Diophantine equation for the three-dimensional quantum Hall effect

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When the Fermi level lies in a gap, the Hall conductivity of three-dimensional electrons in a periodic potential is expressed in a topologically invariant form with a set of three integers. If the magnetic fluxes through the three independent areas of the periodic lattice are rational numbers, one obtains a Diophantine equation relating these numbers and the integers which characterize the Hall conductivity.

I. INTRODUCTION

The quantized Hall effect in two dimensions (2D) has been extensively studied since the pioneering experimental work of von Klitzing, Dorda, and Pepper.[1] Laughlin[2] argued from a general gauge principle that the Hall conductivity should be integrally quantized ($\sigma_{xy}=ne^2/h$, where n is an integer) when the Fermi level lies in a gap of extended states. Then, from the Kubo formula, Thouless, Kohmoto, Nightingale, and den Nijs[3] (TKNN) derived an explicit formula for the Hall conductance of noninteracting electrons in periodic systems. This expression is independent of the detailed structure of the periodic potential.[4] The integer is a topological invariant—the first Chern class of a U(1) principle fiber bundle on a torus.[5] It relates to the structure of the magnetic subbands and thus depends on the flux ϕ of the magnetic field through a unit area of the periodic lattice.

The problem of a 2D crystal in a magnetic field is an old one.[6] The electron energy spectrum has an extremely rich structure as shown by Hofstdater.[6] In fact if ϕ is irrational, it is a Cantor set which consists of infinitely many "bands" with scaling properties.[7] For a rational $\phi=p/q$, each subband carries an integer Hall conductivity. If the Fermi level is in an energy gap such that r bands are completely full, and all others are empty, one has the Diophantine relation

$$r=qs_r+pt_r \ , \tag{1.1}$$

where s_r and t_r are integers. The Hall conductivity is given by $-t_re^2/h$.[3,8]

The solution of (1.1), unfortunately, is not unique. In the weak-potential case we have a restriction $|s_r|\leq p/2$. On the other hand, $|t_r|\leq q/2$ for the strong-potential limit, i.e., the tight-binding case. Thus we do have unique solutions in these two limits. If a gap closes and reopens in the intermediate region, however, t_r will change, although it will still satisfy the Diophantine equation (1.1).

It is interesting to ask whether these results can be generalized to electron states in a three-dimensional periodic potential in a uniform magnetic field. In a previous paper,[9] one of the present authors demonstrated, following the lines of TKNN, that when the Fermi level is in an energy gap in the 3D case, the conductivity tensor can always be written in the form

$$\sigma_{ij}=\frac{e^2}{2\pi h}\varepsilon_{ijk}G_k \ , \tag{1.2}$$

where ε_{ijk} is the unit antisymmetric tensor, and $\mathbf{G}$ is a vector (possibly zero) on the reciprocal lattice of the periodic potential. Moreover, if the magnetic field $\mathbf{B}$ is varied in magnitude or direction, the vector $\mathbf{G}$ remains constant, as long as the Fermi level remains in the gap.

Since $j_i=\sum_k\sigma_{ik}E_k$, (1.2) implies the current is given by $\mathbf{j}=(e^2/2\pi h)\mathbf{E}\times\mathbf{G}$. Then the consequences of (1.2) are the following. (1) For an electric field $\mathbf{E}$ in an arbitrary direction, there can be no current component parallel to $\mathbf{E}$, and so there will be no dissipation. (2) There can be no current component parallel to $\mathbf{G}$. However, there can be a Hall current in the crystal planes perpendicular to $\mathbf{G}$, if $\mathbf{G}\neq\mathbf{0}$. (3) The Hall conductance in each crystal plane perpendicular to $\mathbf{G}$ has a quantized Hall value, ne^2/h. [The value of n is equal to the greatest common divisor of the three integers t_α which appear in (1.5) below.]

The overall question of when there will or will not be an energy gap between bands in a three-dimensional periodic potential has not been extensively investigated; nor has the question of when there will be a nontrivial value of the Hall conductance ($\mathbf{G}\neq\mathbf{0}$). Recently, however, several authors have calculated the energy spectra for some simple cases of 3D periodic systems in a magnetic field, and have indeed found regions of parameters where energy gaps open up.[10–12]

A quantum-mechanical state closely related to the 3D quantized Hall state in a periodic lattice has employed as a description of a three-dimensional chiral spin liquid state by Laughlin and co-workers.[13]

Montambaux and Littlewood[14] presented a physical situation in which the Fermi level is pinned in a gap, in the absence of any disorder. This is the magnetic-field-induced spin-density-wave (SDW) subphases of a 3D quasi-one-dimensional conductor. However, their

description neglected the lattice periodicity along the direction of highest conductivity—an approximation valid for low fields. There it has been stressed that an interesting situation could take place as soon as the field is not aligned along one of the crystallographic axes. This is essentially due to the fact that we have three parameters ϕ_a, ϕ_b, and ϕ_c (instead of one ϕ in 2D), which are the magnetic fluxes in units of h/e through the three independent areas of the periodic lattice. (In this paper, we choose $e>0$, so that the electron charge is $-e$.)

Montambaux and Kohmoto[10] considered a simple geometry in which the field **B** is perpendicular to the *a-b* plane and the *c* axis is tilted with an angle θ in the *B-b* plane, where **a**,**b**,**c** are a set of vectors which span the Bravais lattice. Note that there is no magnetic flux through the *b-c* plane in this geometry. They obtained explicit energy spectra and the quantized Hall conductivities when the Fermi energy lies in a gap for a tight-binding model where the hopping strength in the **b** and **c** directions is weak, compared with the hopping in the **a** direction.

Montambaux and Kohmoto also proposed a generalization to three dimensions of the Diophantine equation (1.1). Specifically, they considered a "rational" magnetic field **B**, which has the form

$$\mathbf{B}=\frac{1}{v_0}\frac{h}{e}\left[\frac{p_a}{q_a}\mathbf{a}+\frac{p_b}{q_b}\mathbf{b}+\frac{p_c}{q_c}\mathbf{c}\right], \tag{1.3}$$

where v_0 is the volume of the unit cell,

$$v_0=\mathbf{a}\cdot(\mathbf{b}\times\mathbf{c}), \tag{1.4}$$

and p_α and q_α are integers ($\alpha=a,b,c$) with $q_\alpha>0$. The reciprocal lattice vector **G** which enters (1.2) for the conductivity tensor may be expanded in terms of the elementary reciprocal lattice vectors dual to **a**,**b**,**c** as

$$\mathbf{G}=-(t_a\mathbf{G}_a+t_b\mathbf{G}_b+t_c\mathbf{G}_c), \tag{1.5}$$

where t_α are also integers. Then the Diophantine equation proposed by Montambaux and Kohmoto states that there exist integers r and s, such that r is the number of filled bands and

$$\frac{r}{Q}=s+t_a\frac{p_a}{q_a}+t_b\frac{p_b}{q_b}+t_c\frac{p_c}{q_c}, \tag{1.6}$$

where $Q=q_aq_bq_c$.

In the case where q_a, q_b, and q_c have a common divisor, the unit cell chosen by Montambaux and Kohmoto is not the smallest possible unit cell in direct space. By choosing the smallest cell in direct space, and hence the largest cell in reciprocal space, we find that the value of Q in (1.6) may be chosen to be the least common multiple of q_a, q_b, and q_c. With this choice of unit cell, the number of filled bands r will of course be smaller (by an integer factor) than for the choice of Montambaux and Kohmoto.

Although Montambaux and Kohmoto derived (1.6) in some special cases, they did not give a general proof of this relation. It is the primary purpose of the present paper to supply such a proof. Specifically, we study generic cases for 3D electrons in a periodic potential in a uniform magnetic field. Namely, the primitive vectors **a**, **b**, and **c** are not necessarily orthogonal to each other, and the magnetic field **B** is aligned in a general direction. In Sec. II, following Ref. 12, we derive the three-dimensional Hall conductivity formula (1.2) by using a particular choice **a**′,**b**′,**c**′ for primitive vectors of the Bravais lattice, which are in general linear combinations of the original vectors **a**,**b**,**c**. With this choice, the expansion coefficients $t_{a'}$, $t_{b'}$, and $t_{c'}$ of the reciprocal lattice vector **G** in the Hall conductivity formula have the meaning of topological invariants—namely, the Chern numbers. In Sec. III we show that the Diophantine equation (1.6) applies for an arbitrary choice of the primitive vectors **a**,**b**,**c**.

II. QUANTIZED HALL CONDUCTIVITY IN A THREE-DIMENSIONAL PERIODIC POTENTIAL

We describe here the derivation of the three-dimensional quantized Hall conductance formula (1.2) for noninteracting electrons in a periodic potential. In order to make this paper self-contained and to establish our notations, we elaborate the proof presented in Ref. 9. The proof is a generalizaton to three dimensions of the arguments of TKNN for the two-dimensional case.[3]

We first note that if the Fermi energy is located in an energy gap, or in an energy region that contains only localized states, then there can be no dissipative current flow for a weak electric field in any direction. It follows that the diagonal elements of σ must vanish for any choice of coordinate axes, and hence σ is purely antisymmetric. Therefore we may write

$$\sigma_{ij}=\frac{e^2}{2\pi h}\varepsilon_{ijk}D_k, \tag{2.1}$$

where **D** is a vector whose value we wish to determine.

One can define three fluxes ϕ_a, ϕ_b, and ϕ_c (instead of one ϕ in 2D) through the three elementary plaquettes of the periodic lattice. The areas of these plaquettes are given by $\mathbf{a}_j\times\mathbf{a}_k$ ($\mathbf{a}_j$ and $\mathbf{a}_k$ are **a**, **b**, or **c**). The flux is written, in units of the quantum h/e, as

$$\begin{aligned}\phi_a&=\frac{e}{h}\mathbf{B}\cdot(\mathbf{b}\times\mathbf{c}),\\ \phi_b&=\frac{e}{h}\mathbf{B}\cdot(\mathbf{c}\times\mathbf{a}),\\ \phi_c&=\frac{e}{h}\mathbf{B}\cdot(\mathbf{a}\times\mathbf{b}),\end{aligned} \tag{2.2}$$

so that the uniform field **B** is totally characterized by these three quantities.

The primitive vectors in the reciprocal lattice are given by

$$\begin{aligned}\mathbf{G}_a&=2\pi(\mathbf{b}\times\mathbf{c})/v_0,\\ \mathbf{G}_b&=2\pi(\mathbf{c}\times\mathbf{a})/v_0,\\ \mathbf{G}_c&=2\pi(\mathbf{a}\times\mathbf{b})/v_0.\end{aligned} \tag{2.3}$$

Since $\mathbf{G}_a$ is perpendicular to the b-c plane, one has $\mathbf{B}\cdot\mathbf{G}_a=2\pi\mathbf{B}\cdot(\mathbf{b}\times\mathbf{c})/v_0=(2\pi h/v_0 e)\phi_a$ and similar relations for $\mathbf{G}_b$ and $\mathbf{G}_c$. So $\mathbf{B}$ is written

$$\mathbf{B}=\frac{1}{v_0}\frac{h}{e}(\phi_a\mathbf{a}+\phi_b\mathbf{b}+\phi_c\mathbf{c}) . \tag{2.4}$$

We shall first consider the case of a "rational magnetic field," where ϕ_a, ϕ_b, and ϕ_c are rational, i.e.,

$$\phi_a=\frac{p_a}{q_a} ,$$
$$\phi_b=\frac{p_b}{q_b} , \tag{2.5}$$
$$\phi_c=\frac{p_c}{q_c} ,$$

where p_α and q_α are integers with no common factor. Let Q be the least common multiple of q_a, q_b, and q_c; then we may write $\phi_a=n_1/Q$, $\phi_b=n_2/Q$, and $\phi_c=n_3/Q$ where n_i are integers. Let p be the greatest common factor of n_1, n_2, and n_3, then we have $n_1=pm_1$, $n_2=pm_2$, and $n_3=pm_3$. Thus we have

$$\phi_a=\frac{p}{Q}m_1 ,$$
$$\phi_b=\frac{p}{Q}m_2 , \tag{2.6}$$
$$\phi_c=\frac{p}{Q}m_3 .$$

From these (2.4) is written

$$\mathbf{B}=\frac{h}{e}\frac{1}{v_0}\frac{p}{Q}\mathbf{c}' , \tag{2.7}$$

where

$$\mathbf{c}'=m_1\mathbf{a}+m_2\mathbf{b}+m_3\mathbf{c} \tag{2.8}$$

is a lattice vector. By definition m_1, m_2, and m_3 do not have a common factor and there is no vector on the Bravais lattice which is a submultiple of $\mathbf{c}'$. Then one can find $\mathbf{a}'$ and $\mathbf{b}'$ such that $\mathbf{a}'$, $\mathbf{b}'$, and $\mathbf{c}'$ are a new set of primitive lattice vectors (see Appendix). The fluxes in the new set of primitive vectors are given by (2.2) with $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ being replaced by $\mathbf{a}'$, $\mathbf{b}'$, and $\mathbf{c}'$. Then (2.7) implies

$$\phi_{a'}=\phi_{b'}=0 ,$$
$$\phi_{c'}=\frac{p}{Q} . \tag{2.9}$$

For electrons in a uniform magnetic field, one may define a set of translation operators $S_{\mathbf{R}}$ which translate the wave function by the vector $\mathbf{R}$ and multiply it by a postion-dependent phase factor, and which commute with kinetic energy.[15] Two operators, $S_{\mathbf{R}}$ and $S_{\mathbf{R}'}$, have the property

$$S_{\mathbf{R}}S_{\mathbf{R}'}=S_{\mathbf{R}'}S_{\mathbf{R}}e^{i2\pi\phi} , \tag{2.10}$$

where $\phi=\mathbf{B}\cdot(\mathbf{R}\times\mathbf{R}')e/h$.

If we now consider the operators $S_{\mathbf{a}'}$, $(S_{\mathbf{b}'})^Q=S_{Q\mathbf{b}'}$, and $S_{\mathbf{c}'}$, it is straightforward to see that they each commute with the Hamiltonian, and they commute with each other. Thus we may choose eigenfunctions of the Hamiltonian in the form

$$\psi_{\mathbf{k},n}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k},n}(\mathbf{r}) , \tag{2.11}$$

where $u_{\mathbf{k},n}$ is invariant under the operators $S_{\mathbf{a}'}$, $S_{Q\mathbf{b}'}$, and $S_{\mathbf{c}'}$ and n is a band index. The absolute value $|u_{\mathbf{k},n}|$ is a periodic function of $\mathbf{r}$ in the "magnetic Bravais lattice" generated by $\mathbf{a}'$, $Q\mathbf{b}'$, and $\mathbf{c}'$ and we shall normalize $u_{\mathbf{k},n}$ in the unit cell of this lattice. The wave vector $\mathbf{k}$ may be restricted to a magnetic Brillouin zone of the form

$$\mathbf{k}=f_1\mathbf{G}_{a'}+\frac{f_2}{Q}\mathbf{G}_{b'}+f_3\mathbf{G}_{c'} , \tag{2.12}$$

where f_1, f_2, and f_3 range from 0 to 1, and $\mathbf{G}_{a'}$, $\mathbf{G}_{b'}$, and $\mathbf{G}_{c'}$ are the fundamental reciprocal lattice vectors of the original lattice, given by (2.2) with $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ being replaced by $\mathbf{a}'$, $\mathbf{b}'$, and $\mathbf{c}'$. The phase of $u_{\mathbf{k},n}$ gives the fiber of the principal U(1) bundle over the two-torus which is the magnetic Brillouin zone, except possibly for some isolated points in the Brillouin zone where two bands become degenerate. They give singularities on the magnetic Brillouin zone. (This assumes that the potential has no special symmetry other than translation.)

If the Fermi energy lies in an energy gap between two bands n and $n+1$, then the conductivity tensor is given, according to the Kubo-Greenwood formula, by

$$\sigma_{ij}=\frac{e^2}{i4\pi^2h}\int d^3k\sum_{n'\le n}\int d^3r\left[\frac{\partial u^*_{\mathbf{k}n'}}{\partial k_i}\frac{\partial u_{\mathbf{k}n'}}{\partial k_j}-\frac{\partial u^*_{\mathbf{k}n'}}{\partial k_j}\frac{\partial u_{\mathbf{k}n'}}{\partial k_i}\right] , \tag{2.13}$$

where the space integral is over a unit cell of the magnetic Bravais lattice, and the $\mathbf{k}$ is over the magnetic Brillouin zone (see Fig. 1). The k integral is written

$$\int d^3k=\int_0^1 df_3(\mathbf{G}_{c'}\cdot\mathbf{c}')\Big/c'\int_{S(f_3)}d^2k$$
$$=2\pi\Big/c'\int_0^1 df_3\int_{S(f_3)}d^2k ,$$

where $S(f_3)$ is a surface which is parallel to the $G_{a'}$-$G_{b'}$ plane in the magnetic Brillouin zone (see Fig. 1). From (2.1) and (2.13) we obtain

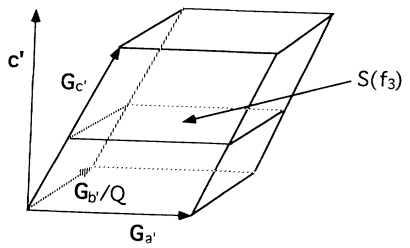

FIG. 1. The magnetic Brillouin zone.

$$\mathbf{D}\cdot\mathbf{c}'=\frac{\pi h}{e^2}\sum_{ijk}\varepsilon_{ijk}\sigma_{ij}c'_{k'}$$
$$=\sum_{n'\le n}\int_0^1 df_3\sigma_{n'}(f_3)\ , \tag{2.14}$$

where

$$\sigma_{n'}(f_3)\equiv\frac{1}{i}\int_{S(f_3)}d^2k\int d^3r[\nabla_k\times(u^*_{\mathbf{k}n'}\nabla_k u_{\mathbf{k}n'})]\cdot\frac{\mathbf{c}'}{|\mathbf{c}'|}\ . \tag{2.15}$$

If the Stokes theorem is applied naively to the k integral over the surface $S(f_3)$, then $\sigma_{n'}(f_3)$ represents the net phase change of $u_{\mathbf{k},n'}$ around the perimeter of $S(f_3)$ and is necessarily an integer times 2π. However, this argument is rather incomplete. If there are no points of degeneracy between the band n' and any other band, this integer is a topological invariant, and is independent of f_3. The essential point here is that the magnetic Brillouin zone is topologically a three-torus. Thus the cross section $S(f_3)$ is a two-torus and in general it is not possible to define a global phase on it. Then the phase of the state defines a principal U(1) bundle over the two-torus. Now the expression in (2.15) represents 2π times a Chern number of the fiber bundle which is necessarily an integer. A detailed account of this point can be found in Ref. 5. If there is a point of degeneracy between n' and another band, the value of $\sigma_{n'}(f_3)$ may change discontinuously, as a function of f_3, but the sum of the contributions of the two bands will not change. Since we have assumed that there is an energy gap between bands n and $n+1$, so that there is no point of contact between them, it follows that $\sum_{n'\le n}\sigma_{n'}(f_3)$ is an integer, independent of f_3, and that the quantity $\mathbf{c}'\cdot\mathbf{D}$ is an integer multiple of 2π.

In a similar manner, we may prove that $\mathbf{a}'\cdot\mathbf{D}$ and $Q\mathbf{b}'\cdot\mathbf{D}$ are also integer multiples of 2π. Moreover, by choosing a different magnetic Brillouin zone, where the roles of $\mathbf{a}'$ and $\mathbf{b}'$ are interchanged, we can establish that $\mathbf{b}'\cdot\mathbf{D}$ is itself an integer multiple of 2π. It then follows that $\mathbf{D}$ is a vector $\mathbf{G}$ on the reciprocal lattice generated by $\mathbf{G}_{a'}$, $\mathbf{G}_{b'}$, and $\mathbf{G}_{c'}$ as

$$\mathbf{G}=-(t_{a'}\mathbf{G}_{a'}+t_{b'}\mathbf{G}_{b'}+t_{c'}\mathbf{G}_{c'})\ . \tag{2.16}$$

The magnetic Brillouin zone is a three-torus. Each band has three topological invariants (first Chern numbers) on the two-tori obtained by slicing the three-torus in three different manners. The three integers $t_{a'}$, $t_{b'}$, and $t_{c'}$ are the sums over these integers over the filled bands. Avron, Seiler, and Simon[16] found that every quantized invariant on a d-dimensional torus T^d is a function of the $d(d-1)/2$ sets of TKNN integers obtained by slicing T^d by the $d(d-1)/2$ distinct T^2. In 3D, the three TKNN integers are precisely related to $t_{a'}$, $t_{b'}$, and $t_{c'}$.

Finally, we must consider irrational values of the magnetic field $\mathbf{B}$. It can be shown that if E_F lies in an energy gap for some specified $\mathbf{B}$, then it must be also inside the gap for all magnetic fields in some neighborhood of $\mathbf{B}$.[17] The value of $\mathbf{G}$ cannot change, however, as long as E_F is inside a gap.[17,18] Therefore the value of $\mathbf{G}$ throughout the neighborhood is determined by the value at the rational magnetic fields, and is a vector on the reciprocal lattice, as claimed.

III. DIOPHANTINE EQUATION

When the Fermi energy is in an energy gap, there exists a relation between the antisymmetric conductivity tensor σ_{ij} and the derivative of the electron density ρ with respect to the magnetic field $\mathbf{B}$, which is an extension of three dimensions of the well-known Widom-Streda formula[19] for the two-dimensional quantized Hall conductance. The three-dimensional version of this formula may be written in the form

$$\sigma_{ij}=-e\varepsilon_{ijk}\frac{\partial\rho}{\partial B_k}\ , \tag{3.1}$$

where the derivative is to be taken with the Fermi level μ fixed inside the gap.

The simplest derivation of this formula follows the lines of Widom's argument. When the Fermi level lies inside a gap, it is reasonable to assume that the frequency- and wave-vector-dependent conductivity tensor $\sigma_{ij}(\mathbf{k},\omega)$ is analytic in the limit $k\to 0$, $\omega\to 0$, with a finite limiting value (possibly zero) which is independent of order of limits taken. Let us consider the ground state of the system in a time-independent magnetic field and electrostatic potential which vary slowly in space, and deviate only slightly from their average values, such that the Fermi level μ remains in the gap at all points in space. If the thermodynamic potential $\Omega=E-\mu N$ is considered to be a functional of the magnetic field $\mathbf{B}(\mathbf{r})$ and the electrostatic potential $\Phi(\mathbf{r})$, then the electron charge density and current are given by

$$-e\rho(\mathbf{r})=\frac{\delta\Omega}{\delta\Phi(\mathbf{r})}\ , \tag{3.2}$$

$$\mathbf{j}(\mathbf{r})=\nabla\times\mathbf{m}(\mathbf{r})\ , \tag{3.3}$$

where

$$\mathbf{m}(\mathbf{r})=-\frac{\delta\Omega}{\delta\mathbf{B}(\mathbf{r})}\ . \tag{3.4}$$

[Strictly speaking, since $\mathbf{B}$ is required to be purely transverse (i.e., $\nabla\cdot\mathbf{B}=0$), only the transverse part of $\delta\Omega/\delta\mathbf{B}$ is well defined, but that is all that is needed to determine the current.]

Now, if we consider a situation where $\mathbf{B}$ is a constant, and Φ varies slowly in space, we may write, to lowest order in the variation $\delta\Phi$,

$$\frac{\delta\Omega}{\delta\mathbf{B}(\mathbf{r})}=\text{const}+\left[\frac{\delta^2\Omega}{\delta\mathbf{B}\delta\Phi}\right]\delta\Phi(\mathbf{r})\ . \tag{3.5}$$

If we also write $j_i=-\sum_i\sigma_{ij}\nabla_j\Phi$, then (3.1) follows directly from (3.2)–(3.5).

If (1.2) and (3.1) are compared, one obtains $\partial\rho/\partial\mathbf{B}=-(e/2\pi h)\mathbf{G}$. When this equation is integrated, we find

$$\rho=\frac{\text{const}}{v_0}-\frac{e}{2\pi h}\mathbf{B}\cdot\mathbf{G}\ , \tag{3.6}$$

where const is a constant which is independent of **B**. Since **G** is a vector on the reciprocal lattice [see (2.16)] one can write $\mathbf{G}=-(t_a\mathbf{G}_a+t_b\mathbf{G}_b+t_c\mathbf{G}_c)$. Using (2.3) and (2.4) we obtain

$$v_0\rho=\text{const}+t_a\phi_a+t_b\phi_b+t_c\phi_c \ . \tag{3.7}$$

Let us first obtain the density of electrons ρ. Since the volume of the magnetic Brillouin zone is $(2\pi)^3/v_0Q$, the density of electrons in a single band is given by $1/v_0Q$. Thus, when there are r bands below the Fermi energy, the density of electrons is

$$\rho=\frac{1}{v_0}\frac{r}{Q} \ . \tag{3.8}$$

Next we shall show that const is an integer. Since Q is the least common multiple of q_a, q_b, and q_c, one can write $Q=n_aq_a=n_bq_b=n_cq_c$, where n_a, n_b, and n_c are integers. Thus from (2.5), (3.7), and (3.8), we have $r=\text{const}\times Q+n_ap_at_a+n_bp_bt_b+n_cp_ct_c$ and $\text{const}\times Q$ has to be an integer. If const is a fraction n/m, then Q must be a multiple of m. When the magnetic field is varied without making a point of contact, however, Q changes and it cannot stay as a multiple of m. Therefore const is an integer s and we finally have

$$\begin{aligned}\frac{r}{Q}&=s+t_a\phi_a+t_b\phi_b+t_c\phi_c\\&=s+t_a\frac{p_a}{q_a}+t_b\frac{p_b}{q_b}+t_c\frac{p_c}{q_c} \ ,\end{aligned} \tag{3.9}$$

which is nothing but the Diophantine equation (1.6) stated in Sec. I.

Now if $\mathbf{a}'$, $\mathbf{b}'$, and $\mathbf{c}'$ are chosen as the primitive lattice vectors, we have $\phi_{a'}=\phi_{b'}=0$ [see (2.9)] and (3.9) is reduced to

$$\frac{r}{Q}=s+t_{c'}\frac{p}{Q} \ , \tag{3.10}$$

which has the same form as the 2D Diophantine equation (1.1).[20] To see this in greater detail let us choose the z direction to be parallel to **B**. Since $\mathbf{c}'$ is parallel to **B**, $(\mathbf{G}_{a'})_z=(\mathbf{G}_{b'})_z=0$ and $(\mathbf{G})_z=-(t_{c'}\mathbf{G}_{c'})_z=-t_{c'}\times 2\pi/c'$ and from (1.2) one has

$$\sigma_{xy}=-\frac{e^2}{h}\frac{t_{c'}}{c'} \ . \tag{3.11}$$

Thus (3.10) and (3.11) are almost the same as the 2D formulas. Here we want to emphasize that though (3.10) looks like a special case of (3.9), actually it is completely equivalent to (3.9). To see this we note that from the expressions of $\mathbf{B}\cdot\mathbf{G}$ one easily obtains

$$t_{c'}\phi_{c'}=t_a\phi_a+t_b\phi_b+t_c\phi_c \ . \tag{3.12}$$

Moreover from (2.6) and (2.9) one has

$$t_{c'}=m_1t_a+m_2t_b+m_3t_c \ . \tag{3.13}$$

The solution of the Diophantine equation (3.9) for **G** [see (1.5)], unfortunately, is not unique. This, however, must be so since **G** depends on the periodic potential (weak-potential limit, tight-binding limit, etc.).

We speculate that the solution of (3.10) is unique with restrictions $|s|\le p/2$ in the weak-potential limit and $|t_{c'}|\le Q/2$ for the tight-binding limit in analogy with the 2D case.

The current is determined by the conductivity tensor with components being $\sigma_{xy}=-\sigma_{xy}$, $\sigma_{yz}=-\sigma_{zy}$, and $\sigma_{zx}=-\sigma_{xz}$ ($\sigma_{xx}=\sigma_{yy}=\sigma_{zz}=0$) which are given by the reciprocal lattice vector **G** [see (1.2)]. Thus in order to specify the current we still need to calculate the other components of the conductivity tensor which are given by the integers $t_{a'}$ and $t_{b'}$.

Moreover, the conditions for existence of an energy gap are nontrivial in the 3D case.

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APPENDIX

Let q be the greatest common factor of m_3 and m_1. By hypothesis, there is no common factor of q and m_2. Then one can choose four integers s_1, s_2, s_3, and s_4 such that

$$s_3m_3=s_1m_1=q \ , \tag{A1}$$

$$s_2m_2+s_4q=1 \ . \tag{A2}$$

Finally, we may choose

$$\mathbf{a}'=s_3\mathbf{a}-s_1\mathbf{c} \ , \tag{A3}$$

$$\mathbf{b}'=s_4\mathbf{b}-\left[\frac{s_2m_3}{q}\right]\mathbf{c}-\left[\frac{s_2m_1}{q}\right]\mathbf{a} \ . \tag{A4}$$

The vectors $\mathbf{a}'$, $\mathbf{b}'$, and $\mathbf{c}'$ can themselves be used as a set of primitive vectors for the Bravais lattice.

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