbf{A}_1(\mathbf{t}_\alpha)\cdot\boldsymbol{\phi}\times\mathbf{b}]\}\psi_2(\ldots,\mathbf{x}_j+\mathbf{t}_\alpha,\ldots). \quad (16)$$

In the symmetric gauge, $\mathbf{A}_1 = \frac{1}{2}\mathbf{B}_0\times\mathbf{x}$, $\mathbf{t}_\alpha)\cdot\mathbf{A}_1(\boldsymbol{\phi}\times\mathbf{b}) + \mathbf{A}_1(\mathbf{t}_\alpha\cdot\boldsymbol{\phi}\times\mathbf{b}=0$, and the boundary conditions in Eq. (16) are $\boldsymbol{\phi}$ independent. The periodicity of $P_2(\boldsymbol{\phi}) = U_2(\boldsymbol{\phi})P(\boldsymbol{\phi})U_2^\dagger(\boldsymbol{\phi})$ is determined by $H_2(\boldsymbol{\phi})$ alone and is $BZ_2 = m\mathbf{t}_1^\dagger\times m\mathbf{t}_2^\dagger$. So by Eq. (10),

$$k'(P_2) = (i/2\pi)\int_{BZ_2}\mathrm{Tr}(dP_2\,P_2\,dP_2) \quad (17)$$

is an integer.

The Diophantine equation (2) comes from (11): One has

$$(dU_2)U_2^\dagger = -i\mathbf{v}\cdot d\boldsymbol{\phi}\times\mathbf{b} + (iN/2)\boldsymbol{\phi}\times\mathbf{b}\cdot d\boldsymbol{\phi}.$$

The first term on the right-hand side is independent of $\boldsymbol{\phi}$ and does not contribute when Eq. (11) is integrated over BZ. The second term comes from the commutator of the components of the vector $\mathbf{v}$ which is proportional to Nb. Since this term is linear in $\boldsymbol{\phi}$ it survives the integration in Eq. (11) over the periods. Combining Eqs. (11, (13), and (17) gives

$$m^2\sigma_j d_j = k_j' + Nmd_j. \quad (18)$$

This says that k_j' of Eq. (17) is a multiple of m, $k_j' = mk_j$ and gives Eq. (2) if $m\neq 0$.

Suppose that $H(\boldsymbol{\phi})$ is translation invariant in one direction, say, $\mathbf{t}_1$. $H_2(\boldsymbol{\phi})$ is then constant in $\boldsymbol{\phi}$ along the $\mathbf{t}_2$ direction. It follows that $P_2(\boldsymbol{\phi})$ is a function of a single coordinate $\boldsymbol{\phi}\cdot\mathbf{t}_1$ and so any two-form constructed from it, in particular $dP_2\,P_2\,dP_2$, must vanish identically. This implies that $k_j = 0$.

Consider the case of discrete translation invariance. Suppose that $q = q_1q_2$ where q_α is the number of periods in the α direction, $\alpha = 1,2$. The period of $H(\boldsymbol{\phi})$ is now smaller by a factor of q. From (15) and (17), and a translating argument, we see that k' of Eq. (17) is a multiple of q. If q and m are relatively prime, this gives Eq. (4).

To summarize, we have derived a Diophantine equation for the Hall conductance of interacting electrons on a two-dimensional torus, in arbitrary background fields. In cases where the background fields have symmetries, the equation constrains (and sometimes actually determines) the Hall conductance and the degeneracy of eigenvalues.

This work was supported in part by the U. S.–Israel Binational Science Foundation under Grant No. 84-00376 and by the Israel Academy of Sciences. One of us (L.G.Y.) is an Alfred P. Sloan Research Fellow.

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