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Possible States for a Three-Dimensional Electron Gas in a Strong Magnetic Field

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If a three-dimensional semimetal or doped semiconductor is placed in a sufficiently strong magnetic field, then a change in its transport properties will occur. If the electron-impurity interaction is dominant, then the magnetic field will produce localization of the electron wavefunctions, sometimes described as magnetic freezeout. If the electron-electron interaction is more important, then some type of collective transition may occur. Spin-density waves, charge-density waves, valley-density waves, excitonic insulators, and Wigner crystallization have been proposed to occur under various circumstances. As a generalization to three-dimensions of the integral quantized Hall effect, we show that for electrons in periodic or quasiperiodic potential, when the Fermi level lies in an energy gap, the zero temperature conductivity tensor is given by $\sigma_{ij} = (e^2/2\pi h)\sum_k \epsilon_{ijk}G_k$, where $\vec{G}$ is a reciprocal-lattice-vector of the potential. We discuss the effect of impurities and dislocations on this result.

1. INTRODUCTION

In view of the dramatic behavior of two-dimensional electron systems in a strong magnetic field — particularly, the manifestations of the integral and fractional quantized Hall effects [1] — it is natural to ask whether there are phenomena of similar interest that might occur in bulk semiconductors or semimetals. This subject has actually been studied, theoretically and experimentally, over a long period of time, but the range of possible behaviors in strong magnetic field is only partially understood. It is the purpose of this talk to give a brief review of the subject, and to present a few recent results.

2. UNIFORM ELECTRON GAS

One of the earliest theoretical treatments of a three-dimensional electron system in a strong magnetic field was that of Celli and Mermin [2]. They considered a simple model, with one type of carrier, with an isotropic effective mass, in a uniform positive background, in a magnetic field which was smaller than the critical value necessary to completely polarize the spins of the electrons. Using a Hartree-Fock approximation with a screened Coulomb interaction, they found that at sufficiently low temperatures the uniform electron gas is necessarily unstable to the formation of a spin-density wave (SDW), whose wave vector is chosen to span the Fermi surface, in the direction parallel to the magnetic field, for the electrons in any occupied Landau level. The reason for this instability arises from the one-dimensional nature of the electron energies in a strong magnetic field. For each of the occupied Landau levels, the energy is only a function of the component k_z of the wavevector parallel to the field $\vec{B}$, and independent of the quantum number which describes the location of the orbit in the plane perpendicular to $\vec{B}$. Then no matter how small the magnitude of the spin-density wave, it can open up an energy gap over a finite fraction of the Fermi surface, if its wave vector is properly chosen, and this will generally lower the energy of the system. We shall discuss some properties of the SDW state in Section 4 below.

In other situations, various other instabilities may occur. When the magnetic field is sufficiently strong, so that the electrons are completely spin-polarized, a spin-density wave is not possible. Depending on the parameters of the system, various types of charge-density waves (CDWs) have been predicted to occur [3–8]. In most cases, one predicts the simultaneous occurrence of CDWs with wavevectors in several directions. In all probability, the ground state in this case will be an insulating Wigner crystal of electrons.

In a model with several equivalent electron valleys, still other possibilities exist. For example, one may form a valley-density wave state (VDW), in which there are in effect two CDWs, 180° out of phase, with identical wave vectors, that are formed from electrons in two different valleys [5,9]. Such a state can have the same gain in exchange energy as the ordinary CDW, but will have a lower cost in direct energy, due to the cancellation of the principal electric charge inhomogeneity. Other VDW states, which may have still lower energy, can be formed by mixing together the electron states from several valleys. Depending on the parameters of the system, especially the anisotropy of the valleys and the electronic g-factors, a VDW state may have higher or lower energy than a state composed of independent SDWs from electrons in various valleys [10].

In a semimetal, with equal numbers of holes in the valence band and electrons in the conduction band, there is yet another fashion in which the system may lower its energy when placed in strong magnetic field. In the "excitonic insulator" state, the Fermi surface is eliminated by a spontaneous admixture of states in the Brillouin zone vicinity of the electron pocket with states in the region of the hole pocket [11,12].

In all of the states mentioned above, the ground state of the system has a lower translational symmetry than the original crystal structure, which one would have found before the magnetic field was applied, and which is still observable in the presence of $\vec{B}$, if the temperature is raised above the critical temperature for onset of the instability. The broken symmetry may be manifested in one or more of the following quantities —

the electron density, the spin-density, the orbital electron current, or the spin-transport current — which will have non-zero expectation values at wave vectors which are not reciprocal-lattice-vectors in the original structure [11]. Another possibility, in a semimetal, is a discontinuous change in the electron and hole concentration, which could occur via a first order transition with no change in symmetry [11,13].

The classification of a structure as CDW, VDW or excitonic insulator will depend on the location in reciprocal-space of the most important new components of the Fourier transform of the electron charge-density, and these distinctions may actually be arbitrary in the case of some semimetal band structures.

3. FIELD-INDUCED LOCALIZATION

The previous discussion has ignored completely effects of the random impurity potential. Although impurities may be absent, or have negligible concentration in an ideal semimetal, the number of impurities is at least equal to the carrier concentration in any bulk semiconductor. The electron-impurity interaction is normally at least as strong as the Coulomb interaction between carriers, which was responsible for the phase transition in the idealized models mentioned above. Therefore, one may expect that impurities are likely to seriously disrupt the electronic ground state of a doped semiconductor in a strong magnetic field, and may well produce a qualitative change in the behavior of the system [14,15].

The classic description of the effects of a sufficiently strong magnetic field on a doped semiconductor, at low temperatures, involves a process called "magnetic freeze-out" [16,17]. Roughly, when the magnetic length $l \equiv |eB/\hbar c|^{-1/2}$ becomes smaller than the mean distance between impurities, the low-lying electron states are localized in the vicinity of a single impurity. The ground state of the system is then an electrical insulator, although various mechanisms can lead to a finite conductivity for temperature $T \neq 0$.

The narrow gap semiconductor InSb [18,19] is the classic example where magnetic freezeout has been observed. At low temperatures, in sufficiently strong magnetic fields, the electrical resistivities ρ_{xx} and ρ_{zz}, for conduction perpendicular or parallel to $\vec{B}$, respectively, are found to increase with $\ell n \rho \propto 1/T$. The Hall resistance ρ_{xy} is found to increase in a similar manner. This is consistent with an interpretation that the current is carried by excited electrons in a conduction band with energy higher than that of the localized electron states, and the number of carriers decreases at low temperature, as the electrons "freeze out" of the conduction band.

Several experiments on $Hg_xCd_{1-x}Te$ [20–23], and recent experiments on n-type Ge [24], have shown important differences from the behavior described above. In these experiments, the Hall constant $R_H \equiv \rho_{xy}/B$ was found to depend weakly on magnetic field and temperature, in the same region where the resistivities ρ_{xx} and ρ_{zz} were found to increase sharply with increasing B or decreasing T. Thus it appears as if the density of carriers in these materials remains roughly constant, while the mobility is sharply decreasing.

The Hall resistance in $Hg_xCd_{1-x}Te$ has been cited as evidence for the importance of electron-electron interactions in that system, with the result that the electrons are behaving like a very "viscous liquid," or perhaps a "disordered Wigner-crystal" [20–23]. (Evidence from electronic specific heat and other measurements have also been cited in support of these descriptions.) However, it may also be possible to explain the transport measurements in terms of uncorrelated electron motion, in the regime of "hopping conductivity," or "phonon-assisted tunneling."

According to our present understanding, a collection of non-interacting electrons at $T = 0$, in a strong random impurity potential may undergo a metal-to-insulator transition, with increasing magnetic field, as the electron states at the Fermi level are converted from extended to localized states. The onset of insulating behavior may then be described as "field-induced localization."

If the magnetic field is not much greater than the critical field for localization, the localization length of the states near the Fermi energy may be considerably larger than the distance between impurities. The most likely mechanism for electrical conduction at low temperatures, in this regime, is phonon-assisted tunneling of electrons between localized states near the Fermi level [25]. In the limit $T \to 0$, this should lead to the behavior $\ell n \rho_{xx} \propto T^{-1/4}$ characteristic of variable range hopping in three dimensions. At higher temperatures, however, other temperature dependences might be expected, as the typical hopping length becomes equal to the localization length. At any fixed low temperature, the resistance should increase strongly with increasing magnetic field, as the localization length gets shorter, and there is decreasing overlap of electron states near the Fermi level.

The behavior of the Hall resistance, in the hopping regime, is the subject of some controversy [25,26]. It is clear that the value of ρ_{xy} must be small compared to ρ_{xx} but it is not evident what the precise behavior should be. In most calculations, it appears that ρ_{xy} increases at a rate which is much slower than ρ_{xx} (e.g., $\rho_{xy} \propto \rho_{xx}^{1/2}$) but it could also be that ρ_{xy} is almost independent of B and T in some range.

It must be noted that the Hall resistance is quite difficult to measure when ρ_{xy} is very much smaller than ρ_{xx}. Therefore it is only possible to study the behavior of ρ_{xy} in a limited range of T and B. We also note that if ρ_{xy} is roughly constant, when $\rho_{xx} \to \infty$, this implies that the elements of conductivity tensor all go to zero, with $\sigma_{xy} \propto \sigma_{xx}^2$.

The effects of electron-electron interactions on hopping conductivity and on the localization transition itself are not well understood in general [25]. However, there is good theoretical indication that in the presence of a strong magnetic field, interactions should have little effect on the nature of the localization transition, at least on the metallic side [27,28]. Measurements on Ge give some additional support to this view [24].

4. TRANSPORT PROPERTIES OF THE SPIN-DENSITY WAVE STATE

Even if the actual behavior of a three-dimensional doped semiconductor in strong magnetic field is dominated by the electron-impurity interaction, it is of interest to inquire what the properties should be of an SDW or CDW state such as the Celli-Mermin state, for electrons in a uniform positive background. The insights gained from this exercise may be useful for understanding some other systems that are realizable in nature. Also, it may be possible to construct a conducting layer which is free of impurities and which is sufficiently thick so that some three dimensional effects may be manifest. For example, it might be possible to create a structure with a graded composition of $Ga_{1-x}Al_xAs$ in which there is a uniform density of electrons $n \approx 10^{16}/cm^3$ in a layer up to 2000 Å thick, with donors removed several hundred Ångstroms from either side of the layer [29].

Most interesting are the transport properties of the Celli-Mermin state at $T = 0$ [30]. If the spin-density wave is pinned in the crystal, because of interactions with the lattice or because of interaction with an arbitrarily small desnity of impurities, then the electrical resistance will be infinite, for an electric field parallel to the wave vector $\vec{Q}$ of the SDW. (This direction is parallel to the magnetic field if the carriers have an isotropic effective mass tensor, or if the magnetic field is appled along a principal axis of the mass tensor; however $\vec{Q}$ may be tilted relative to $\vec{B}$ in the more general case.) On the other hand, *current flow perpendicular* to $\vec{Q}$ will be unaffected by the SDW, *and occurs without dissipation.* (This will be true even if a weak random impurity potential is present. See below.)

There will be a finite Hall resistance for current flow perpendicular to $\vec{Q}$, which is given by the classical formula

$$\rho_{xy} = B_z/nec \quad . \tag{1}$$

(The z axis here is taken parallel to $\vec{Q}$.) In the Celli-Mermin state, the magnitude of $\vec{Q}$ is related to the density by

$$Q = \pi nhc/eB_z \quad . \tag{2}$$

Thus the results above can be summarized by the following description of the conductivity tensor: all elements are zero except for

$$\sigma_{yx} = -\sigma_{xy} = Q\,e^2/\pi h \quad . \tag{3}$$

Note that Hall conductance contributed by one period of the spin-density wave system is equal to $2e^2/h$ which is consistent with the formula for a two-dimensional quantized Hall effect.

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

The results quoted for the Celli-Mermin state are actually a special case of a general theorem. For a three-dimensional electron system in a periodic potential, if the Fermi level lies inside a gap in the energy spectrum, then the conductivity tensor is necessarily of the form

$$\sigma_{ij} = \frac{e^2}{2\pi h} \sum_k \epsilon_{ijk} G_k \quad , \tag{4}$$

where ϵ_{ijk} is the unit antisymmetric tensor, and $\vec{G}$ is a *reciprocal lattice vector* (possibly zero) of the potential. The theorem is proved in Appendix A, below, for non-interacting electrons in an external potential, but the argument applies equally well to an interacting electron system, in the Hartree-Fock approximation, where the periodic potential might result from one or more spin-density waves or charge density waves produced, self-consistently, by the electrons themselves. The theorem applies also to a correlated electron system, if the electron-correlations can be calculated by perturbation theory from a Hartree-Fock state. The theorem also applies to a quasiperiodic potential, where the potential contains several incommensurate periodicities. A closely related theorem has been derived by H. Kunz [31].

Equation (4) is the generalization to three dimensions of the familiar formula for the conductivity tensor in the two-dimensional integral quantized Hall effect. If one considers a highly correlated electron state, analogous to the Laughlin state for the two-dimensional electron gas [1], which *cannot* be obtained by perturbation theory from a state of the non-interacting electron field in an arbitrary periodic potential, then a generalization of the fractional quantized Hall effect is allowed. In this case the reciprocal lattice vector $\vec{G}$, which occurs in Eq. (4), would be divided by an integer greater than unity.

If $\vec{G} = 0$ in Eq. (4), then the crystal is simply an insulator at $T = 0$, which is not very interesting. If $\vec{G} \neq 0$, however, the resistance is zero along the crystal planes perpendicular to $\vec{G}$, and the Hall conductance per crystal plane is quantized.

Equation (4) for the conductivity tensor applies even in the presence of a random impurity potential, provided the impurity potential is not too strong, and provided that the long range order of the periodic potential is not destroyed. Specifically, when impurities are introduced, the diagonal elements of the conductivity tensor remain zero, and the Hall conductance remains constant, as long as the Fermi level remains in an energy gap, or as long as there exist only localized states at the Fermi energy [32]. These results can be derived by arguments similar to the various derivations of the quantized Hall effect in two dimensions [1,33,34]. For example, one can easily extend the argument given in Ref. 34, in which one considers a geometry where an annulus of impure material is sandwiched between an inner and outer annulus of material without the impurity potential. The requirements of charge and energy conservation as one varies the magnetic flux through the hole in the annulus can then be used to show that the Hall conductance is identical in the three parts of the sample, provided that this impurity potential is weak enough that there are no extended states at the Fermi energy anywhere in the

interior of the sample.

6. EFFECT OF DISLOCATIONS

A breakdown in the quantized Hall conductance can occur if there are dislocations in the periodic potential. If the periodic potential gives rise to a finite quantized Hall conductivity, characterized by a non-zero value of $\vec{G}$ in Eq. (4), and if an isolated dislocation has a Burger's vector $\vec{b}_{\rm dis}$ which is not perpendicular to $\vec{G}$, then it can be shown that there will necessarily be extended states at the Fermi energy in the vicinity of the dislocation, which carry an electric current along the dislocation. (These states are analogous to the current-carrying edge-states, which occur in the two-dimensional quantized Hall effect.)

The direction of the current depends on the sign of the Burger's vector, and the magnitude depends on the precise Fermi level of electrons in the extended states of the dislocation. A variation δE_F in the Fermi level will lead to a change in the current δI, which is given by [35]

$$\delta I = \left(\frac{\vec{G} \cdot \vec{b}_{\rm dis}}{2\pi} \right) \frac{e}{h} \delta E_F \quad . \tag{5}$$

Conservation of current requires that in any steady state, the Fermi level must be constant along the length of an isolated dislocation. If an isolated dislocation begins and ends at two surfaces of a sample which are at different voltages, the Fermi level in the dislocation will be determined by the voltage at the surface where the electrons enter the dislocation; dissipation will then occur at the exit point of the dislocation where electrons are injected into the surface states above the surface Fermi level or holes are injected below the Fermi level. On the other hand, if two dislocations come close together at some point in the interior of the sample, there may be tunneling between the two dislocations, so that dissipation can also occur at such points.

It is interesting to consider a model in which there exist a number of dislocations each of which begins at a random point on the surface of a sample and executes a random walk until it hits the same or a different surface. If there is a voltage difference between two opposite faces of the sample, then the dislocations will carry a net current from one face to the other. The magnitude of this current turns out to be equivalent to a finite diagonal conductivity in the sample, given by [35]

$$\sigma \approx \frac{e^2}{h} \left(\frac{\vec{G} \cdot \vec{b}_{\rm dis}}{2\pi} \right) \frac{\tau d}{6} \quad , \tag{6}$$

where d is the step length of the random walk, and τ is the line-density of the dislocations in the interior of the sample. (The random walk model in fact leads to a value of τ which is independent of distance from the surface.) As an example, if we assume that τ is of order d^{-2}, and $\vec{b}_{\rm dis} \| \vec{G}$, then the value of σ is of order $\sigma_{xy} b_{\rm dis}/d$. The diagonal conductivity becomes comparable to the Hall conductivity if $\tau^{-1/2} \approx d \approx b_{\rm dis}$.

When the density of dislocations is sufficiently high so that tunneling between dislocations is important, then the dissipation associated with current flow will occur in the interior of the sample, rather than at the surfaces. The magnitude of σ_{xx} should not be much affected, however, until actual localization of the states below the Fermi level sets in.

7. FURTHER REMARKS

Because of the currents that may be carried by dislocations, grain boundaries, and sample surfaces, one would never expect to see a precise quantization of the Hall conductivity in an actual bulk sample, as one observes in the two-dimensional case. Nevertheless there could occur approximate plateaus in the Hall conductivity that might be identified with the three-dimensional quantized Hall effect.

In experiments on the Bechgaard salts — a family of organic materials with a highly anisotropic layered structure — there have been observed a series of phase transitions in strong magnetic fields at low temperatures, and a series of plateaus in the Hall resistivity [36]. The phase transitions have been attributed to a series of spin-density wave instabilities in the plane of the layers, and the Hall plateaus have been described in terms of the quantized Hall effect in the plane of the layers. However, in experiments thus far, one has not entered a regime where the diagonal resistivity ρ_{xx} is small compared to the Hall resistivity, as would be expected in the quantized Hall effect. Thus the interpretation of the data has required some additional assumptions.

The quantized Hall effect has been observed in multilayer GaAs-GaA/As heterostructures, under conditions where there is a substantial tunneling matrix element between adjacent electron layers [37]. In this case, there was vanishing diagonal resistance parallel to the layers, and the value of the Hall conductance could be interpreted as $2e^2/h$ per layer, provided that several exterior layers are excluded from consideration, presumably as a result of a strong perturbation which has produced localized electron-states in those layers.

We note that an important difference between the case of a multi-layer heterostructure and the hypothesized Celli-Mermin state is that in the first case the periodicity is fixed by the sample preparation, while in the latter, the period of the spin-density wave in the thermodynamic ground state depends continuously on the applied magnetic field. The spin-density wave state would therefore not give rise to a plateau in the Hall conductivity in the Celli-Mermin state. One might observe hysteresis in the Hall conductivity when the magnetic field is varied, if the spin-density wave is pinned by defects or boundaries of the sample.

A phase transition in the semimetal graphite, in strong magnetic fields, has been attributed to a CDW or VDW state, analogous to the Celli-Mermin SDW state, with wavevector perpendicular to the graphite planes [5,14]. In pure graphite, because of the equal numbers of electrons and holes, we expect there will be no Hall conductance, and the material should eventually become an insulator $(\vec{G} = 0)$ at $T = 0$.

An amusing theoretical application of Eq. (4), with $\vec{G} \neq 0$ may be the case of an *undoped* semiconductor in multi-megagauss fields. If the cyclotron energy is large compared to the appropriate energy gaps, magnetic breakdown may occur along a crystal plane which is roughly perpendicular to the applied magnetic field, and a non-zero quantized Hall conductance may be predicted for currents in this plane.

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APPENDIX A. DERIVATION OF THE 3-D QUANTIZED HALL CONDUCTIVITY

We describe here the derivation of the three-dimensional quantized Hall conductance formula, Eq. (4), for non-interacting electrons in a periodic potential. The proof is a generalization to three-dimensions of the arguments of Thouless *et al.* for the two-dimensional case [38].

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 the diagonal elements of $\overleftrightarrow{\sigma}$ must vanish for current flow in any direction of space. It follows that $\overleftrightarrow{\sigma}$ is purely antisymmetric, so we may write

$$\sigma_{ij} = \frac{e^2}{2\pi h} \sum_k \epsilon_{ijk} Q_k \quad , \tag{A1}$$

where $\vec{Q}$ is a vector whose value we wish to determine.

Let $\vec{a}$, $\vec{b}$, $\vec{c}$ be a set of primitive lattice vectors for the periodic potential, and let $v_0 = \vec{a} \cdot (\vec{b} \times \vec{c})$ be the volume of the unit cell. We shall first consider the case of a "rational magnetic field," which we define as a field of the form

$$\vec{B} = \frac{p}{s} \frac{\vec{a}'}{v_0} \frac{hc}{e} \quad , \tag{A2}$$

where p and s are integers, and $\vec{a}'$ is a vector on the Bravais lattice. Without additional restrictions on $\vec{B}$, we may assume that p and s have no common factor, and that there is no vector on the Bravais lattice which is a submultiple of $\vec{a}'$. The last condition implies that $\vec{a}'$ may be written as

$$\vec{a}' = m_1 \vec{a} + m_2 \vec{b} + m_3 \vec{c} \quad , \tag{A3}$$

where m_1, m_2, and m_3 are three integers which have no overall common factor. It is then possible to choose two other vectors $\vec{b}'$ and $\vec{c}'$ on the Bravais lattice such that $\vec{a}' \cdot (\vec{b}' \times \vec{c}') = v_0$. To see this, let q be the greatest common factor of m_1 and m_2. By hypothesis, there is no common factor of q and m_3. Then one can choose four integers s_1, s_2, s_3 and s_4 such that

$$s_1 m_1 + s_2 m_2 = q \quad , \tag{A4}$$

$$s_3 m_3 + s_4 p = 1 \quad . \tag{A5}$$

Finally, we may choose

$$\vec{b}' = s_1 \vec{b} - s_2 \vec{a} \tag{A6}$$

$$\vec{c}' = s_4 \vec{c} - \left(\frac{s_3 m_1}{q}\right) \vec{a} - \left(\frac{s_3 m_1}{q}\right) \vec{b} \quad . \tag{A7}$$

Since the vectors $\vec{a}'$, $\vec{b}'$ and $\vec{c}'$ can themselves be used as a set of primitive vectors for the Bravais lattice, we shall drop the primes and write $\vec{B} = (p/s)(hc/e)(\vec{a}/v_0)$.

For electrons in uniform magnetic field, one may define a set of translation operators $S_{\vec{R}}$ which translate the wavefunction by the vector $\vec{R}$ and multiply it by a position dependent phase factor, and which commute with the kinetic energy [39]. Two operators, $S_{\vec{R}}$ and $S_{\vec{R}'}$ have the property

$$S_{\vec{R}} S_{\vec{R}'} = S_{\vec{R}'} S_{\vec{R}} e^{i\phi} \quad , \tag{A8}$$

where $\phi = \vec{B} \cdot (\vec{R} \times \vec{R}')e/\hbar c$.

If we now consider the operators $S_{\vec{a}}$, $S_{\vec{b}}$ and $(S_{\vec{c}})^s = S_{s\vec{c}}$, 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

$$\psi_{\vec{q},n}(\vec{r}) = e^{i\vec{q}\cdot\vec{r}} u_{\vec{q},n}(\vec{r}) \quad , \tag{A9}$$

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

$$\vec{q} = t_1 \vec{G}_a + t_2 \vec{G}_b + \frac{t_3}{s} \vec{G}_c \quad , \tag{A10}$$

where t_1, t_2 and t_3 range from 0 to 1, and $\vec{G}_a$, $\vec{G}_b$ and $\vec{G}_c$ are the fundamental reciprocal lattice vectors of the original lattice, given by $\vec{G}_a = 2\pi(\vec{b} \times \vec{c})/v_0$, etc. The overall phase of $u_{\vec{q},n}$ can be chosen such that $\vec{u}$ is a continuous function of $\vec{q}$, except possibly for some isolated points in the Brillouin zone where two bands become degenerate. (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

$$\sigma_{ij} = \frac{e^2}{2\pi^2 h} \int d^3q \sum_{n' \leq n} \mathrm{Im} \int d^3r \frac{\partial u^*_{\vec{q},n'}}{\partial q_i} \frac{\partial u_{\vec{q},n'}}{\partial q_j} \quad , \tag{A11}$$

where the space integral is over a unit cell of the magnetic Bravais lattice, and the $\vec{q}$ is over the magnetic Brillouin zone. Then we may write

$$\vec{Q}\cdot\vec{a} = \frac{\pi h}{e^2}\sum_{ijk}\epsilon_{ijk}\sigma_{ij}a_k = \sum_{n'\le n}\int_0^1 dt_1\sigma_{n'}(t_1)\ , \tag{A12}$$

where

$$\sigma_{n'}(t_1) \equiv \frac{1}{2\pi}\int d^3r \oint_C d\vec{q}\cdot \mathrm{Im}\left(u^*_{\vec{q},n'}\frac{\partial}{\partial\vec{q}}u_{\vec{q},n'}\right)\ , \tag{A13}$$

and the contour C runs around the edge of the magnetic Brillouin zone at fixed value of t_1. Here we have used the property $\vec{a}\cdot\vec{G}_a = 2\pi$, $\vec{a}\cdot\vec{G}_b = \vec{a}\cdot\vec{G}_c = 0$.

The quantity $\sigma_{n'}(t_1)$ is $(1/2\pi)$ times the net phase change of $u_{\vec{q},n'}$ around the perimeter of the Brillouin zone and is necessarily an integer. Furthermore, if there are no points of degeneracy between band n' and any other band, this integer is a topological invariant, and is independent of t_1. If there is a point of degeneracy between n' and another band, the value of $\sigma_{n'}(t_1)$ may change discontinuously, as a function of t_1, but the sum of the contributions of the two bands will not change. It follows that $\sum_{n'\le n}\sigma_{n'}(t_1)$ is an integer, independent of t_1, and that the quantity $\vec{a}\cdot\vec{Q}$ is an integer multiple of 2π.

In a similar manner, we may prove that $\vec{b}\cdot\vec{Q}$ and $s\vec{c}\cdot\vec{Q}$ are also integer multiples of 2π. Moreover, by choosing a different Brillouin zone, where the role of $\vec{b}$ and $\vec{c}$ are interchanged, we can establish that $\vec{c}\cdot\vec{Q}$ is itself an integer multiple of 2π. It then follows that $\vec{Q}$ is a vector on the reciprocal lattice generated by $\vec{G}_a$, $\vec{G}_b$ and $\vec{G}_c$.

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

To derive the theorem for a quasiperiodic potential, we note that an incommensurate system can always be approximated, in an arbitrarily large region by a potential where there is a rational relation between the constituent wavevectors. If there exists a gap at the Fermi energy in the incommensurate case, there must be a similar gap in the approximating rational case, and the conductivity tensors should also be similar. The value of $\vec{Q}$ in the rational case should always correspond to one of the principal Fourier components of the constituent potential, or to some lower order harmonic combination of these. In the limit of the incommensurate system, the wavevector $\vec{Q}$ should then coincide with a finite order Bragg peak in the quasiperiodic potential.

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