BLOCH ELECTRONS

in a

MAGNETIC FIELD

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Institut Fourier Grenoble, May 30 2006
At the occasion of Yves Colin de Verdière 60th birthday

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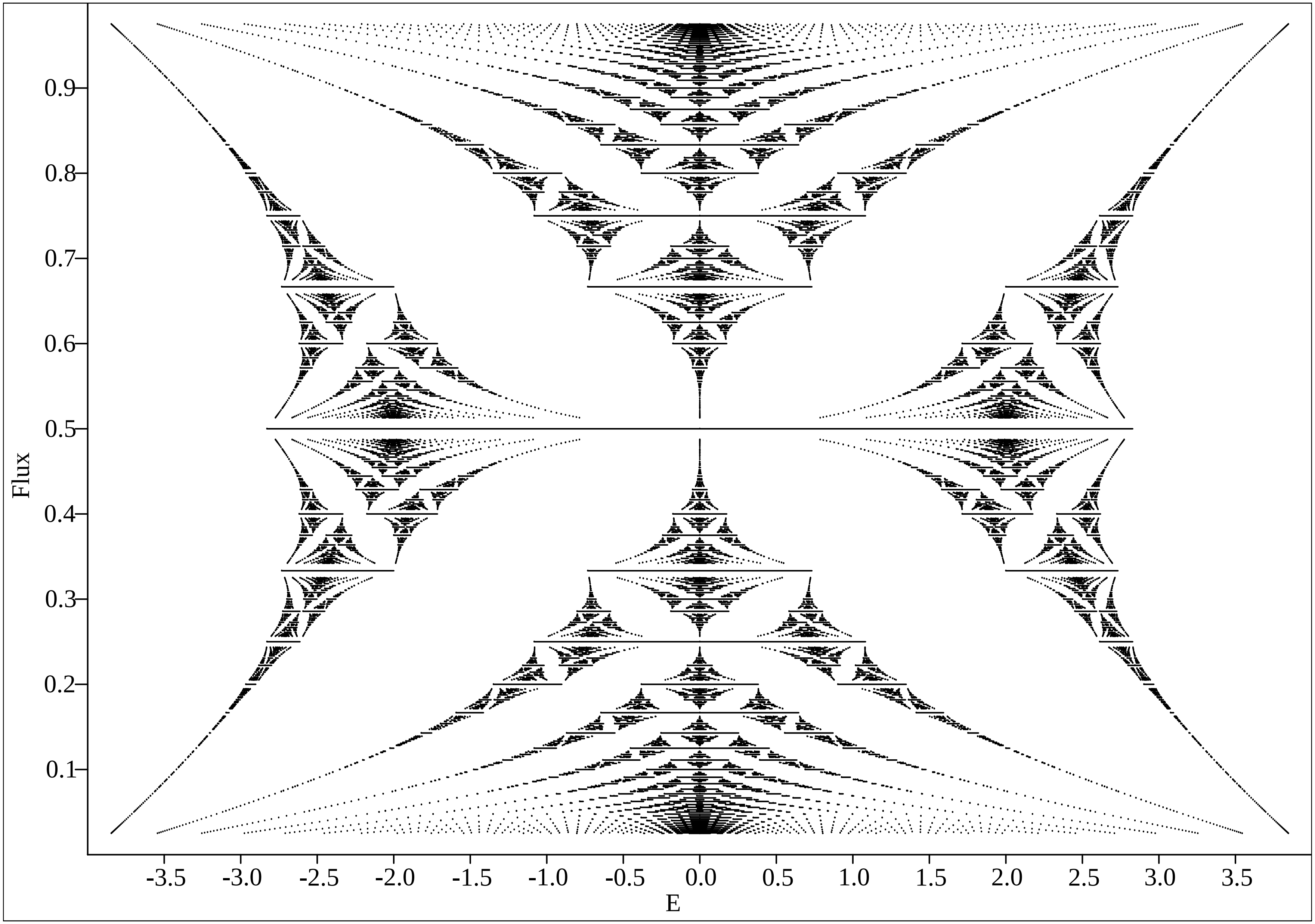
60 Years Ago !

Yves Colin Altherr's Geburtsvisitenkarte zurück
Am 29.11.2005 um 08.27 Uhr ist Yves Colin Altherr geboren!
Gewicht: 2760g, Grösse: 44cm
Erstes Foto von Yves Colin

Today !

30 Years Ago !



1976 : The Hofstadter Spectrum !

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3. Magnetic Oscillations
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History

1. *Early Times: Experiments*
   (a) Superconductivity (Kamerlingh–Onnes 1911)
   (b) Magnetic Oscillation:
   Shubnikov–De Haas (1930)
   De Haas–Van Alphen (1930)

2. *Early Times: Theory*
   (a) Bloch theory (1928)
   (b) Landau (1930), diamagnetism of metals
   (c) Peierls (1933), effective band Hamiltonians

3. *Semiclassical Approach 50–65*:
   (a) Onsager (1952) and magnetic oscillations
   (b) The Lifshits–Kosevich formula (1954)
   (c) Harper 1955
   (d) The Russian School, Landau, Zeldovitch, Azbell, (58–65)
   (e) Magnetic breakdown (Pippard 1964)

4. *Hofstadter's Spectrum 1976*:
   (a) Theoretical calculations (1960–65) ;
   (b) Hofstadter Ph.D. Thesis: numerical calculation of Harper's model
   (c) Wannier–Claro (1978–80)

5. *Rigorous Results 1980–1990*:
   (a) Gap labeling Theorem (1981)
   (b) Metal-Insulator transition (1979–95)
   (c) Semiclassical Analysis *(Helffer–Sjöstrand, J. B.–Rammal)*
   (d) Transport

6. *Modern Experiments 1980–1990*:
   (a) Sharvin & Sharvin
   (b) The Quantum Hall Effect
   (c) Grenoble's experiments

7. *Today*: the amazing graphene

Low Magnetic Fields

- Free Hamiltonian $H = P^2/2m_*$

  $P = (P_1, P_2, P_3) =$ momentum. $m_* =$ mass

- With B a magnetic field $P \to P - qA$

  $q =$ charge of carriers, $A =$ *vector potential*

$$\partial_1 A_2 - \partial_2 A_1 = B$$

$$\partial_2 A_3 - \partial_3 A_2 = \partial_3 A_1 - \partial_1 A_3 = 0$$

- Quasi-momentum $K = (P - qA)/\hbar$

$$[K_1, K_2] = -\imath \frac{qB}{\hbar}, \qquad [K_3, K_1] = 0 = [K_3, K_2]$$

- $qB/\hbar$ is an *effective Planck constant*. Then

$$H = \frac{\hbar^2}{2m_*}(K_1^2 + K_2^2 + K_3^2) = H_B + \frac{\hbar^2}{2m_*} K_3^2$$

H_B is the *Landau* Hamiltonian.

- Energy spectrum of H_B: eigenvalues

$$E_n = \hbar\omega_c(n+\frac{1}{2}) \qquad n \in \mathbb{N} \qquad \omega_c = \frac{qB}{m_*}$$

with multiplicity $qB/\hbar$ per unit area.

THE MOTION IS BIDIMENSIONAL.

With a periodic potential V *(Bloch electrons)*

$$H = H_B + \hbar^2 K_3^2/2m_* + V$$

At $B = 0$ band spectrum: $E_j(k)$ ($k \in \mathbb{T}^3 =$ *quasi-momentum*)

Fourier: $E_j(k) = \sum_{m\in\mathbb{Z}^3} E_{j,m} e^{\imath k\cdot m}$

Peierls ('33): *substitute* K to $k \Rightarrow$
Effective band Hamiltonian

$$H_{Peierls} = \sum_{m\in\mathbb{Z}^3} E_{j,m} \; e^{\imath K\cdot m}$$

This is the lowest order term of a semiclassical expansion for H near the energies of the band E_j.

(J.B., Helffer–Sjöstrand, 1980's)

Magnetic Oscillations

Equations of motion

$$\frac{dK}{dt} = \frac{\imath}{\hbar}\,[H_{Peierls}, K] \quad \Rightarrow \quad \frac{dK_3}{dt} = 0$$

In the Peierls approximation this gives

$$\frac{dk_1}{dt} = -\frac{qB}{\hbar^2}\,\frac{\partial E_j}{\partial k_2} \qquad\qquad \frac{dk_2}{dt} = \frac{qB}{\hbar^2}\,\frac{\partial E_j}{\partial k_1}$$

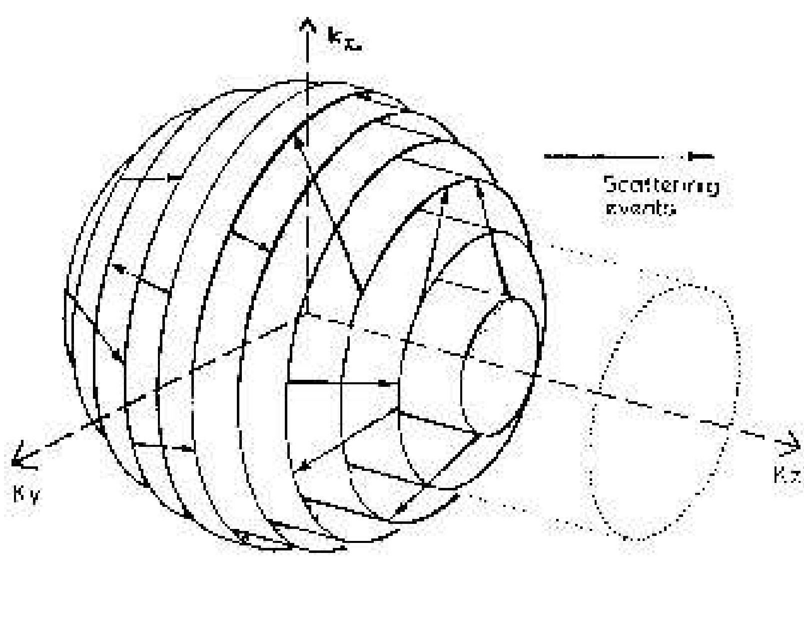
Thus $E(k)$ is conserved, the motion is perpendicular to the B-axis. In solids only the electrons with energy
$E_F + O(k_B T)$ (E_F= Fermi energy, T= Temperature)
participate to the current. Thus motion is confined on the *Fermi surface* $E_j(k) = E_F$.

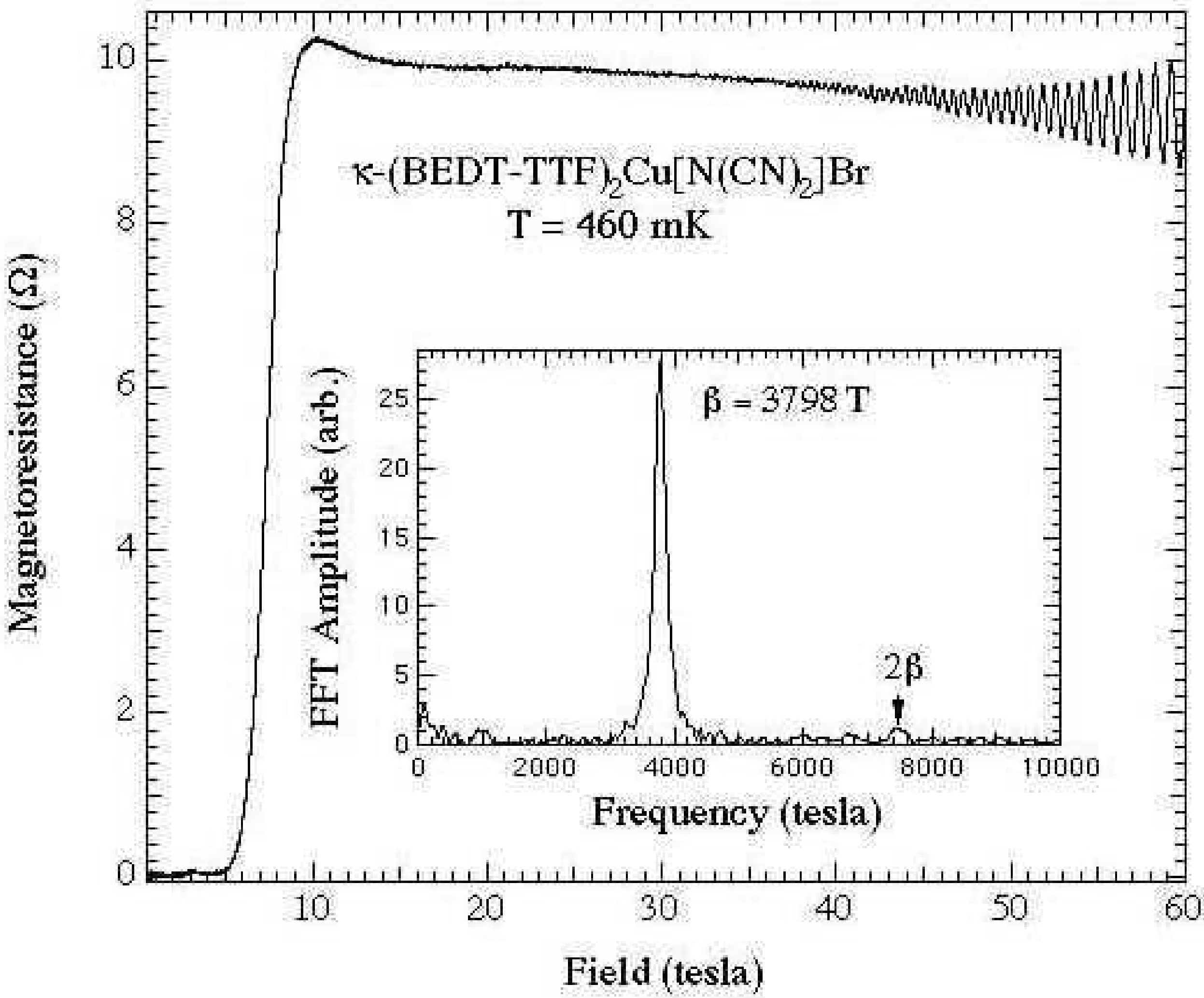
Bohr–Sommerfeld quantization formula selects the quantized orbits (ν is the *Maslov* index)

$$\oint_{\mathrm{orb}} k_1 dk_2 = -2\pi \frac{qB}{\hbar}\,(n+\nu)\,, \qquad n \in \mathbb{Z}$$

- The quantization conditions select cylinders.
- As $B \uparrow$ the radius of these cylinders $\uparrow$ until one of them, with index n, gets out of the Fermi surface.
- Then its area equals the maximum $A_{\max}$ of a section of the Fermi surface perpendicular to B.
- As B continues to increase the cylinder with index $n-1$ dominates leading to oscillation in the *free energy* with period

$$\Delta\left(\frac{1}{B}\right) = \frac{2\pi q}{hA_{\max}}$$





Resistance oscillations (Shubnikov–de Haas)

Inset: Fourier analysis of signal as a function of $1/B$

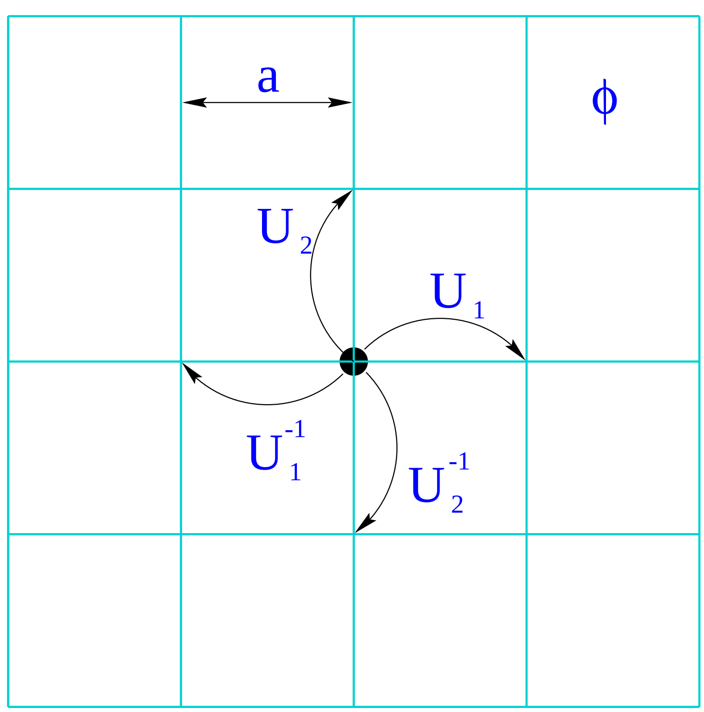
Algebraic Approach

The Peierls operators $e^{\imath K_1} = U_1$ and $e^{\imath K_2} = U_2$ are called *magnetic translations* and satisfy

$$U_1 U_2 = e^{2\imath\pi\alpha} U_2 U_1 \,, \qquad \alpha = \frac{\phi}{\phi_0} = \frac{Ba^2}{h/e} \,.$$

The simplest band model is the *Harper Hamiltonian*

$$H_H = U_1 + U_1^{-1} + U_2 + U_2^{-1} \,.$$



a = lattice spacing

ϕ = flux through unit cell

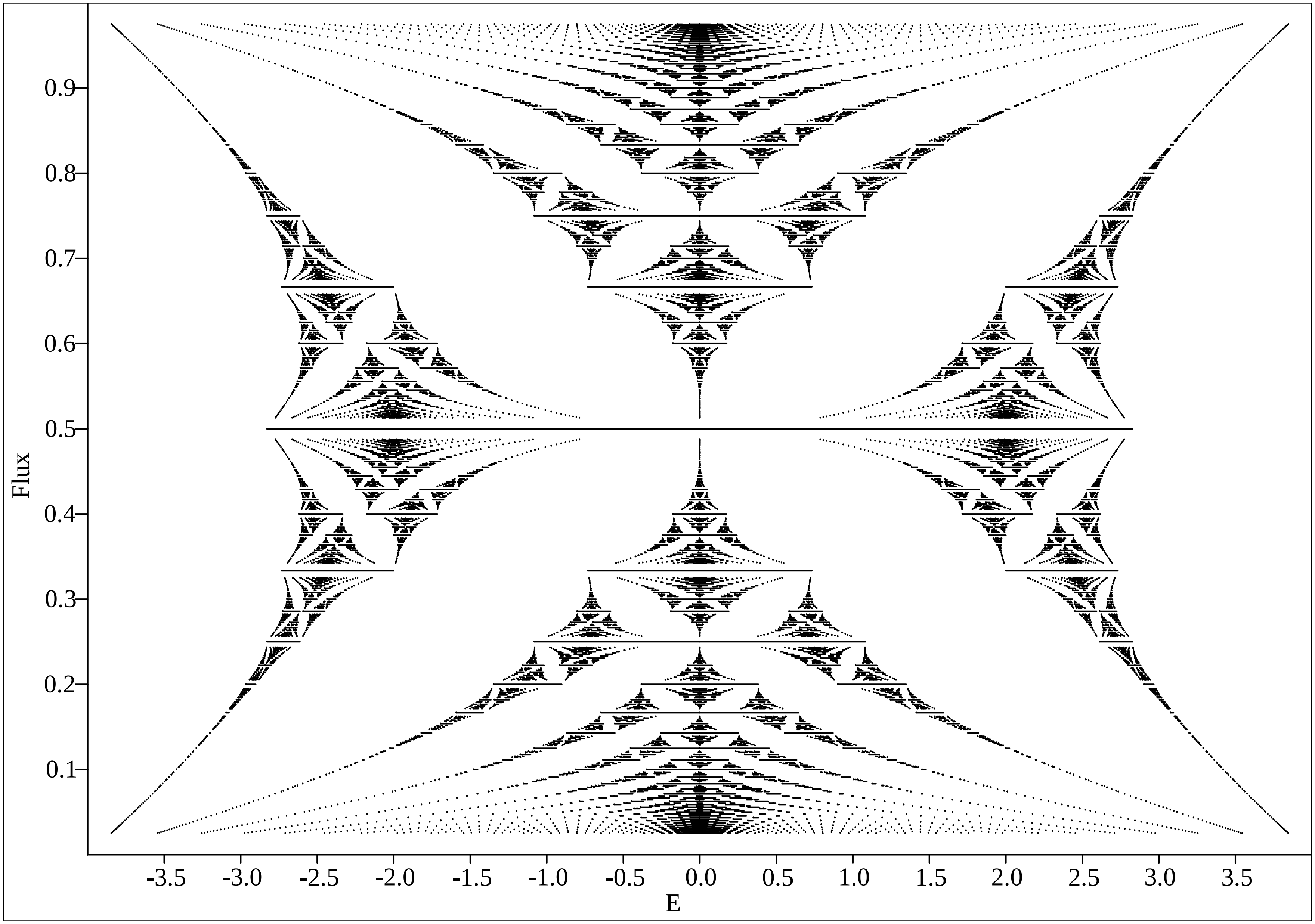
For $\alpha = p/q \in \mathbb{Q}$ a faithful representation of $U_1,\ U_2$ is given by

$$U_i = e^{\imath k_i}\, u_i\,, \qquad u_1 u_2 = e^{2\imath\pi p/q} u_2 u_1\,, \qquad u_i^q = \mathbf{1}$$

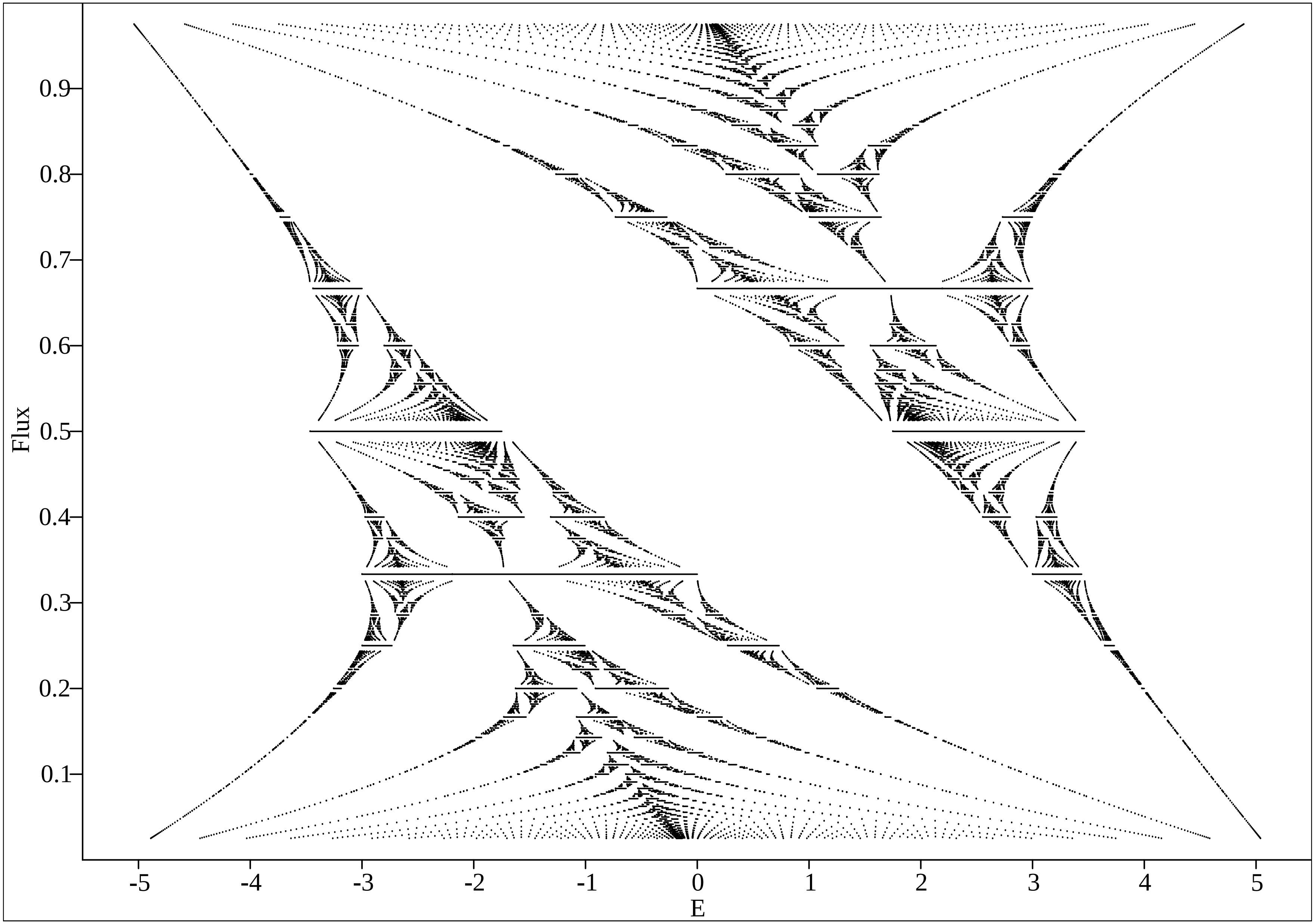
$$u_1 = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{bmatrix}$$

$$u_2 = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & e^{2\imath\pi p/q} & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 0 & \cdots & e^{2\imath\pi(p-1)p/q} \end{bmatrix}$$

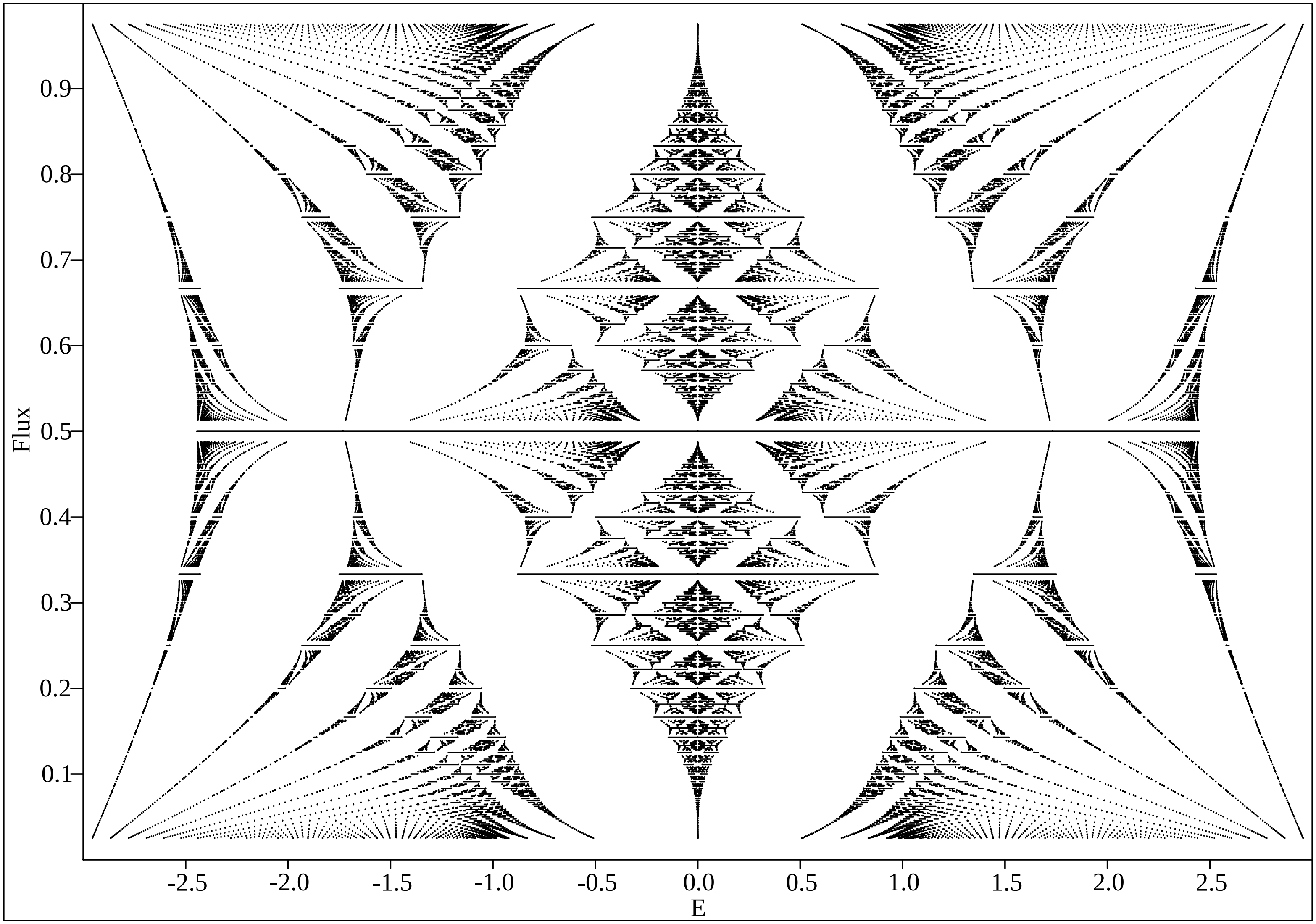
Then any Peierls Hamiltonian becomes a function $k \in \mathbb{T}^2 \mapsto H(k) \in M_{q\times q}(\mathbb{C})$, easy to diagonalize on a computer.



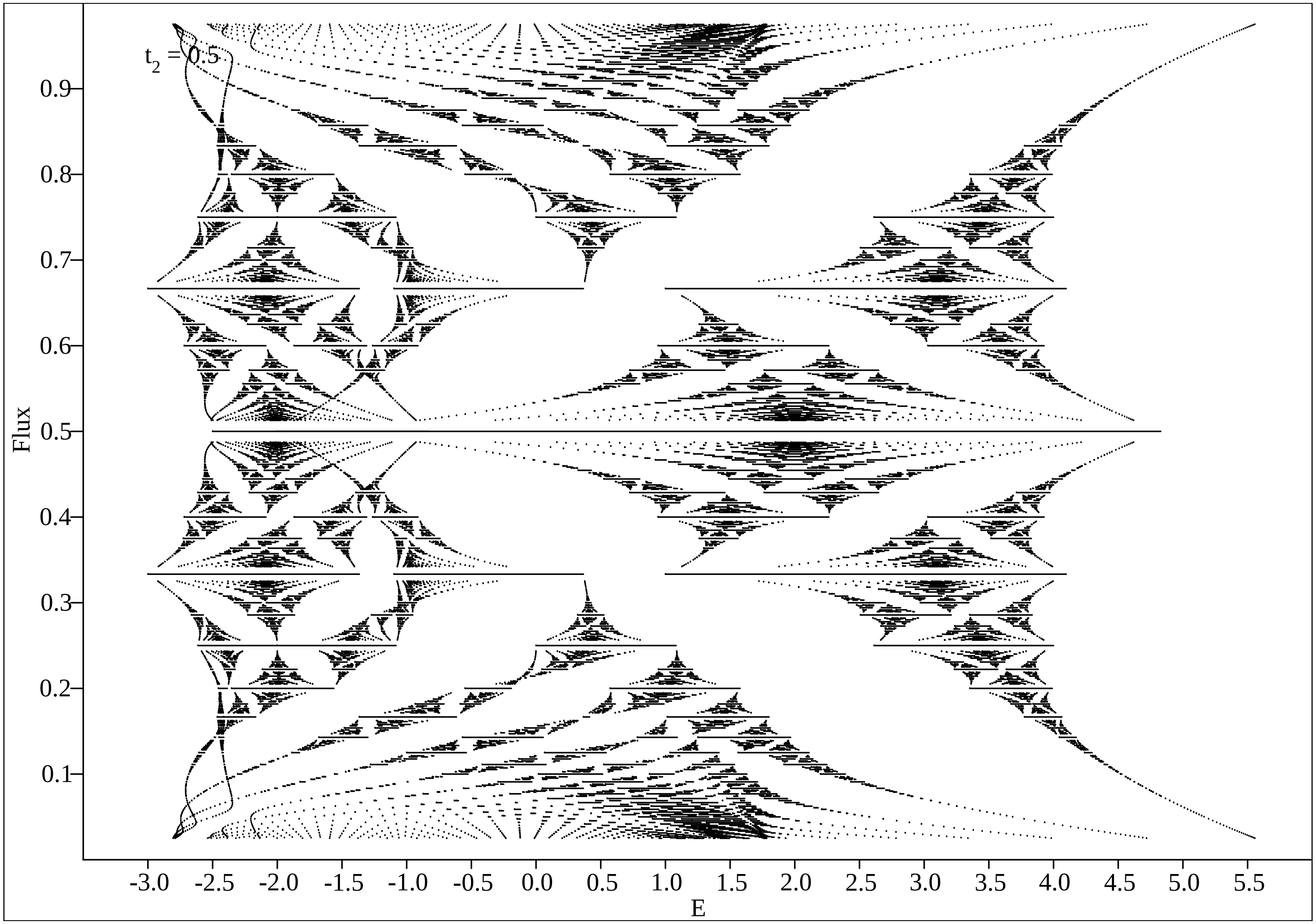
Harper $H = U_1 + U_1^{-1} + U_2 + U_2^{-1}$



Triangle $H = U_1 + U_1^{-1} + U_2 + U_2^{-1} + U_3 + U_3^{-1}$ with $U_1 U_2 U_3 = \imath$



$$\text{Honeycomb } H = \begin{bmatrix} 0 & U_1 + U_2 + U_3 \\ U_1^{-1} + U_2^{-1} + U_3^{-1} & 0 \end{bmatrix} \text{ with } U_1 U_2 U_3 = \mathbf{1}$$



Square lattice with 2nd n.n. $H = U_1 + U_2 + \frac{1}{2}(U_1^2 + U_2^2) + h.c.$

Theorem 1 *Let $H = H^*$ be a polynomial in U_1, U_2 then*

(i) The gap boundaries are Lipschitz continuous functions of the flux where gaps do not close.
(Bellissard '94)

(ii) At gap closure, if not Lipshitz, the gap edges are Hölder continuous of exponent at most $1/2$.
(Haagerup–Rørdam '95)

(iii) The right and left derivatives of a gap edge are explicitly computable at each rational flux and are unequal.
(Bellissard–Rammal '90)

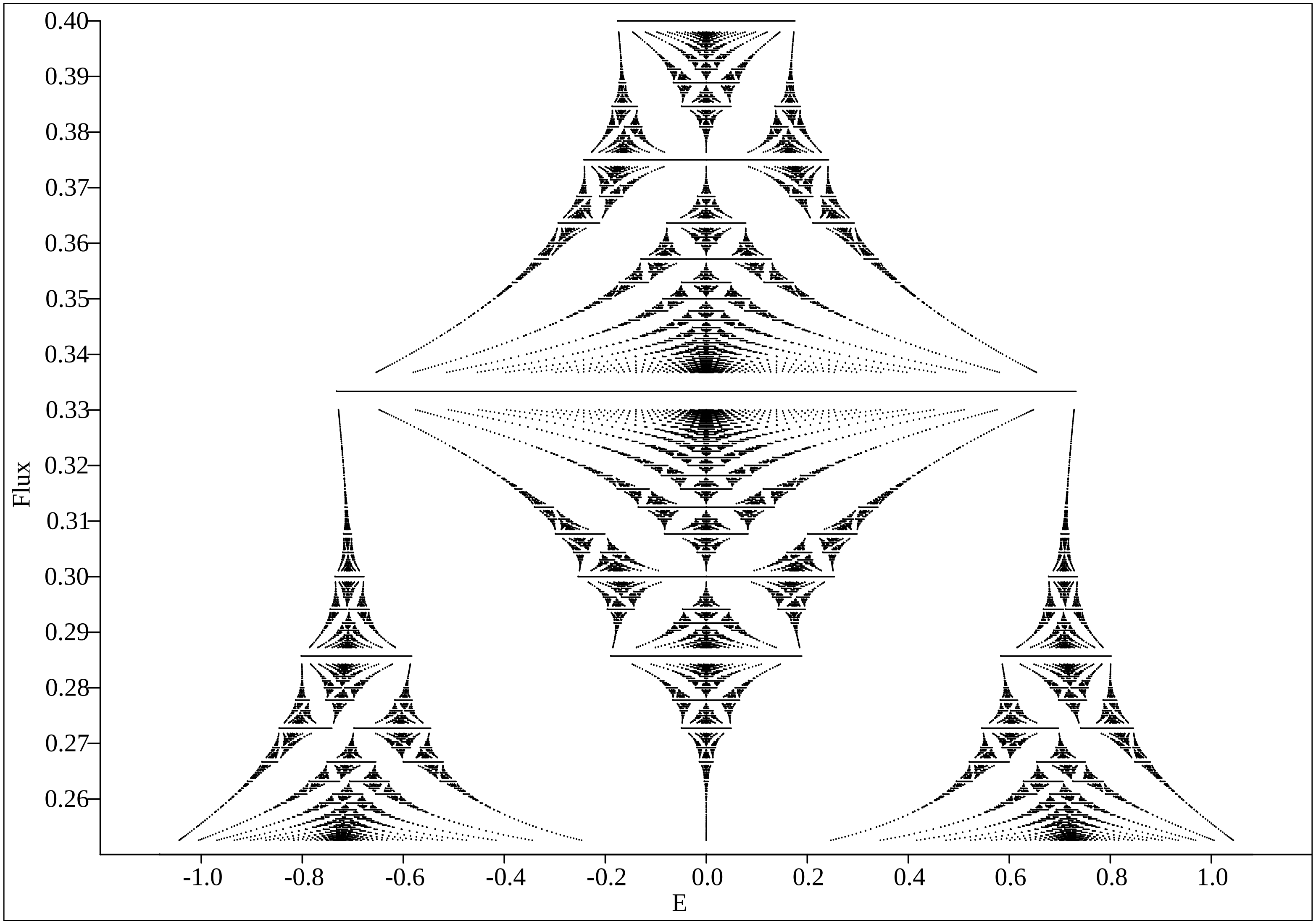
(iv) Near each gap edge and near flux $\alpha = p/q \in \mathbb{Q}$, the energy spectrum admits an asymptotic expansion of the form (Landau sublevels)
(Bellissard–Rammal '90)

$$E_n = e_0 + e_a \left(\alpha - \frac{p}{q}\right) + e_b \left|\alpha - \frac{p}{q}\right| \left(n + \frac{1}{2}\right) + O(\left(\alpha - \frac{p}{q}\right)^2)$$

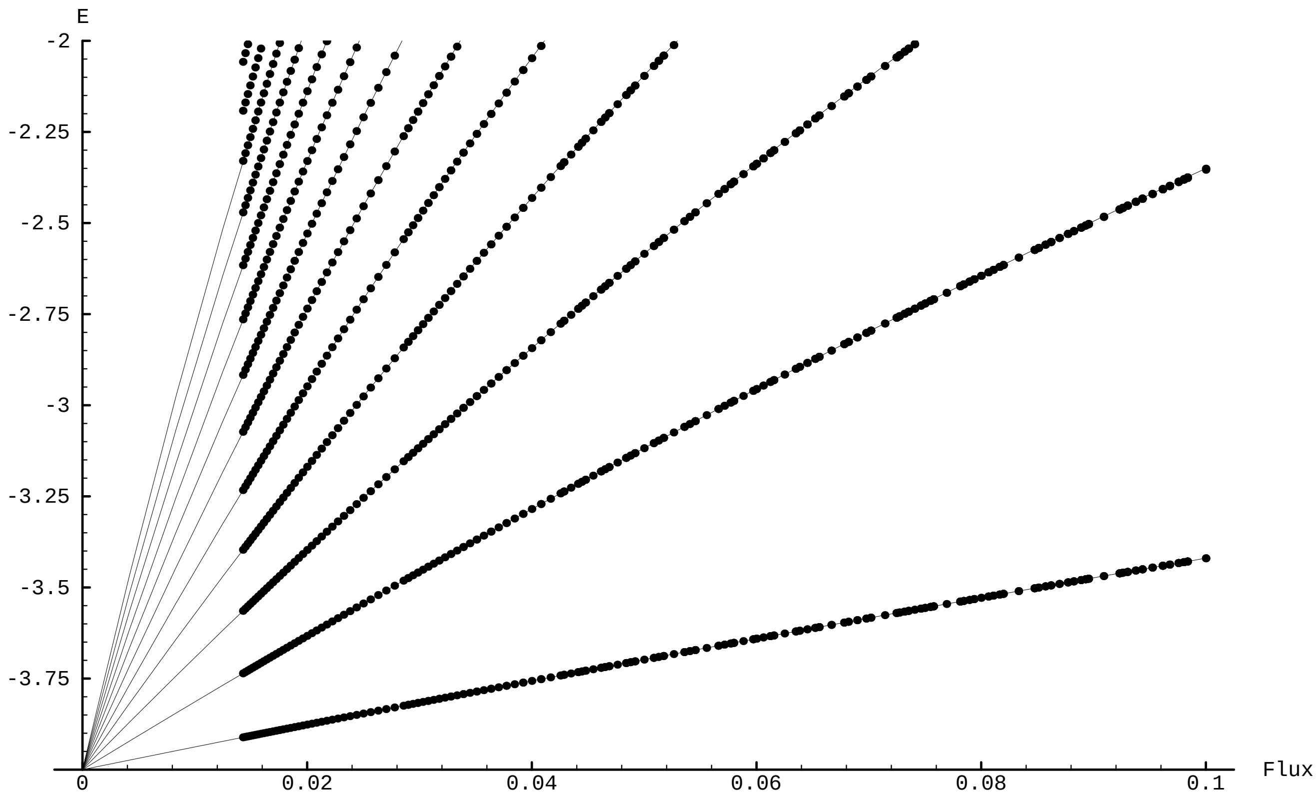
where e_a, e_b are explicitely computable in terms of H.

(v) Near a closing gap with Hölder exponent $1/2$ at rational flux $\alpha = p/q$ the energy spectrum admits an asymptotic expansion of the form (Dirac–Landau sublevels)
(Bellissard–Rammal '90)

$$E_{\pm n} = e_0 \pm e_\pm \left|\alpha - \frac{p}{q}\right|^{1/2} |n|^{1/2} + O(\left|\alpha - \frac{p}{q}\right|^{3/2})$$

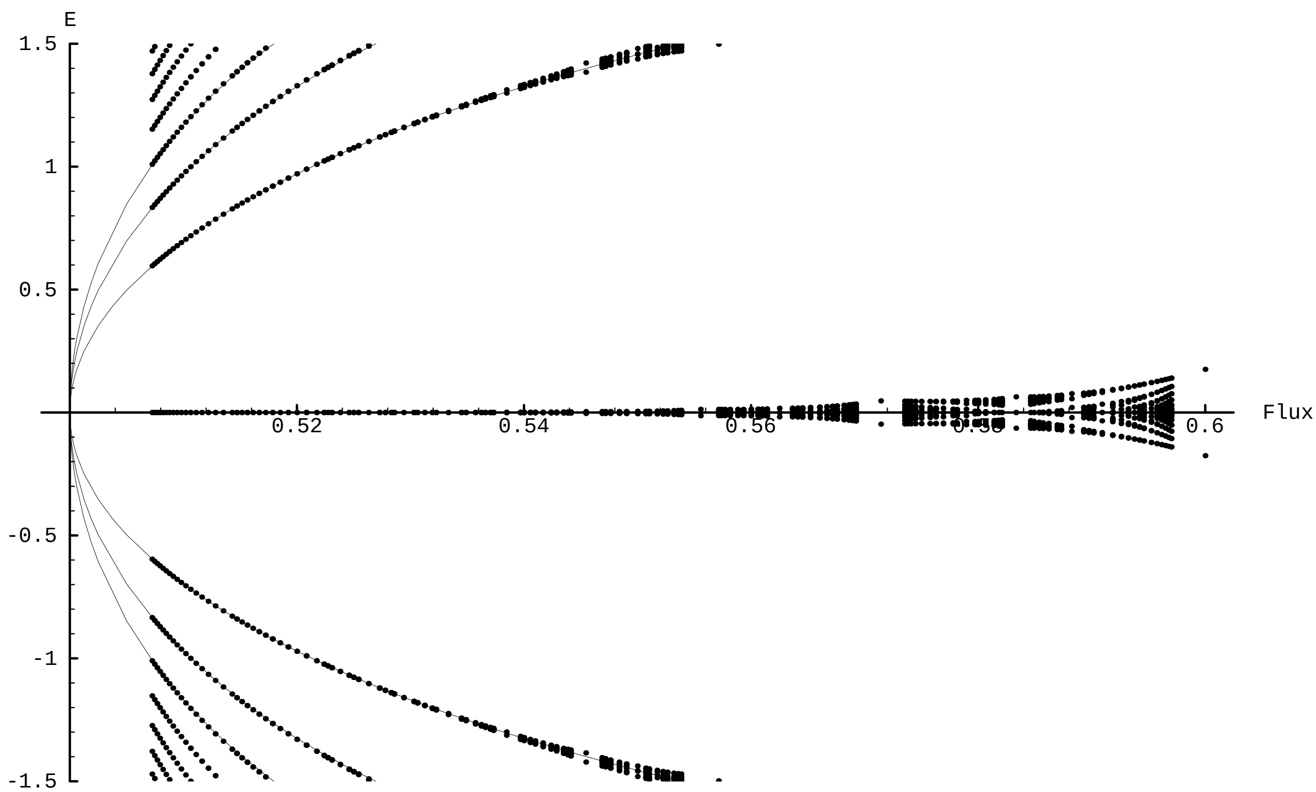


Discontinuity of the gap edge derivatives near $\alpha = 1/3$ in Harper's model



Landau sublevels for Harper's model near $\alpha = 0$

– **Lines:** *semiclassical formula.* **Dots:** *exact numerical diagonalization* –



Dirac–Landau sublevels for Harper's model near $\alpha = 1/2$

– **Lines:** *semiclassical formula.* **Dots:** *exact numerical diagonalization* –

Application to Graphene

C. BERGER *et al.*, *Electronic Confinement and Coherence in Patterned Epitaxial Graphene*, *Science*, **312** (26 May 2006), 1191–1196 .

Carbon monolayers in hexagonal lattice phase grown on surface of a substrate, mostly SiC semiconductor, are called *graphene*.

Electrons in graphene behave like *relativistic massless fermions of spin* 1/2 *(Majorana fermions)*, with velocity $v \approx 10^6 m/s$.

Electrons experience a very low level of dissipation. The coherent length is $1.1\mu m$ at $4K$ and more than $100nm$ at room temperature ! In particular in a small ribbon the interference effects dominate the conductivity.

Thanks to such a low dissipation, experiments show a lot of details when put in a uniform in magnetic field, including fractal behavior reminiscent to Hofstadter's spectrum.

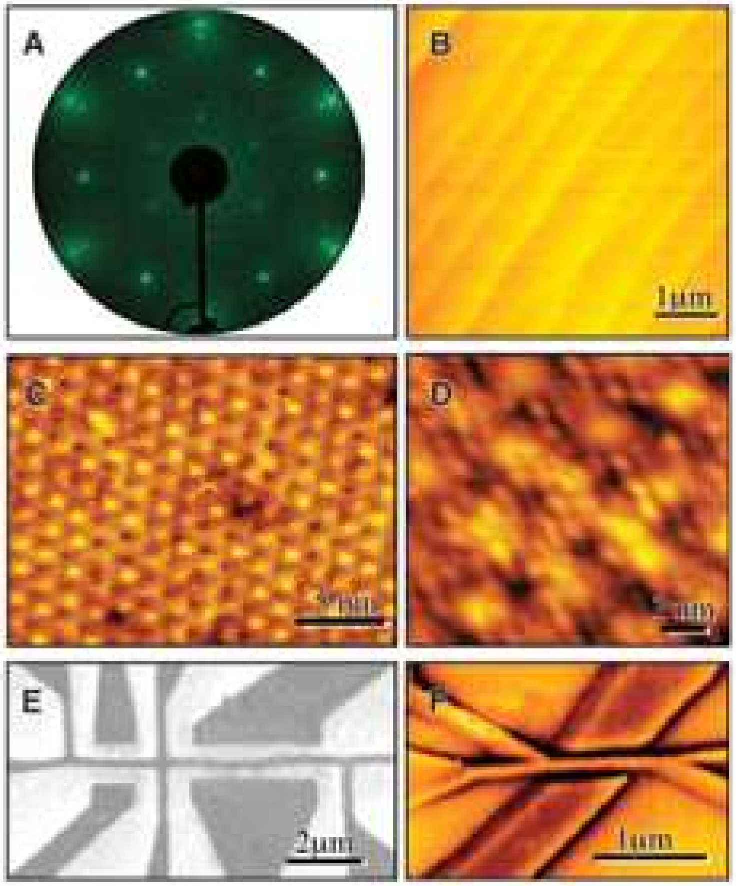


Fig. 1. Production and characterization of EG. **(A)** LEED pattern (71 eV) of three monolayers of EG on 4H-SiC(000$\bar{1}$) (C-terminated face). The outermost hexagon (spots aligned on the vertical) is graphene 1×1 diffraction. Bright sixfold spots aligned on the horizontal are SiC 1×1. The smallest hexagon is the result of a $\sqrt{3} \times \sqrt{3}$ reconstruction of the interfacial layer, as are the spots lying just inside the graphene pattern. Graphene thickness is determined via Auger spectroscopy (attenuation of Si peaks). **(B)** AFM image of graphitized 4H-SiC, showing extended terraces. STM studies indicate that the graphite is continuous over the steps (*1*). **(C)** STM image of one monolayer of EG on SiC(0001). Tunneling conditions (tip bias –0.8 V, current 100 pA) preferentially image structure beneath the graphene layer. Two interface corrugations are apparent, with periods 6×6 (1.8-nm triangular superlattice) and $\sqrt{3} \times \sqrt{3}$ (smaller spots with 0.54-nm spacing) relative to the SiC surface unit cell. **(D)** STM image of interface reconstruction beneath one monolayer of graphene on SiC(0001) obtained after lithography. General features are as seen in (C). **(E)** SEM of patterned EG. Dark regions are the EG (still coated with electron-beam resist). **(F)** EFM of another patterned EG sample, showing a horizontal ribbon (bright contrast) with tapered voltage contacts left and right, which is flanked by diagonally oriented side gates above and below the ribbon. Contrast is obtained through electrostatic forces between the probe and the graphene structure to which potentials are applied, thus allowing functioning devices to be measured.

Science, **312** (26 May 2006), 1191–1196

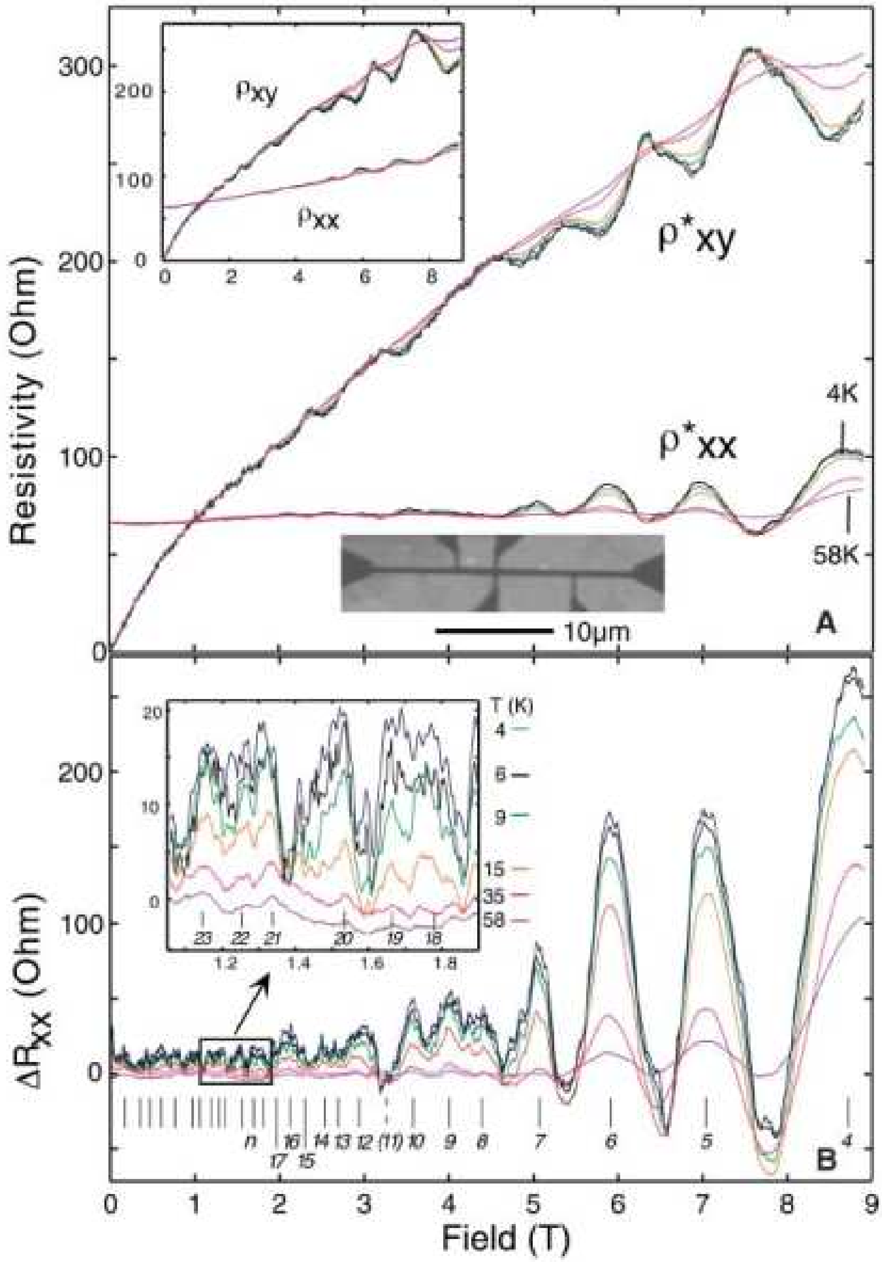


Fig. 2. Magnetotransport of a lithographically patterned graphene Hall bar (SEM micrograph, lower inset) measured at temperatures $T = 4$, 6, 9, 15, 35, and 58 K, and magnetic fields $-9\ \mathrm{T} \leq B \leq 9\ \mathrm{T}$. (**A**) Components of the resistivity tensor ρ are shown (inset; $\rho_{xx} = R_{xx}W^*/L$, $\rho_{xy} = R_{xy}$). ρ^* is derived from ρ: $(\rho^*)^{-1} = \rho^{-1} - (\rho^0)^{-1}$, where $\rho^0_{xx} = 1125$ ohms and $\rho^0_{xy} = 0$. Hence, the slight slope in ρ_{xx} appears to be caused by a conducting layer ρ^0 on top of the graphene layer. The graphene mobility is $\mu^* = 2.7\ \mathrm{m^2/V{\cdot}s}$. (**B**) ΔR_{xx} obtained from the measured R_{xx} by subtracting a smooth background. Peak positions are indicated (peak 11 is missing). The peak character changes near $B = 4.5$ T. The peak amplitudes are essentially constant below 2 T and increase above 2 T. Inset: Detail of the oscillations near $B = 1$ T. The amplitude of the universal conductance fluctuations (noise-like structures) increases with decreasing temperature.

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Coherent Transport

Coherent transport is the one described by the Hamiltonian dynamics without dissipative term. Dissipation occurs only at positive temperature and blurs the effect of coherent transport. Coherence can be recovered from the low temperature behavior of quantities like the conductivity.

Example: rectangular symmetry Hamiltonian

$$H = t_x(U_1 + U_1^{-1}) + t_y(U_2 + U_2^{-1}) \qquad t_x < t_y$$

The conductivity at zero magnetic field ($\alpha = 0$) is anisotropic so that $\sigma_{xx}/\sigma_{yy} \simeq (t_x/ty)^2$. With magnetic field however at finite temperature and low dissipation (through a relaxation time τ)
(Barelli, Bellissard, Claro '99)

$$\frac{\sigma_{xx}}{\sigma_{yy}} \restriction_{\mathrm{B}} \simeq C \left(\frac{\hbar}{\tau}\right)^2 \frac{\sigma_{xx}}{\sigma_{yy}} \restriction_0 \quad \downarrow 0 \quad \text{as} \quad T \downarrow 0$$

At zero temperature the transport is defined through *fractal exponents*.

If $\mathcal{T}$ denotes the *trace per unit volume* defined by

$$\mathcal{T}\left(U_1^{m_1}U_2^{m_2}\right) = \delta_{m_1,0}\,\delta_{m_2,0}$$

then the density of state for the Hamiltonian H is defined by

$$\int_{\mathbb{R}} \mathcal{N}(dE) f(E) = \mathcal{T}\left(f(H)\right)$$

The *spectral exponents* are defined by

$$\int_{E_\epsilon}^{E+\epsilon} \mathcal{N}(dE) \overset{\epsilon\downarrow 0}{\sim} \epsilon^{\delta(E)}$$

or by

$$\int_{\mathbb{R}} \mathcal{N}(dE) \left(\int_{E_\epsilon}^{E+\epsilon} \mathcal{N}(dE')\right)^{q-1} \overset{\epsilon\downarrow 0}{\sim} \epsilon^{(q-1)D_{\mathcal{N}}(q)}$$

Let now ∂_x, ∂_y be the derivations defined by

$$\partial_i U_J = \imath \delta_{ij} \ U_j \qquad i,j \in \{1,2\} = \{x,y\}$$

Then the *diffusion exponents* in direction $i = x, y$ are defined by

$$\int_{-T}^{T} \frac{dt}{T} \mathcal{T}\left(\left| e^{-\imath t H} \partial_i e^{+\imath t H} \right|^q \right) \stackrel{T \uparrow 0}{\sim} T^{q\beta_i(q)}$$

Then the following result holds
(Bellissard, Guarneri, Schulz-Baldes '02)

Theorem 2 *Let $H = H^*$ be a polynomial in U_1, U_2. If the flux α is a Roth number*†*, then*

$$\beta_i(q) \geq D_{\mathcal{N}}(1-q) \qquad \forall\ 0 < q < 1$$

†namely for all $\eta > 0$ $\exists c > 0$ $s.t.$ $|\alpha - m/n| \geq c/n^{2+\eta}$ for all $m/n \in \mathbb{Q}$

Computing the Exponents

How to compute the exponents ?

The spectral exponents are given by the long time behavior of

$$\mathcal{T}\left(A\, e^{\imath t H}\right) \overset{t\uparrow\infty}{\sim} \frac{1}{t^{1+\delta(E)}}$$

whenever A is localized near the energy E of H.

Malgrange ('74): For H a polynomial in real variables, using the Gauss–Manin connection

$$\int_{\mathbb{R}^n} d^n x\, \chi(x)\, e^{\imath t H(x)} \overset{t\uparrow\infty}{\sim} \sum_{\eta; j \leq n} c_{\eta,j}\, \frac{1}{t^{1+\eta}} \ln^j t$$

with χ localized near a critical point of H.

The η's are computed through the eigenvalues of a *monodromy* matrix for the Gauss–Manin connection: $\eta \in \mathbb{Q}$

Using the language of Noncommutative Geometry, it seems that there is an analog of the Gauss–Manin connection for Hamiltonians representing Bloch electrons in a magnetic field.

In particular there should be a long time asymptotic expansion $\mathcal{T}\left(A\, e^{\imath t H}\right)$ where the exponents η are likely to belong to the set of *Gap Labels*.

Can one develop such a theory ?