# Quantized Hall conductance in a glide-plane symmetry

Itzhack Dana [1]
*Department of Nuclear Physics, Weizmann Institute of Science, Rehovot 76100, Israel*

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The quantization of the Hall conductance is investigated for non-interacting electrons in a two-dimensional crystal with glide-plane symmetry. This is the simplest space-group symmetry imposing new general constraints on the Hall conductance, besides those already imposed by magnetic translational symmetry. Both the cases of isolated and degenerate magnetic bands are considered.

The quantization of the Hall conductance in solids can be explained by general arguments of dynamical and/or symmetry nature [1]. In particular, for a perfect crystal, the quantization may be viewed as a consequence of magnetic translational symmetry [2–4]. Let us summarize the main results of refs. [2,3]. Consider non-interacting electrons in a two-dimensional crystal with lattice constants $a$ and $b$ in the $x$ and $y$ directions, respectively. A uniform magnetic field $\boldsymbol{H}$ is applied perpendicular to the crystal. One assumes, for simplicity, a rational number $\varphi$ of flux quanta $hc/e$ through a unit cell:

$$\varphi = eHab/hc = p/q\,, \tag{1}$$

where $p$ and $q$ are relatively prime integers. It is well known (see, e.g., refs. [5,6]) that the spectrum of the problem exhibits a band structure. The eigenfunctions in a magnetic band are denoted by $\psi_{\boldsymbol{\kappa}}$, where $\boldsymbol{\kappa} = (\kappa_1, \kappa_2)$ labels the eigenvalues of the commuting set of magnetic translations $T(q\boldsymbol{a})$ and $T(\boldsymbol{b})$:

$$T(q\boldsymbol{a})\psi_{\boldsymbol{\kappa}} = \exp(\mathrm{i}\kappa_1 qa)\psi_{\boldsymbol{\kappa}}\,, \tag{2a}$$

$$T(\boldsymbol{b})\psi_{\boldsymbol{\kappa}} = \exp(\mathrm{i}\kappa_2 b)\psi_{\boldsymbol{\kappa}}\,. \tag{2b}$$

Here $\boldsymbol{\kappa}$ varies in the magnetic Brillouin zone,

$$0 \leqslant \kappa_1 < 2\pi/qa\,, \quad 0 \leqslant \kappa_2 < 2\pi/b\,. \tag{3}$$

For an *isolated* magnetic band, the case assumed in refs. [2,3,5], $\psi_{\boldsymbol{\kappa}}$ is periodic in $\boldsymbol{\kappa}$ with unit cell (3), up to $\boldsymbol{\kappa}$-dependent phase factors. As pointed out in refs. [3,5], the phase of $\psi_{\boldsymbol{\kappa}}$ may always be chosen so as to satisfy the following periodicity conditions:

$$\psi_{\kappa_1+2\pi/qa,\kappa_2} = \psi_{\boldsymbol{\kappa}}\,, \tag{4a}$$

$$\psi_{\kappa_1,\kappa_2+2\pi/b} = \exp(\mathrm{i}\sigma\kappa_1 qa)\psi_{\boldsymbol{\kappa}}\,. \tag{4b}$$

Here $\sigma$ is an integer which, as shown in ref. [2], is precisely the quantized Hall conductance (in units of $e^2/h$) carried by the magnetic band. As shown in ref. [3], a general consequence of magnetic translational symmetry is that $\sigma$ satisfies the Diophantine equation

$$p\sigma + qm = 1\,, \tag{5}$$

where $m$ is an integer. Eq. (5) admits an infinite number of solutions $(m, \sigma)$ [#1]. The physically allowed solutions depend on the *details* of the periodic potential [2,7,8]. However, as far as *general* arguments, based *only* on magnetic translational symmetry, are concerned, all the solutions are, in principle, allowed.

It is therefore natural to ask which space-group symmetries, if any, may impose new general constraints on $m$ and $\sigma$. We show in this Letter that the simplest such symmetry corresponds to a *non-sym-*

[1] Address after September 1990: Department of Physics, Bar-Ilan University, Ramat-Gan 52100, Israel.

[#1] Eq. (5) always possesses one solution $(m_0, \sigma_0)$ ($-m_0/\sigma_0$ is a neighbor of $p/q$ on the Farey tree). Then $(m, \sigma) = (m_0 - ps, \sigma_0 + qs)$, for all integers $s$, are also solutions.

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*morphic* magnetic space group [9]. More specifically, for a two-dimensional crystal [10], we find that this symmetry is a glide plane perpendicular to the crystal and accompanied by time reversal (because of the presence of $\boldsymbol{H}$ [11]). The corresponding magnetic space group may be denoted, using standard notation [9,10], by $pg'$, where $g'$ denotes the glide plane $g$ accompanied by time reversal (indicated by a prime). For definiteness, we assume that $g$ is parallel to the lattice vector $\boldsymbol{a}$, so that the non-primitive translation associated with it is $\boldsymbol{a}/2$. The operator corresponding to $g'$ may then be written as [12,13]

$$O=T(\boldsymbol{a}/2)KM\,, \tag{6}$$

where $K$ is the complex-conjugation operator (corresponding to time reversal [11]) and $M$ is the mirror-reflection operator.

The necessity to assume a non-symmorphic magnetic symmetry to obtain new general constraints will become evident and will be explained at the end of this paper. Our main results are the general constraints on $m$ and $\sigma$ given by eqs. (11), (13)–(15) below. In particular, eq. (13) is a Diophantine equation for the Hall conductance associated with a pair of magnetic bands which are degenerate because of the glide-plane symmetry.

To derive these results, we start by applying the operator (6) to both sides of eqs. (2). Using the results in refs. [12,13], and assuming an *isolated* magnetic band (i.e., eqs. (4)), we easily find that

$$O\psi_{\boldsymbol{\kappa}}=\exp[\mathrm{i}\phi(\boldsymbol{\kappa})]\,\psi_{-\kappa_1,\kappa_2+\pi p/qb}\,, \tag{7}$$

where $\exp[\mathrm{i}\phi(\boldsymbol{\kappa})]$ is a phase factor. Since both $\psi_{\boldsymbol{\kappa}}$ and $O\psi_{\boldsymbol{\kappa}}$ in (7) satisfy the periodicity conditions (4), this phase factor must be strictly periodic in $\boldsymbol{\kappa}$ with unit cell (3). Thus, the most general form of $\phi(\boldsymbol{\kappa})$ is

$$\phi(\boldsymbol{\kappa})=m_1\kappa_1 qa+m_2\kappa_2 b+f(\boldsymbol{\kappa})\,, \tag{8}$$

where $m_1$ and $m_2$ are arbitrary integers, and $f(\boldsymbol{\kappa})$ is strictly periodic in $\boldsymbol{\kappa}$ with unit cell (3). From (6) we get

$$O^{2q}=T(q\boldsymbol{a})\,. \tag{9}$$

Using (9) in (2b), together with (7), (8), and (4b), we obtain the conditions

$$\sum_{j=0}^{q-1}[f(\kappa_1,\kappa_2+2\pi pj/qb)-f(-\kappa_1,\kappa_2+2\pi p(j+\tfrac{1}{2})/qb)]=m_2\pi p\,,$$

$$p\sigma-2qm_1=1\,. \tag{10}$$

Comparison of (10) with (5) immediately yields the basic constraint on $m$:

$$m=-2m_1\,, \tag{11}$$

i.e., $m$ must be *even*.

We first consider the case of $p$ even ($q$, of course, is then odd). Obviously, eq. (5) with (11) can never be satisfied in this case. Thus, the assumption of isolated magnetic bands, i.e., eqs. (4), cannot be valid. This means that by varying $\kappa_1$ and/or $\kappa_2$ beyond the intervals in (3), $\psi_{\boldsymbol{\kappa}}$ must transform into a function $\psi'_{\boldsymbol{\kappa}}$ belonging to a *different* magnetic band. A similar variation of $\boldsymbol{\kappa}$ in $\psi'_{\boldsymbol{\kappa}}$ will transform $\psi'_{\boldsymbol{\kappa}}$ into a function $\psi''_{\boldsymbol{\kappa}}$ belonging, in general, to a third magnetic band. We show below that a consistent picture is already obtained by assuming the simplest possible situation, namely that $\psi''_{\boldsymbol{\kappa}}$ is equal, up to a $\boldsymbol{\kappa}$-dependent phase factor, to $\psi_{\boldsymbol{\kappa}}$. Thus, instead of an isolated magnetic band, one should speak in this case of a *pair* of magnetic bands, described by a *single* function $\psi_{\boldsymbol{\kappa}}$. Clearly, the magnetic bands in a pair are necessarily degenerate at some points $\boldsymbol{\kappa}$ in the magnetic Brillouin zone (3). In fact, one can show independently, using just symmetry arguments (see appendix A), that each magnetic band is degenerate with a second one along the entire "symmetry line" $\kappa_1=\pi/qa$.

For definiteness, let us assume here that $\psi_{\boldsymbol{\kappa}}$ transforms into $\psi'_{\boldsymbol{\kappa}}$ by varying $\kappa_1$ beyond the interval $[0, 2\pi/qa)$ (the other case, in which this transformation takes place by varying $\kappa_2$ beyond the interval $[0, 2\pi/b)$, can be treated similarly). Then, since $\psi_{\boldsymbol{\kappa}}$ reproduces precisely two magnetic bands, it must be periodic in $\boldsymbol{\kappa}$, up to $\boldsymbol{\kappa}$-dependent phase factors, with unit cell

$$0\leqslant\kappa_1<4\pi/qa\,,\quad 0\leqslant\kappa_2<2\pi/b\,,$$

which is twice as large as the magnetic Brillouin zone (3). In analogy with (4), the phase of $\psi_{\boldsymbol{\kappa}}$ may always be chosen so as to satisfy the following periodicity conditions:

$$\psi_{\kappa_1+4\pi/qa,\kappa_2}=\psi_{\boldsymbol{\kappa}}\,, \tag{12a}$$

$$\psi_{\kappa_1,\kappa_2+2\pi/b}=\exp(\mathrm{i}\sigma_\mathrm{P}\kappa_1 qa/2)\psi_\kappa\,. \qquad (12\mathrm{b})$$

Here $\sigma_\mathrm{P}$ is an integer which, according to the results in ref. [2], gives the *total* Hall conductance carried by the pair of magnetic bands. To derive a Diophantine equation for $\sigma_\mathrm{P}$, we start by considering the effect of the operator (6) on $\psi_\kappa$. Eq. (7) is still valid, but, having in mind the new definition of $\psi_\kappa$ and the conditions (12), the functions appearing on the two sides of (7) belong now to the two different magnetic bands in the pair (i.e., $O$ "exchanges" magnetic bands). In the case that $O$ does not exchange magnetic bands, $-\kappa_1$ on the right-hand side of eq. (7) has to be replaced by $2\pi/qa-\kappa_1$. In both cases, however, we obtain, by repeating the steps leading to eq. (10) (using now eqs. (2), (12), and (8) with $a$ replaced by $a/2$), the Diophantine equation

$$p\sigma_\mathrm{P}-2qm_1=2 \quad (p \text{ even integer})\,. \qquad (13)$$

Unlike eq. (10), eq. (13) is perfectly consistent for $p$ even. It is a general constraint on the total Hall conductance $\sigma_\mathrm{P}$ of a pair, completely analogous to eq. (5) for an isolated magnetic band.

In the case of $p$ odd, eq. (10) immediately yields the following general constraint on the Hall conductance $\sigma$ of an isolated magnetic band:

$$\sigma=\text{odd integer} \quad (p \text{ odd integer})\,. \qquad (14)$$

The assumption of an isolated magnetic band (in the sense of eqs. (4)) is consistent with the fact that, unlike the case of $p$ even (see appendix A), for $p$ odd the glide-plane symmetry does not lead to the degeneracy of two magnetic bands along the symmetry line $\kappa_1=\pi/qa$ [13]. An energy gap then generally "opens" between two magnetic bands along this line.

Let us now assume that the Fermi energy $E_\mathrm{F}$ lies in a gap, and that there are $N$ filled magnetic bands below $E_\mathrm{F}$. For $p$ even, $N$ is generally even since each magnetic band overlaps in energy with a second one (see above and appendix A). For $p$ odd, the parity of $N$ is arbitrary (see the discussion in appendix B). An equation for the measurable Hall conductance $\sigma_\mathrm{H}$ carried by these $N$ magnetic bands is easily derived using eqs. (10), (13), (1), and the fact that $\rho=N/q$ is the number of electrons per unit cell of the crystal:

$$\varphi\sigma_\mathrm{H}-\rho=\text{even integer}\,. \qquad (15)$$

The only difference between eq. (15) and the analogous eq. (2) in ref. [3] (where no glide-plane symmetry is assumed) is that the integer on its right-hand side is constrained to be even. An immediate consequence of this fact is that the vanishing of $\sigma_\mathrm{H}$ may occur only if $\rho$ is even, i.e., if $N$ is an even multiple of $q$. This is consistent, for $\rho=2$, with the one-band effective Hamiltonian approach in the tight-binding limit [5]. In this approach, one usually calculates the energy spectrum for the problem within the energy range of an isolated Bloch band (for $\boldsymbol{H}=0$). However, in the presence of the glide-plane symmetry, a Bloch band is *not* isolated. In fact, as one can easily show, it must be degenerate with a second one along the symmetry line $k_1=\pi/a$ in the Brillouin zone. Thus, instead of an isolated Bloch band, one should use a pair of overlapping Bloch bands in a "one-band" effective Hamiltonian approach to the problem. One then finds precisely $N=2q$ magnetic bands within the energy range of the pair. Now, as shown in ref. [5], a necessary condition for the consistency of the effective Hamiltonian approach is that the value of $\sigma_\mathrm{H}$ for these magnetic bands is zero. The pair of overlapping Bloch bands may be considered as a "valence band", carrying a zero Hall conductance.

By the same arguments as in ref. [3], eq. (15) extends to irrational values of $\varphi$, provided $E_\mathrm{F}$ is in a gap. Actually, $E_\mathrm{F}$ stays in a gap under sufficiently small variations of $\varphi$ (this follows from the general results in refs. [14] and [15]). During these variations, both $\sigma_\mathrm{H}$ and the integer on the right-hand side of (15) are constant (corresponding to a "plateau"), and $\rho$ is then a linear function of $\varphi$. An interesting example of such a variation is given in appendix B.

In conclusion, let us explain why a non-symmorphic magnetic symmetry should be assumed in order to obtain new general constraints on $m$ and $\sigma$ in eq. (5). The effect of a pure point-group operation [12] on $\psi_\kappa$ is, essentially, a direct application of this operation to $\boldsymbol{\kappa}$ (i.e., a rotation by some angle or a reflection about some mirror plane) [13,16]. Thus, such an operation, either combined or not combined with time reversal (which sends $\boldsymbol{\kappa}$ to $-\boldsymbol{\kappa}$ [13,16]), always preserves the length of $\boldsymbol{\kappa}$. On the other hand, the basic equations (4), defining $\sigma$, involve *uniform translations* in the magnetic Brillouin zone. Such translations can be performed only by applying magnetic translations to $\psi_\kappa$ [3,13]. It is then clear that, in order to obtain new general information about $\sigma$ on the basis of eqs. (4), it is necessary to combine pure point-group operations with magnetic translations (this has indeed the effect of uniformly translating $\boldsymbol{\kappa}$, at least in one direction; see, e.g., eq. (7)). The corresponding magnetic space group [9,13,12] is then non-symmorphic. By inspection, we easily find that the simplest such group for a plane lattice [10] is a glide-plane symmetry, $pg'$.

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## Appendix A

We show here that, for $p$ even, each magnetic band is degenerate with a second one along the entire symmetry line $\kappa_1=\pi/qa$. Consider, for each value of $\boldsymbol{\kappa}=\boldsymbol{\kappa}_s$ on this line, the two functions

$$T(l\boldsymbol{a})\psi_{\boldsymbol{\kappa}_s}, \quad O\psi_{\boldsymbol{\kappa}_s}, \tag{A.1}$$

where $O$ is the operator (6) and $l$ is the smallest integer satisfying

$$pl=p/2 \pmod q . \tag{A.2}$$

Since $T(\boldsymbol{a})$ "sends" $\boldsymbol{\kappa}=(\kappa_1, \kappa_2)$ to $(\kappa_1, \kappa_2+2\pi p/qb)$ [3], it is easily verified, using (A.2) and (7), that the two magnetic Bloch functions (A.1) are associated with the same value of $\boldsymbol{\kappa}=\boldsymbol{\kappa}_s+(0, \pi p/qb)$ (which is on the symmetry line $\kappa_1=\pi/qa$). Moreover, the two functions are, obviously, degenerate. Now, using well-known procedures in co-representation theory [11,17] for magnetic symmetry groups [18], one can show [13] that the functions (A.1) induce, for each $\boldsymbol{\kappa}_s$, a co-representation of the *second type* of the symmetry group. This means that the functions (A.1) are different, and thus must belong to two different magnetic bands.

## Appendix B

Given the constraints (13) and (14), it is instructive to check the consistency of eq. (15) as $\varphi$ is varied from $p/q$ ($p$ even and $q$ odd) to $p'/q$ ($p'$ odd). We assume that $p'/q$ is sufficiently close to $p/q$, so that $E_F$ stays in a gap during this variation. Then both $\sigma_H$ and the integer on the right-hand side of eq. (15) are constant. Subtracting eq. (15) for $\varphi=p/q$ from the same equation for $\varphi=p'/q$, we obtain

$$(p'-p)\sigma_H=N'-N , \tag{B.1}$$

where $N$ and $N'$ are the numbers of magnetic bands belong $E_F$ for $\varphi=p/q$ and $\varphi=p'/q$, respectively. Since $p'$ is odd, one may assume that the magnetic bands for $\varphi=p'/q$ are isolated and associated each with an odd value of the Hall conductance $\sigma$ (eq. (14)). Then the parity of $\sigma_H$ is the same as that of $N'$. Using now eq. (B.1) and the fact that $p'-p$ is odd, we immediately conclude that $N$ is always even, in consistency with the known situation for $p$ even.

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