Bloch electron in a magnetic field: Mixed dimensionality and the magnetic-field-induced generalized quantum Hall effect

by Mark Ya. Azbel

The energy spectrum of a Bloch electron in a magnetic field is one-dimensional. This leads to the Peierls instability and the magnetic-field-induced transition to the quantized Hall effect. The wave function is two-dimensional. This decreases the Peierls gap and makes it exponentially vanishing with magnetic field. Disorder lifts the degeneracy and one-dimensionality of the spectrum. High disorder yields a metallic behavior. Intermediate disorder leads to the generalized quantized Hall effect. The latter has a finite magnetoresistance as a semimetal, and Hall plateaus similar to the quantized ones, but they may have any value of the effective charge.

1. Experiment

Experiments [1] in quasi-two-dimensional (2D) Bechgaard salts $(TMTSF)_2X$, $X = ClO_4$, PF_6, ReO_4, have clearly demonstrated Hall resistance plateaus similar to but different from those in the quantized Hall effect (QHE).

In **Table 1** ρ_{xy} and ρ_{xx} are, respectively, the Hall resistivity and magnetoresistivity (per crystallographic z-plane); c is the (smallest) bandwidth along the magnetic field H; ε_F is the Fermi energy; m^* is the effective mass; n is the charge density in the xy plane; j is the filling factor; j_{eff} is the effective filling factor; $\vec{H} \parallel z$. Three features of the Bechgaard salts sound strange for QHE:

1. j_{eff} is orders of magnitude less than j.
2. The effective charge ν is neither an integer nor an odd-denominator fraction.
3. A very high $n \simeq 2 \times 10^{14}$ cm^{-2} implies $k_F \ell \simeq 2000$, $k_F r_c > 100$ (k_F is the Fermi wave vector, $r_c = \hbar k_F c/eH$; ℓ is the mean free path), and thus rules out any localization [2], which is so crucial for QHE.

Gor'kov and Lebed' [3] were the first to understand that quasi-1D materials undergo a magnetic-field-induced transition (MFIT). Although this transition is related to the Peierls instability [4], the gap, which opens at the Fermi energy, leads to a QHE rather than to an insulator. Indeed, a completely filled sub-band is in fact [5] a broadened Landau level which carries electrons *or* holes, whereas a "conventional" Peierls transition yields a "true" band with electron *and* hole currents compensating each other. Defects [5] lead to a generalized QHE (GQHE) with an "irregular" effective charge, in agreement with experiments [6].

In this paper I demonstrate that the physics of the GQHE is related to the "dimensionality mixture" for a 2D Bloch electron in a magnetic field. Its highly degenerate spectrum is quasi-1D, whereas its wave function is 2D. I study the resulting unusual Peierls transition, where defects lift the spectrum degeneracy, make it quasi-2D, and lead to the effective charge ν. The GQHE emerges at intermediate randomness. It is flanked by the QHE on the "very pure sample side" and by a metallic phase on the "dirty sample side." A complete phase diagram, METAL–QHE–GQHE, is presented.

In Section 2, I discuss the Peierls instability in the presence of randomness for $H = 0$ and $H \neq 0$. Section 3 considers the implications of the "1D" spectrum for the magnetic field-induced transition (MFIT). The GQHE is discussed in Section 4, and Section 5 deals with the METAL–QHE–GQHE phase diagram.

2. The Peierls instability

Consider the Peierls instability in magnetic field $\vec{H} \parallel z$. In the plane xy, the dispersion relation in the Bechgaard salts is

$$\varepsilon = \frac{\hbar^2 k_x^2}{2m^*} + a\cos(k_y b), \tag{1}$$

where $\varepsilon_F \simeq 1500$ K, $a \simeq 300$ K, $m^* \simeq 10^{-27}$ g, $b \simeq 7$ Å. The Peierls substitution [7],

$$\hat{k} \to \frac{1}{i}\nabla - \frac{e}{\hbar c}\hat{A},$$

in the vector potential Landau gauge, $A = A_y = -Hx$, yields the Schrödinger equation for the wave function ψ:

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\psi}{\partial x^2} + a\cos\left(\frac{b}{i}\frac{\partial}{\partial y} + \frac{eHb}{c\hbar}x\right)\psi = \varepsilon\psi. \tag{2}$$

Choosing $\psi = \chi\exp(ik_y y)$, one finds

Table 1 Experimental conditions and results.

"Common" QHE	*Bechgaard salts*
Conditions	
Two-dimensional	Quasi-two-dimensional ($c/\varepsilon_F < 0.003$)
$\frac{heH}{m^*c} > \lvert$ *Potential* $\rvert$	$\frac{heH}{m^*c} \ll \lvert$ *Potential* $\rvert$
No periodic potential	Strong periodic potential along y
$j \equiv nch/eH \simeq 1$	$100 \leq j \leq 250$
Results	
$\rho_{xy} = \frac{h}{e^2 j}$	$\rho_{xy} = \frac{h}{e^2 j_{\text{eff}}\nu}$, $j_{\text{eff}} \ll j$, $\nu \simeq 1$
$\rho_{xx} = 0$	$\rho_{xx} \neq 0$
Electrons or holes	Electron $\Leftrightarrow$ hole transitions

$$\chi'' + \frac{2m^*}{\hbar^2}\left[\varepsilon - a\cos\frac{eHb}{c\hbar}(x - x_0)\right]\chi = 0, \tag{3}$$

$$x_0 = -\frac{c\hbar k_y}{eH}. \tag{4}$$

This is the Mathieu equation. Its gaps are $\propto \exp(-2000/H_T)$, where H_T is the magnetic field in teslas. Clearly, they are absolutely negligible. However, Equation (3) in $x_1 = x - x_0$ is effectively the Schrödinger equation in a 1D periodic potential. Thus, it is unstable [3] with respect to the Peierls gap formation [4]. The perturbative SDW potential $V_0\cos(2k_F x)$ generates a gap Δ at $\varepsilon = \varepsilon_F$ and decreases the electron energy by $\simeq \Delta^2 \ln(\varepsilon_F/\Delta)$. For sufficiently small Δ, this is always beneficial, since the SDW energy increase is $\propto \Delta^2$. The gap formation is clearly related to the 1D nature of the spectrum, i.e., to the degeneracy of the spectrum with respect to k_y. The wave function remains [8] 2D. To make the impact of this "dimensionality difference" explicit, consider the Peierls gap formation in more detail in a "conventional" 1D case (when $H = 0$) and in the Equation (3) situation. When defects are present, this analysis turns out to be of importance.

3. 1D Schrödinger equation

Consider the 1D Schrödinger equation with a periodic potential $u(x)$:

$$\psi'' + \frac{2m^*}{\hbar^2}(\varepsilon - u)\psi = 0. \tag{5}$$

When $\varepsilon > \max u$, the exact solution to Equation (5) in the allowed band may be presented in the form

$$\psi_\pm = k^{-1/2}\exp\left(\pm i\int k\,dx\right), \tag{6}$$

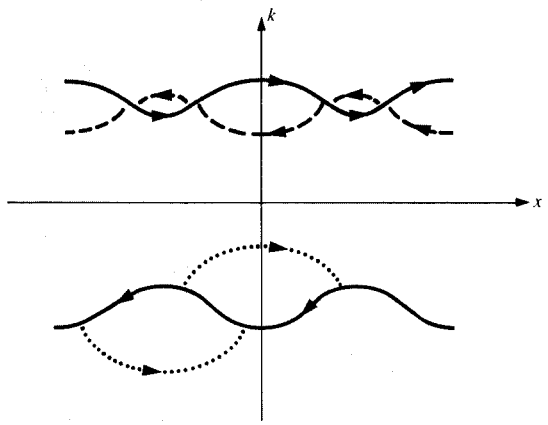

Figure 1

One-dimensional nesting in a magnetic field. Dashed lines—closed orbits with clockwise and anticlockwise motion. Dotted lines—"best nesting" in Equation (3); largest closed-orbit areas with clockwise electron and anticlockwise hole motion.

where $k(x)$ is determined by the equation

$$k^2 = \frac{2m^*}{\hbar^2}(\varepsilon - u) + \frac{3k'^2 - 2kk''}{4k^2}. \tag{7}$$

In the quasi-classical limit, $k^2 \simeq 2m^*(\varepsilon - u)/\hbar^2$—see **Figure 1**.

A perturbative potential V nests the two branches, generating a gap

$$\Delta = \int \psi_+ V \bar{\psi}_- dx. \tag{8}$$

By Equation (8), the largest gap is provided by

$$V = V_0 \mathrm{Re}(\psi_+ \bar{\psi}_-). \tag{9}$$

Then

$$\Delta = V_0 \int |\psi_+ \psi_-|^2 dx \simeq V_0. \tag{10}$$

Defects lead to a random contribution to u in Equation (5) (and to localization). Still, the choice(s) of the perturbative potential may allow for the gap $\Delta \simeq V_0$ in the spectrum.

The picture for Equation (3) is drastically different, since $\chi = \chi(x - x_0)$ depends on the orbit center coordinate x_0. One *cannot* choose the same "good for all x_0" factor V of Equation (9). The "2D nature" of the wave function results in a gap, which is *much smaller* than V_0 and which $\to 0$ when $H \to 0$. The "best" nesting in Equation (3) (leading to the largest gap) is related to the largest closed-orbit areas (dotted lines in Figure 1), which may correspond to clockwise electrons or anticlockwise holes. [For the best nesting in Equation (2), see [9]]. The quantization of magnetic flux through closed orbits leads to the Landau levels. Magnetic breakdown tunneling between the orbits broadens the levels into Landau sub-bands separated by narrow gaps. If the Fermi energy is in the largest gap, then the corresponding filling factor is

$$j_{\mathrm{eff}} \simeq \frac{1}{2\pi}(\textit{dotted area}) \propto H^{-1}. \tag{11}$$

In the quasi-classical limit, electron and hole orbits are almost degenerate; hence easy electron-hole and hole-electron transitions occur.

The largest gap is [5, 9]

$$\Delta \propto V_0 H^{-1/3}. \tag{12}$$

Given the relation between Δ and V_0, thermodynamics determines V_0. The minimum of the combined electronic $[\propto \Delta^2 \ln(\varepsilon_F/\Delta)]$ and SDW $(\propto \Delta^2)$ energies yields [5, 9]

$$\ln V_0^{-1} \propto j_{\mathrm{eff}}^{2/3}. \tag{13}$$

The random potential W contribution to Equations (2) and (3) lifts the spectrum degeneracy. Hence, it may be impossible to generate the gap for all x_0's at the same energy. Even the best nesting may leave a small density of states at the Fermi energy. Physically this is most explicit in the quasi-classical limit $(k_F r_c \gg 1)$ when $|\nabla W| \ll (v/c)eH$, where $\vec{v} = 1/\hbar\, \partial\varepsilon/\partial\vec{k}$ is the velocity. Then, in the leading approximation we find the Lorentz equation $\hbar\dot{\vec{k}} = (e/c)\dot{\vec{r}} \times \vec{H}$ and

$$\vec{r} = \vec{r}_0 + \frac{\hbar c\vec{H}}{eH^2} \times (\vec{k} - \vec{k}_0). \tag{14}$$

Now the conservation of the total energy ε_t implies, by Equation (14),

$$\varepsilon_t = \varepsilon(\vec{k}) + W(\vec{r}) = \varepsilon(\vec{k}) + W\left[\vec{r}_0 + \frac{\hbar c\vec{H}}{eH^2} \times (\vec{k} - \vec{k}_0)\right]. \tag{15}$$

Thus, the kinetic energy

$$\varepsilon(\vec{k}) = \varepsilon_t - W\left[\vec{r}_0 + \frac{\hbar c\vec{H}}{eH^2} \times (\vec{k} - \vec{k}_0)\right] \tag{16}$$

changes with k and depends on the initial $\vec{r}_0$ and k_0. (Note that when $W = 0$, ε is conserved.) The corresponding smearing of the gap may be much larger than the conventional broadening $\hbar/\tau = \hbar v/\ell$, where τ is the mean free path time. For instance, if one considers an "average" variation W over distances of order ℓ, then the characteristic gap smearing is

$$\delta W \simeq (W/\ell) r_c \equiv \frac{W}{\Omega\tau} = \frac{\hbar}{\tau}\frac{W}{\hbar\Omega} \gg \hbar/\tau,$$

since $W \gg \hbar\Omega = (\hbar eH/m^*c)$—see Table 1. If $\delta W > \Delta$, then any nesting yields states at ε_F (although their density may be low). They lead to finite dissipation and magnetoresistivity.

4. GQHE theory

The theory of the GQHE may be constructed by introducing into Figure 1 the probability p of a magnetic breakdown and the probability matrix $\hat{\tau}$ of random intra- and inter-branch scattering per unit time. The average distance traveled along x is $\simeq r_c/q$, where $q \equiv 1 - p$. If $r_c/q \ll \ell$, then the orbit is effectively closed, and one may expect a "conventional" QHE. This, in particular, happens when $\ell \to \infty$. If $r_c/q \gg \ell$, then scattering occurs before an electron "learns" that its orbit is closed, and it may "presume" it to be effectively open. This happens, in particular, when $q = 0$ (truly open orbit). To understand the physics of the general situation, consider first the latter case. Suppose the electric field E is along the ξ direction, and let η be a coordinate perpendicular to ξ (the crystallographic axes are x and y). Then the Lorentz equation

$$\hbar\dot{\vec{k}} = \left(\frac{e}{c}\dot{\vec{r}} \times \vec{H}\right) + e\vec{E} \tag{17}$$

implies that

$$\xi = \xi_0 - \hbar c(k_y - k_0)/eH. \tag{18}$$

The total energy ε_t conservation

$$\varepsilon_t = \varepsilon(\vec{k}) - eE\xi \tag{19}$$

yields

$$\varepsilon(\vec{k}) = \varepsilon_t - e(\xi_0 + \hbar c k_0/eH)E + \hbar c k_\eta E/H. \tag{20}$$

[Note that, in contrast to Equation (16), Equation (20) is an exact formula.] The energy $\varepsilon(\vec{k})$ slowly decreases until, close to the self-crossing (at $H = 0$) energy ε^{sc}_{min}, an orbit has a reflection point. The corresponding change in the energy is large, so one must consider a "complete" Bloch dispersion, e.g.,

$$\varepsilon = \cos(k_x b_x) + a\cos(k_y b) \qquad a < 1. \tag{21}$$

After the reflection, k_y decreases, and the increase in the energy, by Equation (20), ultimately also leads to the reflection in the vicinity of the hole self-crossing energy ε^{sc}_{max}, and so on—see **Figure 2**. By Equation (19),

$$\Delta\xi = \frac{\Delta\varepsilon}{eE} \qquad \Delta\varepsilon = \varepsilon^{sc}_{max} - \varepsilon^{sc}_{min}; \tag{22}$$

i.e., $\Delta\xi$ is finite, but usually *very large*, and $E > \Delta\varepsilon/eL$ leads to nonlinearity (L is the sample size along ξ). By Equation (17), the average velocity $\langle\dot{\eta}\rangle$ along η is

$$\langle\dot{\eta}\rangle = -\frac{cE}{H} + \frac{c\hbar}{eH}\lim_{\Delta t\to\infty}\frac{\Delta k_\xi}{\Delta t}, \tag{23}$$

where $\Delta k_\xi \neq 0$. Equation (23) gives a renormalized "conventional" Hall velocity ($-cE/H$). (A closed orbit is periodic, and its $\Delta k_\xi = 0$.) To calculate $\langle\dot{\eta}\rangle$, complement Equation (20) with the Hamilton equation

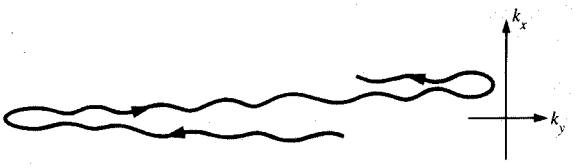

Figure 2

Open orbit (in $\vec{k}$-space) in crossed electric and magnetic fields.

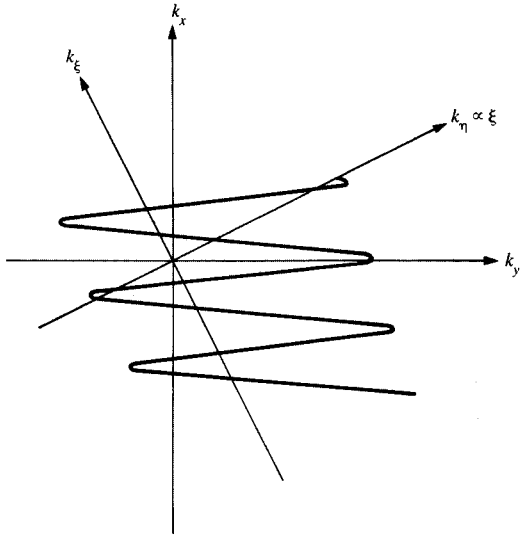

Figure 3

Orbit center motion.

$$\dot{r} = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial\vec{k}},$$

which with Equation (18) relates k_ξ in Equation (17) to $\dot{k}_\eta$:

$$\frac{1}{\hbar}\frac{\partial\varepsilon}{\partial k_\xi} = \dot{\xi} = -\hbar c\dot{k}_\eta/eH. \tag{24}$$

Equations (20) and (24) allow one to calculate $k_\eta(t)$ and $k_\xi(t)$. Then Equation (23) determines $\langle\dot{\eta}\rangle$,

$$\langle\dot{\eta}\rangle = \frac{\nu cE}{H} \qquad \nu = 1 - \frac{2\pi\,|k_x^{min}|}{b\displaystyle\int_0^{2\pi/b}|k_x|\,dk_y}. \tag{25}$$

The orbit is extended along η, but $\langle\dot{\eta}\rangle \propto E$ is usually very small. See **Figure 3** for the orbit center motion.

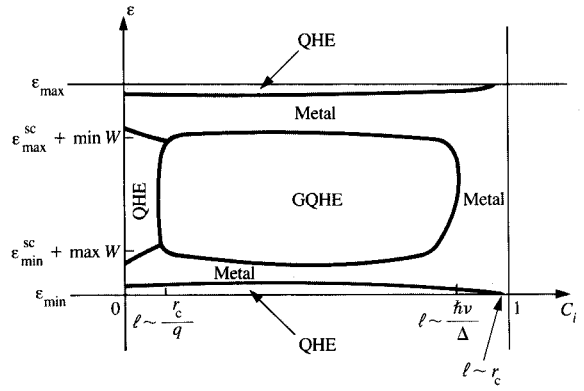

Figure 4

METAL-QHE-GQHE phase diagram.

Now consider a general case with finite ℓ and q. In the quasi-classical limit, we have

$$1 - q = p \propto \exp\left(-\int |k_x|\, dx\right). \tag{26}$$

Calculating the integral in the classically forbidden region [generated by the gap Δ from Equation (12)], one arrives at

$$\ln p^{-1} \simeq j_{\text{eff}}^{4/3}\, V_0^2. \tag{27}$$

Now, solving the master equation, one determines the Hall resistivity per plane [5]:

$$\rho_{xy} = \frac{\hbar}{e^2 \nu j_{\text{eff}}}, \tag{28}$$

where j_{eff} is an integer and ν is the effective charge. In a general case [5],

$$\nu = 1 - \frac{2\pi}{bS} \frac{|k_x^{\min}| + \dfrac{1-q}{q}\displaystyle\int_0^T \hat{\tau}_*^{-1} |k_x| dt}{1 + \dfrac{1-q}{q}\displaystyle\int_0^T \hat{\tau}_*^{-1} dt}. \tag{29}$$

Here

$$S = \int_0^{2\pi b} |k_x| dk_y$$

is the orbit area, T is the period:

$$T = \frac{c}{eH}\frac{\partial S}{\partial \varepsilon},$$

and the subscript * denotes the interbranch scattering. Clearly, ν may take any value and can be of either sign in the GQHE.

5. METAL–QHE–GQHE phase diagram

When a sample is sufficiently dirty, $\hbar v/\ell > \Delta$, there is no gap nor a MFIT. When a sample is very clean, $\ell > r_c/q$, the orbits are closed, $k_x^{\min} = 0$ in Equation (29), and $\nu = 1$; i.e., one observes MFI QHE.

Until now I have discussed only orbits which are open at $H = 0$. If the Fermi energy corresponds to a closed (at $H = 0$) orbit, then the Landau sub-band is exponentially narrow, $\propto \exp(-k_F r_c)$, and it makes "exponentially little sense" to open a gap in it. Since $k_F r_c \gg 1$ implies no localization [2], the phase is metallic, with a conventional Hall effect. Localization, together with QHE, develops near the band edges, where $k_F r_c \lesssim 1$. (Note that throughout the paper I assume a 2D situation.)

According to Equation (16), when

$$(W_{\max} - W_{\min}) < (\varepsilon^{sc}_{\max} - \varepsilon^{sc}_{\min}),$$

there are two boundaries between open and closed orbits, at

$$\varepsilon = \varepsilon^{sc}_{\max} + W_{\min}$$

and at

$$\varepsilon = \varepsilon^{sc}_{\min} + W_{\max}.$$

Thus, at $T = 0$ the 2D phase diagram in the energy ε-impurity concentration (C_i) plane appears as in **Figure 4**. The following are some remarks concerning the diagram:

1. The boundaries between the GQHE and the QHE are obviously smeared.
2. The boundaries between the GQHE and metallic phases have in fact a complicated shape, since the Landau spectrum is complicated in the vicinity of self-crossing orbits [10].
3. There are two "quasi-mobility edges" at METAL–QHE boundaries. These are not "true" mobility edges, since an unrealistically large $L \gg \ell \exp(2\pi\ell/b)$ implies localization at all energies.

References and note

1. For a review and references, see L. P. Gor'kov, *Sov. Phys. Isp.* **27,** 809 (1984) and *Proceedings of Yamada Conference XV on Quasi-1-D Conductors, Physica* **B143** (1986).
2. When $H = 0$, the 2D localization length ξ is of the order $\exp(k_F \ell) \simeq 10^{1000}$. When $H \neq 0$, one may assume the scaling $\ln \xi \simeq k_F \ell F(r_c/\ell)$, with ξ being finite and independent of ℓ when $\ell \to \infty$. Then $r_c \ll \ell$ yields $\xi \propto \exp(k_F r_c) > 10^{40}$. Note that in the latter case adjacent orbit centers are separated by distances which are small compared to the orbit size r_c and allow for easy inter-orbit tunneling and "delocalization," if the random potential changes little at r_c.
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