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BLOCH ELECTRONS IN RATIONAL AND IRRATIONAL MAGNETIC FIELDS.

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Abstract: *States of crystal electrons in a homogenous magnetic field are of considerable practical and theoretical interest: they are the basis of the magneto-oscillatory effects which yield in turn most informations on Fermi surfaces, provided a theory connecting zero and finite magnetic field Bloch states exists. This is achieved by the semiclassical Peierls-Onsager theory which explains experimental results at least for nondegenerate bands. However, this method lacks a rigorous first principle derivation. Recently such a rigorous treatment has been developed; the obtained electronic spectra are in agreement with semiclassical results for simple bands; they show, moreover the splitting of degenerate bands and the detailed structure of magnetic breakdown.*

Another intriguing aspect of the problem is the coexistence of two pace lengths: lattice constant and Landau orbit diameter, which are almost always incommensurate ("irrational" versus "rational" magnetic fields). As a consequence the spectrum exhibits an extremely complicated fine structure, related to the "chaotic" properties of certain maps.

This is largely a theoretical talk about recent advances in the theory of crystal electrons in magnetic fields, apparently a problem in the trivial class of one particle quantum mechanics; so I feel obliged to point out our motivation for this work: why is it nontrivial, amusing, maybe even important?

1. Geometrical considerations: Let me start with some remarks on the geometry or the kinematics of electrons in a periodic potential and a magnetic field and explain the terms rational and irrational fields, which, in geometrical terms, denotes commensurate and incommensurate pace lengths.

Fig.1 illustrates the point: the crystal lattice is the pavement on which the electrons have to walk. Without a magnetic field, they can freely adjust their pace to the lattice constant; as a result there is a continuum of energies, but whenever electron wavevectors and reciprocal lattice are commensurate there is the energy stationarity and splitting characteristic of a band edge.

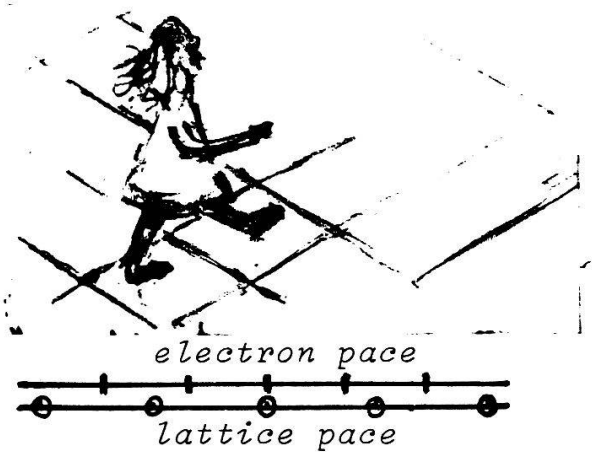

Fig.1: "Don't step on a crack"

Now in a homogenous magnetic field the crystal electrons meet with <u>two</u> characteristic lengths, or rather <u>two</u> characteristic areas: the quantized areas of the cyclotron orbits $\pi\langle r^2\rangle_n = \pi\, n\, \hbar c/eB$, where n denotes the Landau quantum numbers, and the areas of the lattice mesh projected onto the plane perpendicular to the field. Fig.2 shows such a projection and the first 3 cyclotron orbits; if the two shaded areas are commensurate, one calls such fields rational; the general rationality condition was first formulated by Brown /1/ and Fischbeck /2/ 20 years ago:

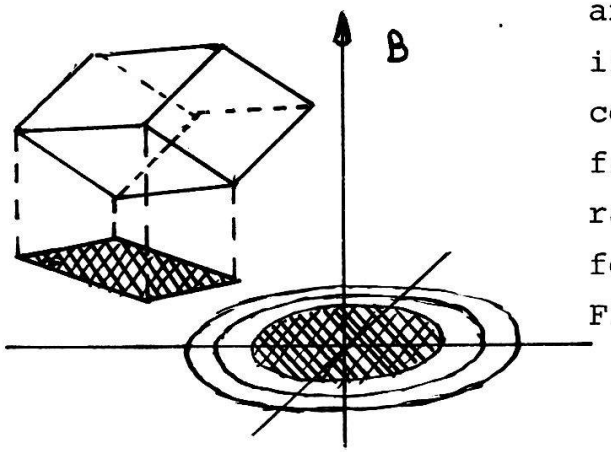

Fig.2: Projection of a lattice mesh onto the plane perpendicular to B, quantised cyclotron orbits.

$$e\vec{B}/\hbar c = 2\pi\,(1/N)\,(\vec{R}/\Omega) \qquad \ldots (1)$$

where Ω is the volume of the unit cell, $\vec{R}$ a lattice vector and l, N integers.

The authors just mentioned have then constructed the group of symmetry operations of the problem, the magnetic translation group, a generalisation of the ordinary lattice translations that includes phase factors to account for the vector potential. In the case of rational magnetic fields in the sense of eq.(1) this group is finite (though nonabelian) and has irreducible representations of dimension N,where N ist the denominator of the rational number in (1). Hence Fischbeck and Brown could do all the usual group theoretical classifications of states; in particular as a result of strictly geometrical arguments one recognizes that for a rational field 1/N there must be N-fold degeneracy of the eigenstates according to the dimension of the irreducible symmetry group representation.

But this result, beautiful, because based only on symmetry considerations, gives rise to a serious puzzle: the degeneracy g jumps erratically as we go from one rational field to another one nearby. So, e.g. for a typical solid, B = 1T (10kG) corresponds to $1/N \sim 1/10^5$, $g = 10^5$; but $B' = (1+10^{-12})T$ corresponds to $1'/N' = 10^7/(10^{12}-1)$ and hence to a $g' = 10^{12}-1$.

To avoid this "degeneracy catastrophe" one must speculate that - as we go from B' to B - the spectrum is bunched together in such a way that observable quantities show a less erratic behaviour. This is in fact the case, as I will show in the next section; but to replace speculation by calculation, one needs dynamics in addition to geometry.

2. Semiclassical dynamics: Let us look at the Hamiltonian for the problem

$$H = (\vec{p}-e\vec{A}/c)^2/2m + V_{per.}(\vec{r}) \qquad (2)$$

For A = 0 it has plane-wave-like Blochfunctions as eigenfunctions, for $V_{per.} = 0$ it has squareintegrable Landau functions. The latter, in momentum representation, look like $\exp(-p^2/B)$; i.e. they exhibit an essential singularity at B = 0 and do not go over into $\delta(p-p_o)$, that is into plane waves.

For these reasons a perturbation treatment of either $\vec{A}$ or V_{per} is problematic.

The effective Hamiltonian or Peierls-Onsager method avoids this problem; instead of the full Hamiltonian (2) one considers electrons in one particular Bloch band only and treats the effect of a (weak) Lorentz-force semiclassically:

$$\dot{\vec{p}} = e\,\vec{v} \times \vec{B} = e\,\vec{v} \times \mathrm{rot}\vec{A} \qquad (3)$$

But for electrons in a band with dispersion $E_n(k)$ one has the wellknown result $\langle\vec{v}\rangle = \nabla_k E_n(k)$ and one obtains from (3) the textbook arguments summarized in fig.3:

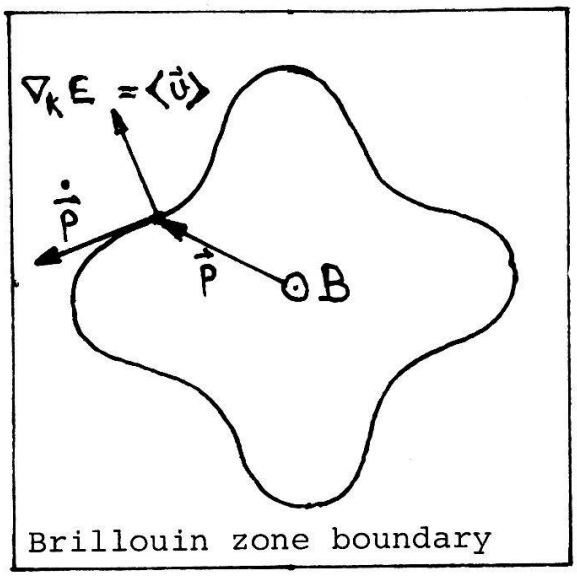

Fig.3: Semiclassical dynamics in a twodimensional Brillouin zone.

under the influence of the magnetic field the state of the electron moves on the energy surface in planes normal to the field. For closed orbits one applies Bohr-Sommerfeld quantization and arrives at the band cyclotron orbits that are in fact observed in all kinds of magneto oscillatory effects and form the basis of much of our knowledge of Fermi surfaces. Harper /3/, Azbel /4/ and others have formalized this argument and introduced a semiclassical effective Hamiltionoperator

$$H_{eff} = E_n((\vec{p}-e\vec{A}(\vec{r}))/\hbar) \qquad (4)$$

where E_n takes the functional form of the dispersion $E_n(\vec{k})$ with the operators $\vec{p}$ and $\vec{A}(\vec{r})$ in the argument. It is easy to show that the classical Hamilton equation $\dot{\vec{p}} = -\partial H_{eff}/\partial r$ leads back to (3); in that sense (4) is a consistent semiclassical ansatz.

Hofstadter /5/ has made an exhaustive study of the spectrum of (4) in the simple case that $E_n(\vec{k})$ is a twodimensional quadratic tight binding band, lattice constant a, of the form

$$E_n(\vec{k}) = 2\cos k_x a + 2\cos k_y a\ . \qquad (5)$$

The problem can then be reduced to a onevariable eigenvalue equation in the form of a difference equation

$$a_{n+1} + 2\cos(2\pi\alpha n-\nu)\, a_n + a_{n-1} = \varepsilon a_n \qquad (6)$$

$\alpha = a^2B/2\pi(\hbar c/e)$ is precisely the dimensionless ratio of flux through the unit cell a^2 to flux quantum which occured already in the rationality condition (1) and, for rational fields, takes on the value 1/N.

Hofstadters numerical results for the spectrum for rationals up to N = 50 is shown in fig.4. "This graph", to quote Hofstadter,

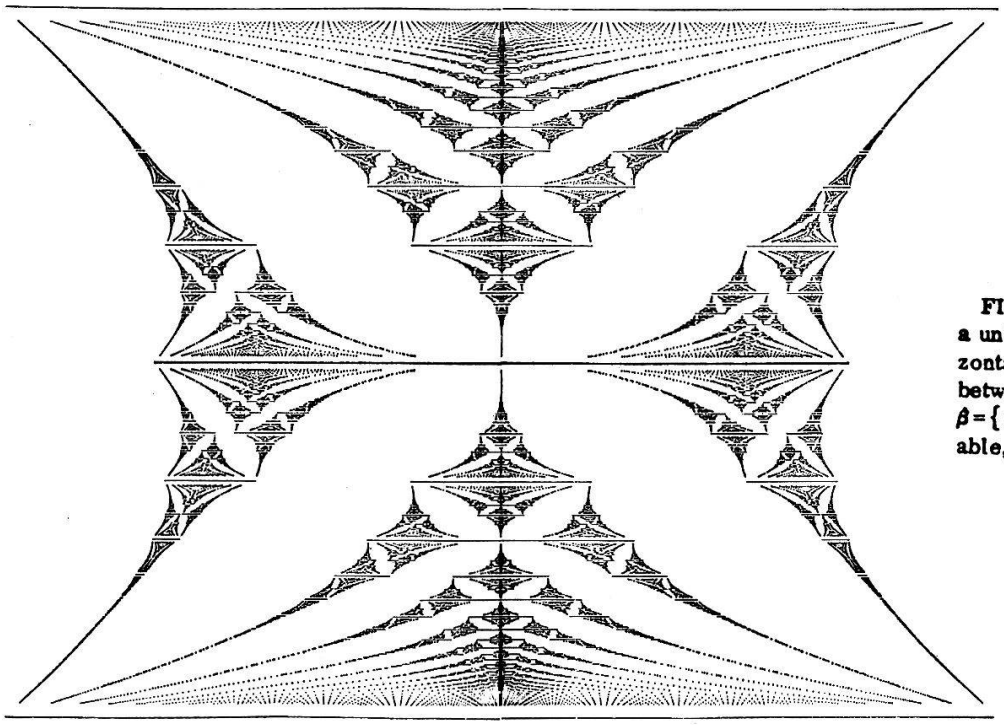

FIG. 4 : Spectrum inside a unit cell. ϵ is the horizontal variable, ranging between +4 and −4, and $\beta=\{\alpha\}$ is the vertical variable, ranging from 0 to 1.

"has some very unusual properties. The large gaps form a very striking pattern somewhat resembling a butterfly; perhaps equally striking are the delicacy and beauty of the fine-grained structure. These are due to a very intricate scheme, by which bands cluster into groups, which themselves may cluster into larger groups, and so on." This nesting structure can roughly be described as follows: subareas of the graph are reduced and slightly distorted replicas of the entire graph and can be decomposed themselves into an (infinite) sequence of ever finer self-replicas.

As a result for irrational, that is almost all fields, one concludes that the spectrum is singular continuous,

it consists of uncountably many points, between any pair of which there is a finite gap: this is homeomorphic to the Cantor set. We do not know, however, the fractal dimension of the graph, because we don't have an analytical expression for the distortion and reduction of the graph in each of the subsequent nesting steps; all we know is that for a given denominator N there are N bands in the spectrum, which become ever narrower as N increases.

So now we have degeneracy and number of subbands growing with N, band width shrinking with N. What do observable quantities look like? As an example we have looked at the density of states g(λ) and the integrated density of states n(λ); fig.5 from Wannier, Ray, Obermair /6/.

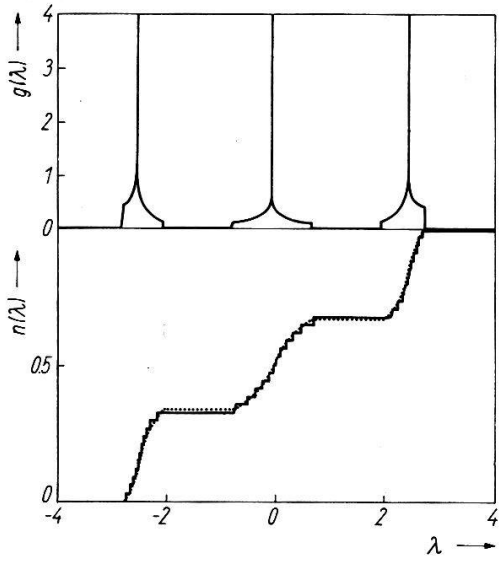

Fig. 5. Density of states $g(\lambda)$ and integrated density of states $n(\lambda)$ for a rational magnetic field represented by the denominator 3. $g(\lambda)$ is typical of "erratic" behavior: three pagoda-like energy bands ($p/q = \frac{1}{3}$). In the integrated density of states $n(\lambda)$ this "erratic" aspect recedes. The integral of the upper curve (dotted outline, $p/q = \frac{1}{3}$) does not differ much numerically from the integral for $p/q = 11/34$ (solid line) although the analytic structure of the two curves is totally different

Two features, I hope, are evident: (a) The degeneracy catastrophe drops out. (b) The density of states g(λ) is still dramatically dependent on N; for 1/N = 11/34 (not shown for g(λ) there would be 34 logarithmic singularities instead of the 3 shown in the figure. Thermodynamic quantities, however, which are integrals like n(λ), are dominated by the "large" structures (3 high steps); the 34 small steps are only a finer detail hard to resolve in practice. The large structures are determined by the leading term in a continued fraction expansion of the quantity α; e.g. here α = 11/34 = 1/(3 + 1/11); i.e. 3 high steps.

Three remarks to conclude this section:
(a) The difference equation (6) can also be interpreted as a description of electrons on a linear chain with a (commensurate or noncommensurate) periodic substrate underlaid, which brings us back to the naive geometric pictures of section 1 but also shows the close relationship to commensurate - incommensurate phase transitions. (b) The existence of finite gaps in the spectrum is essential for an understanding of the quantum Hall effect, cf. Thouless et al. /7/. Such gaps are in fact a consistent feature of the spectrum shown in fig.4. (c) Eq. (6) can be transformed to a twodimensional discrete mapping and studied in this context.

3. First principle calculation. In spite of the obvious success of the semiclassical methods just described, there are some serious deficiencies: (a) A rigorous derivation from first principle quantum mechanics is lacking. (b) The method does not work for degenerate bands, in the magnetic breakdown region and in the socalled Landau regime, i.e. weak periodic potential, strong magnetic field. (c) The widths of the magnetic subbands obtained semiclassically may be an artefact of the method (these widths might be accessible to an experimental test in de Haas-van Alphen or similar experiments).

A rigorous calculation of the spectrum of the full Hamiltonian (2) appeared highly desirable, cf. Schellnhuber and Obermair /8/. To show the essence of our approach let me return briefly to the Landau problem: no periodic potential, free electrons in a homogenous magnetic field. The motion along the field, assumed in z-direction, will be neglected in all that follows. We then have a classical phase space of 4 dimensions, spanned by the veriables $x,y;p_x,p_y$. The Hamiltonian reduces to the kinetic energy

$$H_o = m/2\ v^2 \tag{7}$$

which, written in terms of the canonical momenta, becomes

$$H_o(x,y,p_x,p_y) = 1/2m\ [(p_x-eA_x)^2 + (p_y-eA_y)^2] \tag{8}$$

The functional dependence of H on x and y is obviously dependent on the gauge chosen for $\vec{A}$. The classical circular orbits are,

of course, gauge independent, but the wavefunctions representing eigenstates of (8) depend critically on the gauge. Moreover, the two degrees of freedom, x and y, are coupled in a gauge dependent way.

A number of authors /8/9/10/ have therefore lately proposed a purely algebraic formulation of the problem: technically it can be described as a canonical transformation from x, y, p_x, p_y to a new set of 2 pairs of conjugate operators q, Q, p, P. If one writes $\vec{A} = 1/2\ B(-y,x,0)$ in the symmetric gauge, the terms of H_o are $(p_x + eBy/2)^2$ and $(p_y - eBx/2)^2$. Defining $\alpha = eB/\hbar c$ and

$$P = +\alpha^{-1/2} p_x/\hbar + \alpha^{1/2} y/2 \ ; \ p = +\ldots - \ldots$$
$$Q = -\alpha^{-1/2} p_y/\hbar + \alpha^{1/2} x/2 \ ; \ q = +\ldots + \ldots \qquad (9)$$

one easily checks that $[Q,P] = i$; $[q,p] = i$, all other commutators vanish and H_o reads

$$H_o = \hbar\omega_c/2\ (P^2 + Q^2) \qquad (10)$$

This is a onedimensional harmonic oscillator; the (q,p) degree of freedom has dropped out altogether; this gives rise to the continous degeneracy of the Landau levels.

If one now introduces a periodic potential $V_{per}(x,y)$ again, the simplest possible ansatz being $V = 2v_o\ (\cos Gx + \cos Gy)$, $G = 2\pi/a$, then one has, in the new variables, a coupling of the 2 degrees of freedom in the potential. For rational magnetic fields it is possible to decouple again (for technical details cf. /8/) with two separation constants (κ,λ) that span the magnetic Brillouin zone and one obtains a set of Hamiltonians

$$H(\kappa,\lambda) = \hbar\omega_c/2(P^2 + Q^2) + 2v_o(\cos\sqrt{\eta}(Q+\lambda) + \cos\sqrt{\eta}(P-\lambda)) \qquad (11)$$

η is now the inverse of the rationality parameter α in eq.(6) and takes on values $\eta = 2\pi\ N/l$.

Let me summarize the results of our extensive numerical studies in the last two figures: Fig.6 shows the spectrum at the Γ-point of the magnetic B.Z. for $N/l = 4/3$ as a function of the amplitude v_o of the periodic potential. For small v_o one sees the 3fold splitting of the Landau levels in full agreement with group theory predictions for $l = 3$. On the other hand for large

v_o the magnetic subbands are bunched together in groups of 4 (N = 4) within the limits of the zero field bands in accordance with the semiclassical theory for $\alpha = 1/N = 3/4$. Notice also that the second lowest and third lowest group of 4 states arise from one, twofold degenerate zero field band.

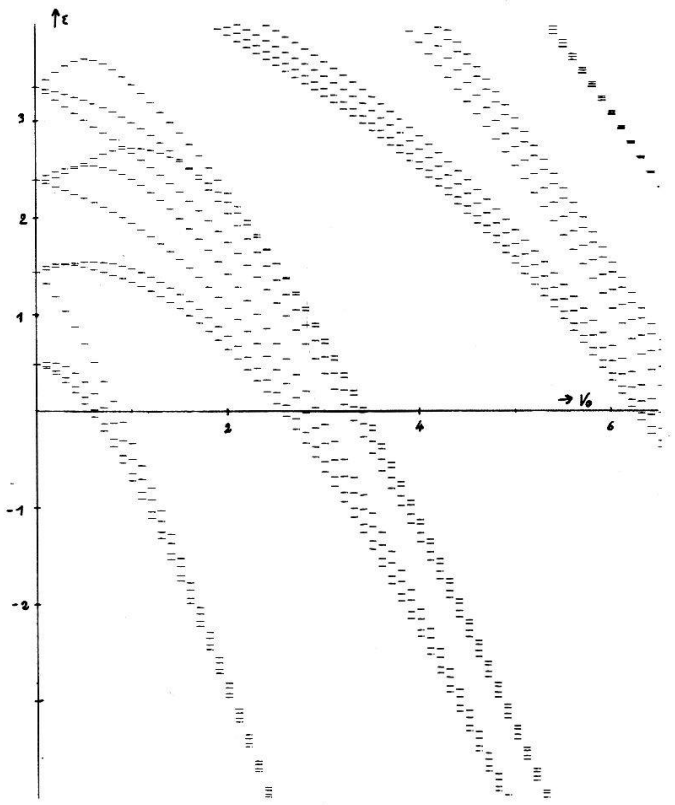

Fig.6: Evolution of the Γ-point spectrum of the magnetic B. Z. with growing lattice potential v_o . For v_o=0, i.e. on the ε-axis, one recognizes the Landau levels, for large v_o the fully developed magnetic subband centers, from /11/

The excellent agreement between first principle and semiclassical calculations is seen in fig.7a for the lowest zero field band for N=5, l=1 and a fixed, large value of v_o: positions and linewidths are nearly identical. Fig.7 shows the splitting of the degenerate second lowest band into 2 groups of N=5 magnetic subbands; this is an exact result, where the semiclassical method breaks down.

4. Conclusion. The different pieces of theory for Bloch electrons in magnetic fields, some fundamental, some ad hoc, begin to form a coherent picture. Predictions from group theory and from the semiclassical approach are, within the limits of their applicability, confirmed by first principle calculations for rational fields. For irrational fields the spectrum goes to a Cantor set. Experimental tests for the new predictions (intrinsic line widths, gap structure, splitting of degenerate bands) remain to be developed.

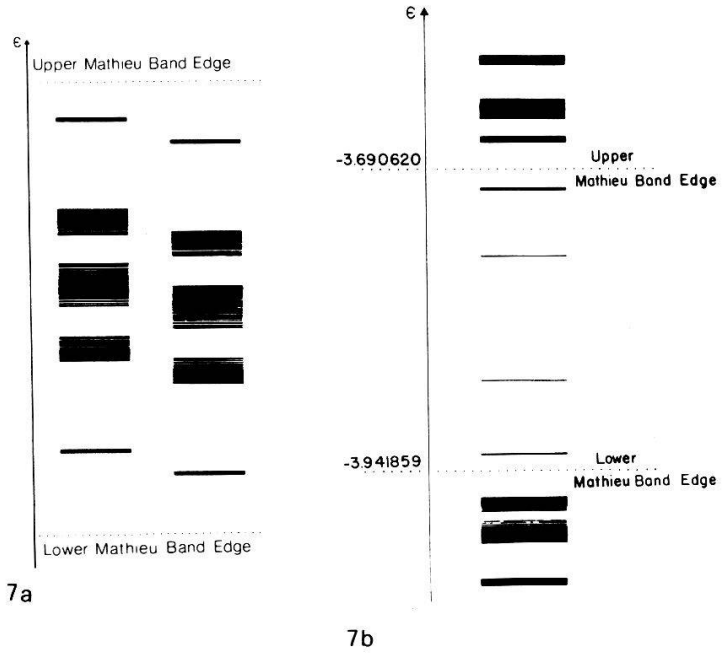

Fig.7a (left): First principle and semiclassical spectrum in the lowest band, N=5. Fig.7b (right): First principle spectrum for degenerate 2nd lowest band shows splitting.

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