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LETTER TO THE EDITOR

Quantised Hall conductance in a perfect crystal

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Abstract. Using magnetic translation symmetry, the Hall conductance of an isolated magnetic band in units of e^2/h is shown to satisfy the Diophantine equation $p\sigma + qm = 1$, where p and q are relatively prime integers giving the number of flux quanta per unit cell area, $\varphi = p/q$, and m is an integer. This equation holds for a general periodic Schrödinger Hamiltonian with an arbitrary magnetic field and is a direct consequence of the q-fold degeneracy of magnetic bands. Extension to general real φ gives the equation $\varphi\sigma_{\mathrm{H}} - \rho =$ integer with σ_{H} the Hall conductance and ρ the number of electrons per unit cell, from which σ_{H} is uniquely determined once ρ, φ and the gap structure are given.

Since the experimental discovery of the quantum Hall effect by von Klitzing *et al* (1980), there has been much theoretical interest in explaining this effect either by general dynamical arguments (Laughlin 1981, Prange 1981, Thouless 1981, Halperin 1982) or by exploiting the symmetry of the problem (Thouless *et al* 1982, Streda 1982a, b, MacDonald 1983, 1984). The symmetry approach has led to a very interesting Diophantine equation for the integer Hall conductance in two limiting cases of strong and weak magnetic fields (Thouless *et al* 1982, Streda 1982a, b, MacDonald 1983, 1984). This equation was derived by combining symmetry arguments with perturbation theory, and it shows explicitly how the Hall conductance of a solid can be written as an algebraic sum of well defined conductances of the split sub-bands (Thouless *et al* 1982, MacDonald 1983).

In this Letter we prove that a Diophantine equation for the Hall conductance is a general result following just from magnetic translational symmetry. Namely, it does not involve specific models, and it is not limited to strong or weak magnetic fields. We show that an isolated magnetic band (or sub-band) carries an integer Hall conductance σ, in units of e^2/h, satisfying the equation

$$p\sigma + qm = 1. \tag{1}$$

Here p and q are relatively prime integers with $p/q = (eBab)/(hc) = \varphi$, where φ is the number of flux quanta per unit cell area ab of the crystal (a and b are the lattice constants), and m is an integer. If there are N filled magnetic bands, then, by introducing ρ, the number of electrons per unit cell $\rho = N/q$, equation (1) gives

$$\varphi\sigma_{\mathrm{H}} - \rho = \text{integer} \tag{2}$$

where σ_{H} is the measurable integer Hall conductance for N magnetic bands.

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In the limit of strong magnetic field equation (1) is equivalent to the Diophantine equation of Thouless *et al* (1982) for the rth gap in a Landau level

$$r = s_r q + t_r p \tag{3}$$

where s_r and t_r are integers. Equation (1) is obtained by subtracting from equation (3) the same equation for $r-1$ and by using the result that $\sigma = t_r - t_{r-1}$. Although equation (1) is derivable from equation (3) (or from analogous equations in other models (MacDonald 1983)), it turns out to be a general result of symmetry, as is shown below. The Diophantine equation in the form (2) was first written by Wannier (1978) in the context of locating the energy gaps when a Bloch band 'splits' into magnetic bands. It was then used by Streda (Streda 1982a, b) in the discussion of the quantum Hall effect in the tight-binding limit (weak magnetic fields). Similar equations were shown to yield a labelling of the gaps in the energy spectrum of the Schrödinger equation with an almost periodic potential (Johnson and Moser 1982) and the quantisation of particle transport (Thouless 1983). We prove that equations (1) and (2) are exact results for a perfect two-dimensional crystal in a uniform rational magnetic field. Thus we show for the first time that these equations are a consequence of the q-fold degeneracy of magnetic bands, and that they have an identical form over the whole range of magnetic field. In particular, we show that the existing claims in literature (Thouless *et al* 1982, MacDonald 1983) of the need to exchange p and q in the weak and strong limits do not apply to equations (1) and (2). This is so in spite of the fact that in Harper's equation p and q are exchanged for weak and strong magnetic fields.

We have two derivations of equation (1). The first is differential geometric in character and will not be given here. The second, which we shall present, is based entirely on the magnetic translational symmetry of the problem (Zak 1964a, b). More precisely, it becomes evident from this derivation that equation (1) is a consequence of the q-fold degeneracy in a magnetic band (or sub-band) (Zak 1964a, b). For an isolated magnetic band the magnetic Bloch functions $\psi_{k_1k_2}$ can be chosen as eigenfunctions of the commuting magnetic translations $T(q\boldsymbol{a})$ and $T(\boldsymbol{b})$ (Dana and Zak 1983, Dana 1983). Following arguments similar to those given in Weinreich's book (Weinreich 1965), the phase of $\psi_{k_1k_2}$ can be chosen to satisfy the following periodicity conditions:

$$\psi_{k_1+2\pi/qa,k_2} = \psi_{k_1k_2} \tag{4a}$$

$$\psi_{k_1,k_2+2\pi/b} = \exp(\mathrm{i}\sigma k_1 qa)\psi_{k_1k_2} \tag{4b}$$

where σ is an integer which, according to Thouless *et al* (1982), is precisely the Hall conductance of the magnetic band. Since the operator $T(\boldsymbol{a})$ commutes with the Hamiltonian and does not belong in general (for $q > 1$) to the commuting set, the function $T(\boldsymbol{a})\psi_{k_1k_2}$ is degenerate with $\psi_{k_1k_2}$ and, for an isolated magnetic band, it belongs to the same band. In addition, it is associated with the quasi-momentum $(k_1, k_2 + 2\pi p/qb)$ (Zak 1964a, b). We therefore have

$$T(\boldsymbol{a})\psi_{k_1k_2} = \exp(\mathrm{i}mk_1qa)\psi_{k_1,k_2+2\pi p/qb} \tag{5}$$

where m is an integer and the phase in (5) is chosen consistent (Weinreich 1965) with equation (4b). Applying $T(\boldsymbol{a})$ q times to equation (5) and using equation (4b), we find the relation

$$\exp(\mathrm{i}k_1qa)\psi_{k_1k_2} = \exp[\mathrm{i}(p\sigma + qm)k_1qa]\psi_{k_1k_2}$$

from which equation (1) follows.

It is easily verified that equation (1) determines σ modulo q. Thus, for $p/q = \frac{7}{11}$, a case considered by Thouless *et al* (1982), equation (1) is solved by $\sigma = -3 + nq$, $n = 0, \pm 1, \ldots$. In the work by Thouless *et al* (1982) perturbation theory was used to limit m, namely $|m| \leqslant p$. With this restriction the only admissible values of σ are $\sigma_1 = -3$, $\sigma_2 = 8$, which are associated with the sub-bands of a split Landau level for a square lattice. In MacDonald's work (1983) a hexagonal lattice is considered, where again perturbation theory poses restrictions on m and σ. It should be noted that equation (1) is symmetric with respect to the integers m and σ. While σ has the meaning of a Hall conductance, the meaning of m eludes us. Equation (1) determines m modulo p.

Unlike equation (1), which describes a physically unmeasurable quantity and determines it only modulo q, equation (2) describes the physically measurable Hall conductance σ_{H}. We argue that equation (2) determines σ_{H} uniquely, given φ, ρ in the gaps and the gap structure of the Hamiltonian. First, we argue that energy gaps in the spectrum are stable under small perturbations and therefore persist under slight variations of φ. Although we do not have a rigorous proof of this stability, we believe that this is a technical question which should be provable by standard methods of perturbation theory (Kato 1976). There is also ample numerical evidence that such stability is indeed true (Thouless *et al* 1982, Wannier 1978, Hofstadter 1976). Since this Letter was first written at the end of 1983, this has been proven by Avron and Simon (1985). Given this, the Fermi energy can be assumed to stay in a gap under small variations of φ. It can be shown (Avron *et al* 1985) that ρ, σ_{H} and the integer on the RHS of equation (2) are all continuous functions of φ provided the Fermi energy stays in a gap. It then follows that equation (2) extends to all φ (irrationals included). It is easy to see that for irrational φ equation (2) has at most one solution. Since in general the φ can be approximated by irrationals and there is a unique way of varying the Fermi energy in a gap at the rational φ to the gap at neighbouring irrational fluxes, the uniqueness of σ_{H} follows.

Equation (2) is thus an exact result which determines σ_{H} uniquely once φ and ρ and the gap structure are given under the condition that the Fermi energy stays in a given gap. It is therefore of interest to discuss its physical consequences.

(*a*) Suppose $(\rho, \sigma_{\mathrm{H}})$ solves equation (2). Then $(\rho \pm 1, \sigma_{\mathrm{H}})$ is also a solution (provided $\rho \pm 1$ corresponds to E_{F} in a gap). This expresses the fact that a full valence band does not contribute to the Hall conductance.

(*b*) Suppose $(\rho, \sigma_{\mathrm{H}})$ solves equation (2). Then $(1 - \rho, -\sigma_{\mathrm{H}})$ is also a solution (provided $1 - \rho$ corresponds to E_{F} in a gap). This expresses the celebrated electron–hole duality.

(*c*) $\sigma_{\mathrm{H}} = 0$ implies that ρ is an integer.

(*d*) For free electrons, i.e. when the periodic potential is zero, the integer on the RHS of equation (2) is zero.

(*e*) It is instructive to compare equation (2) with the thermodynamic formula (Streda 1982a, b)

$$\sigma_{\mathrm{H}} \frac{e^2}{h} = ec \left(\frac{\partial N(E)}{\partial B} \right)_{T, E_{\mathrm{F}}}$$

where $N(E) = \rho/(ab)$ in our case. In a plateau of the Hall conductance it integrates to $\varphi\sigma_{\mathrm{H}} - \rho = \text{const}$. The constant on the RHS is generally different for different plateaus. This is similar to equation (2) except that in the former the constants and σ_{H} are not constrained to be integers.

(*f*) Equation (2) can be read as an equation for ρ given σ_H and φ. It says that in a plateau ρ increases linearly in φ with slope σ_H, and when σ_H jumps so does ρ. In a slightly different context, Baraff and Tsui (1981) discussed these variations in ρ as a function of φ.

(*g*) For irrational fluxes it is a trivial exercise to show that equation (2) has at most one solution. If for a given flux and density E_F is in a gap, it will be so for neighbouring fluxes (Avron and Simon 1985). This determines the conductivity also for rationals. For rational fluxes equation (2) has infinitely many solutions. In particular, for a given fixed rational φ, σ_H cannot be determined without additional information.

(*h*) Even though the 'Diophantine' equation is generally valid, this does not mean that different crystals will have identical conductivities. This is because for the same irrational flux, they may have different densities that correspond to E_F in a gap.

(*i*) Even if two crystals can be deformed continuously to each other, this does not mean that they have identical conductivities. The reason is that for finite deformations the non-degeneracy condition (E_F lying in a gap) may, and will, be violated in general. In fact, this is precisely what one expects from the Wigner–von Neuman no-crossing theorem: varying the crystal gives energy bands that depend on three parameters, 2*k* vectors and one shape variable. With three parameters Wigner and von Neuman tell us that there will be points of crossing. At crossings, σ_H jumps.

In conclusion, we derive in this Letter an exact equation (1) for the integer Hall conductance of a perfect crystal. This equation holds for any periodic Schrödinger Hamiltonian over the whole range of magnetic field. Equation (1) is a consequence of the *q*-fold degeneracy of magnetic bands and remains identical in the weak and strong magnetic field limits, despite the fact that in Harper's equation *p* and *q* are exchanged in these limits.

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