Effective Hamiltonians for perturbed periodic quantum systems and their geometry

Stefan Teufel, Universität Tübingen

Workshop on *Macroscopic Limits of Quantum Systems*

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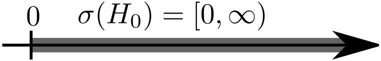
based on joint works with

- **Silvia Freund,**
- **Domenico Monaco, Gianluca Panati, Adriano Pisante**,
- **Nicolai Rothe**

1. Introduction: Band spectra

- $H_0 = -\Delta_x$ on $L^2(\mathbb{R}^2_x)$



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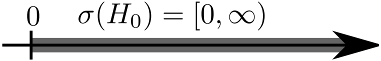
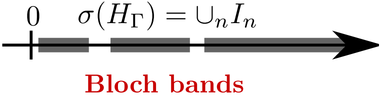


- $H_\Gamma = -\Delta_x + V_\Gamma(x)$



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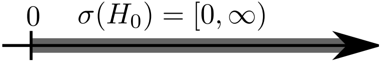

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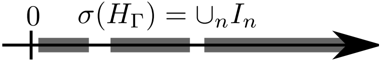
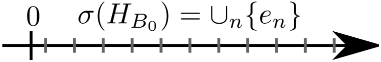


Bloch bands

with $V_\Gamma(x+\gamma) = V_\Gamma(x)$ for all $x \in \mathbb{R}^2$, $\gamma \in \Gamma \sim \mathbb{Z}^2$

- $H_{B_0} = (-\mathrm{i}\nabla_x + A_0(x))^2$

with $\mathrm{d}A_0 = B_0 = \mathrm{const.}$



Landau levels

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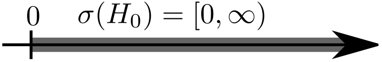

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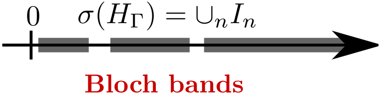

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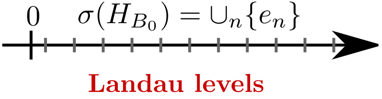
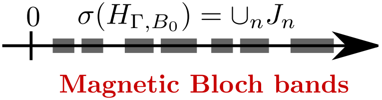


- $H_{\Gamma,B_0} = (-\mathrm{i}\nabla_x + A_0(x))^2 + V_\Gamma(x)$



with Γ and B_0 commensurable

1. Introduction: Peierls substitution

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$$H_0 \sim k^2 \, .$$

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And H_Γ is thus unitarily equivalent to an orthogonal sum of multiplication operators by functions E_n on $P_n\mathcal{H}$,

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$$H_\Gamma \sim \bigoplus_{n=1}^{\infty} E_n(k) \qquad \text{on} \qquad \bigoplus_{n=1}^{\infty} P_n\mathcal{H} \;\cong\; \bigoplus_{n=1}^{\infty} L^2(\mathbb{T}^2)\,.$$

- We have exactly the same structure for H_{Γ,B_0} up to one caveat:

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  There is no natural isomorphism between $P_n\mathcal{H}$ and $L^2(\mathbb{T}^2)$ anymore.

  Instead $P_n\mathcal{H}$ is naturally isomorphic to a space of L^2-sections $L^2(\Xi_n)$ of a certain vector bundle Ξ_n over the torus $\mathbb{T}^2$.

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For $\varepsilon > 0$ let

$$W^\varepsilon(x) := W(\varepsilon x) \qquad \text{and} \qquad A^\varepsilon(x) = A(\varepsilon x)$$

be the scaled potentials. For $\varepsilon \ll 1$ they are slowly varying on the scale of the lattice and give rise to small fields.

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- Fourier transformation turns $\widetilde{H}_0 = \big(-\mathrm{i}\nabla_x + A^\varepsilon(x)\big)^2 + W^\varepsilon(x)$ into the pseudo-differential operator

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- Peierls substitution for Bloch bands:
The restriction of $\widetilde{H}_\Gamma = \big(- \mathrm{i}\nabla_x + A^\varepsilon(x) \big)^2 + V_\Gamma(x) + W^\varepsilon(x)$ to one of the subspaces $\mathrm{ran}\widetilde{P}_n \cong L^2(\mathbb{T}^2)$ under Bloch-Floquet transformation is close to
$$\widetilde{H}_\Gamma \big|_{\mathrm{ran}\widetilde{P}_n \cong L^2(\mathbb{T}^2)} \overset{\varepsilon \ll 1}{\sim} E_n\big(k + A^\varepsilon(\mathrm{i}\nabla_k) \big) + W^\varepsilon(\mathrm{i}\nabla_k) \, .$$

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- Peierls substitution for magnetic Bloch bands:

  $\widetilde{H}_\Gamma = \big(-\mathrm{i}\nabla_x + A_0(x) + A^\varepsilon(x) \big)^2 + V_\Gamma(x) + W^\varepsilon(x)$ restricted to one of the subspaces $\mathrm{ran}\widetilde{P}_n \cong L^2(\Xi_n)$ under magnetic Bloch-Floquet transformation should in some sense be close to

$$\widetilde{H}_\Gamma \big\vert_{\mathrm{ran}\widetilde{P}_n \cong L^2(\Xi_n)} \overset{\varepsilon \ll 1}{\sim} E_n\big(k + A^\varepsilon(\mathrm{i}\nabla_k) \big) + W^\varepsilon(\mathrm{i}\nabla_k) \, .$$

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- Bellisard '88, '89
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- Freund, T. '13: unitary equivalence for magnetic Bloch bands, but A bounded

2. Bloch bundles and Wannier functions

Gapped group of bands: Let $I \subset \mathbb{N}$ be a finite index set such that

$$\{E_n(k) \,|\, n \in I\} \subset \sigma(H(k))$$

is separated uniformly in k by a gap from the rest of the spectrum of $H(k)$. Typically $\{E_n(k) \,|\, n \in I\}$ are the bands below the Fermi energy.

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Put $P_I(k) = \sum_{n \in I} P_n(k)$ and $P_I := \int^{\oplus} P_I(k) \mathrm{d}k$, then $\mathrm{ran} P_I$ is an invariant subspace for $\widehat{H}_\Gamma$ and $\mathcal{F}^{-1} \mathrm{ran} P_I$ is an invariant subspace for H_Γ.

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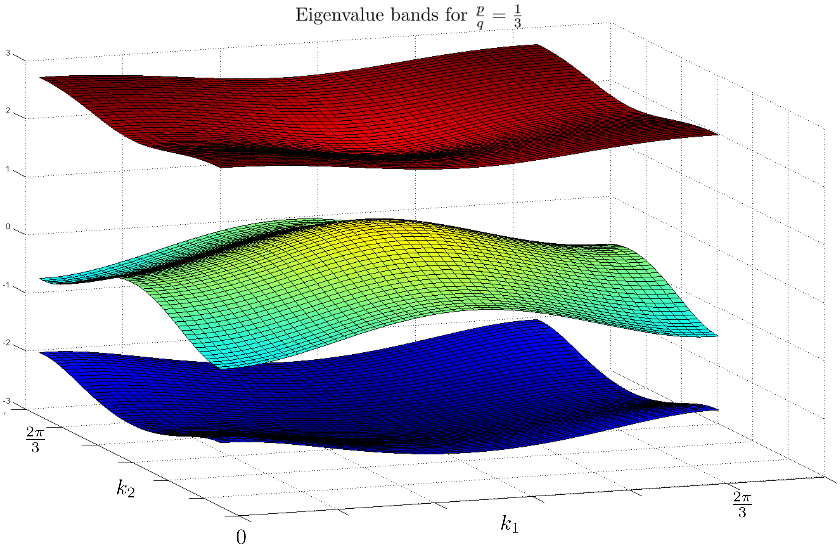

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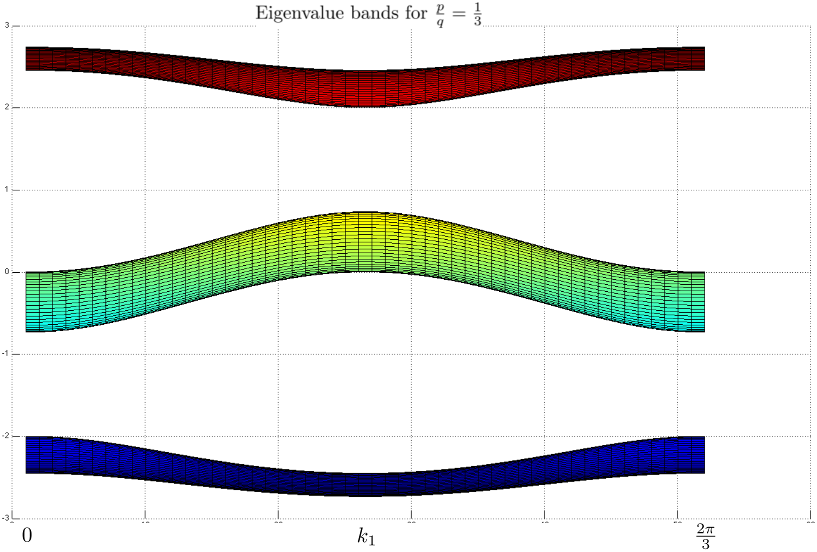

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Composite Wannier functions $(w_1, \ldots, w_m)$ for $\mathcal{F}^{-1} \mathrm{ran} P_I$ with $\mathrm{rank} P_I(k) \equiv m$ are functions in $L^2(\mathbb{R}^2)$ such that

$$\{T_\gamma w_j \mid \gamma \in \Gamma, j = 1, \ldots, m\}$$

is an orthonormal basis of $\mathcal{F}^{-1} \mathrm{ran} P_I$.

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The Bloch bundle Ξ_I associated to the group of bands $\{E_n(k) \,|\, n \in I\}$ is the rank-m vector bundle $\Xi_I \xrightarrow{\pi_I} \mathbb{T}^2$ given by

$$\Xi_I := \{(k, \varphi) \in \mathbb{R}^2 \times \mathcal{H}_{\mathrm{f}}) \,|\, P_I(k)\varphi = \varphi\}/\sim,$$

where

$$(k, \varphi) \sim (k', \varphi') \quad :\Leftrightarrow \quad k' - k \in \Gamma^* \text{ and } \varphi' = \tau(k' - k)\varphi \,.$$

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The range of P_I in $L^2(\mathbb{T}^2, \mathcal{H}_{\mathrm{f}})$ is thus naturally isomorphic to L^2-sections of the Bloch bundle Ξ_I,

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$$\Omega_I(k) = \mathrm{i}\, P_I(k)[\partial_1 P_I(k), \partial_2 P_I(k)]\,,$$

and the corresponding Chern number is

$$\theta_I = \frac{1}{2\pi}\int_{\mathbb{T}^2} \mathrm{tr}\,\Omega_I(k)\,\mathrm{d}k\,.$$

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The Bloch bundle is called trivializable, if it admits a global frame $(\varphi_1, \ldots, \varphi_m)$, that is a family of smooth functions $\varphi_j : \mathbb{R}^2 \to \mathcal{H}_\mathrm{f}$ that are τ-equivariant,

$$\varphi_j(k + \gamma^*) = \tau(\gamma^*)\varphi_j(k)\,,$$

and form an ONB of $\mathrm{ran} P_I(k)$ for all $k \in \mathbb{R}^2$.

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Such a global frame provides an isomorphism of the range of P_I with $L^2(\mathbb{T}^2, \mathbb{C}^m)$,

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Theorem (Panati '07) In dimensions $d = 2,3$ the Bloch bundle is trivializable if and only if its Chern number(s) vanish.

2. Bloch bundles and Wannier functions

Theorem (Monaco, Panati, Pisante, T. 16')

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$$\int_{\mathbb{R}^d} |x|^2 |w_j(x)|^2 \, \mathrm{d}x = \infty \qquad \text{for at least one } j \in \{1, \ldots, m\}\,.$$

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Composite Wannier functions $(w_1, \ldots, w_m)$ satisfying

$$\int_{\mathbb{R}^d} |x|^{2s} |w_j(x)|^2 \, \mathrm{d}x < \infty$$

for all $j = 1, \ldots, m$ and any $0 < s < 1$ always exist.

3. Peierls substitution for magnetic subbands

The Hofstadter model is the simplest example of a periodic system with magentic field. Its Hamiltonian H_{Hof} is just the discrete Laplacian with costant magnetic field on the square lattice.

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$$H_{B_0}(k) = \begin{pmatrix} 2\cos(k_2) & 1 & 0 & \cdots & \mathrm{e}^{\mathrm{i}qk_1} \\ 1 & 2\cos(k_2 + B_0) & 1 & \cdots & 0 \\ 0 & 1 & 2\cos(k_2 + 2B_0) & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & & & & 1 \\ \mathrm{e}^{-\mathrm{i}qk_1} & 0 & \cdots & 1 & 2\cos(k_2 + (q-1)B_0) \end{pmatrix} .$$

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Alternatively, the Hofstadter model can be obtained from Peierls substitution applied to the band function $E(k) = 2\cos(k_1) + 2\cos(k_2)$, i.e.

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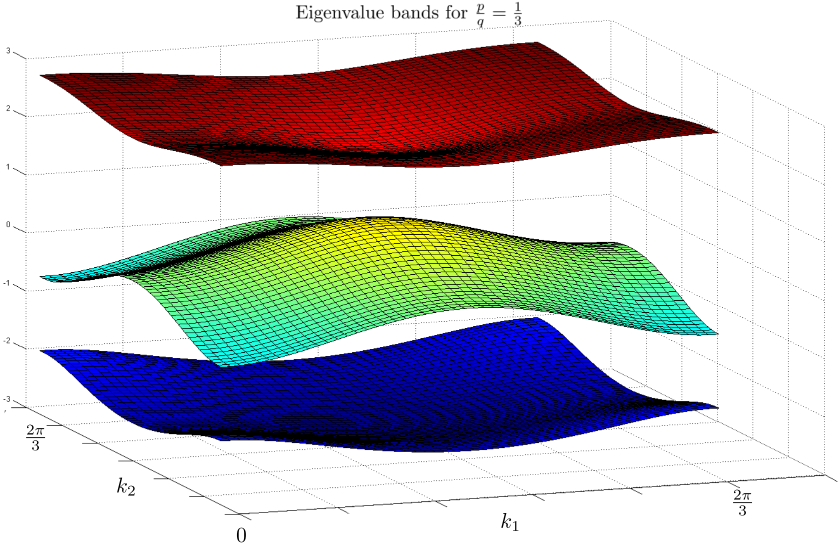
The Hofstadter Hamiltonian can thus also be regarded as the canonical effective Hamiltonian for a Bloch band perturbed by a constant magnetic field B_0 (see De Nittis, Panati '10).

3. Peierls substitution for magnetic subbands



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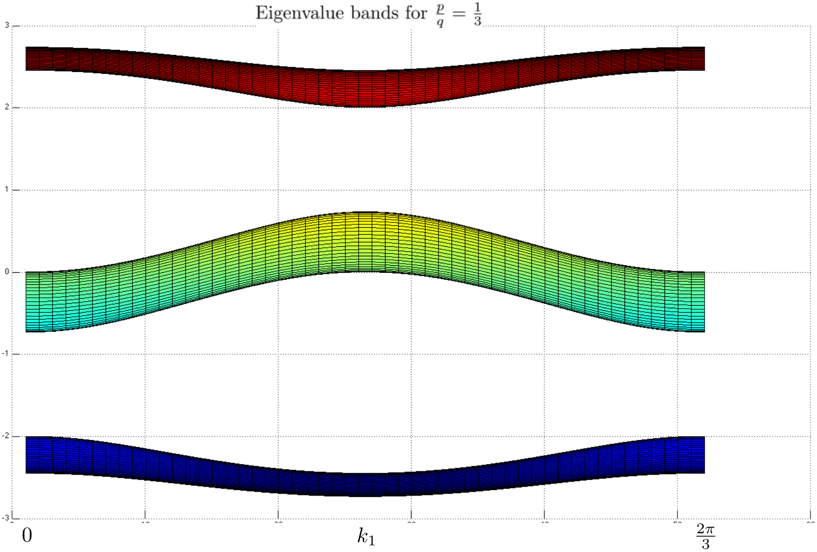

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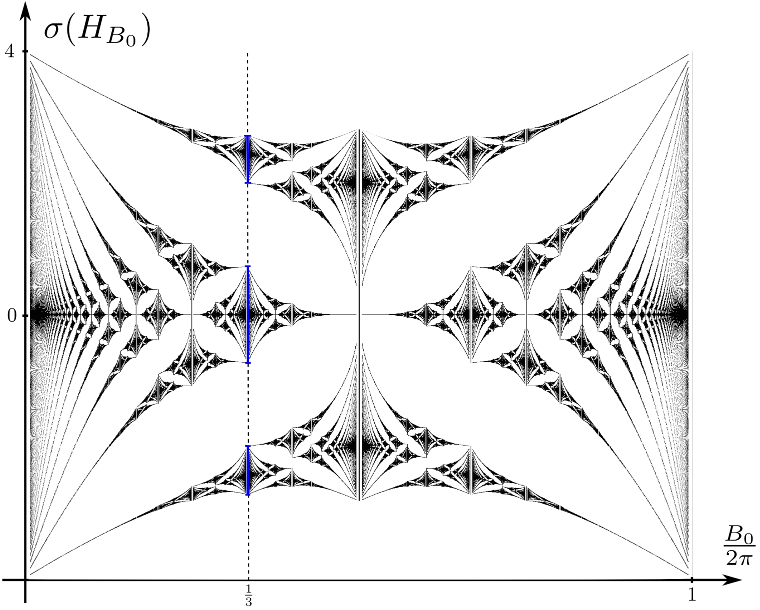

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While this is a beautiful mathematical result, it is not too relevant from the physics point of view.

Our aim is to prove "Peierls substitution", i.e. the stability of the block decomposition for rational values of B_0 under certain types of perturbations and to construct explicit *effective operators* that are unitarily equivalent to the blocks of the perturbed periodic operator.

3. Peierls substitution for magnetic subbands

One would like to understand the effect of additional (non-periodic) electric and magnetic potentials W and A that give rise to small electric and magnetic fields $E = -\nabla W$ and $B = \mathrm{curl} A$.

Let

$$W : \mathbb{R}^2 \to \mathbb{R} \qquad \text{and} \qquad A : \mathbb{R}^2 \to \mathbb{R}^2$$

be smooth functions that are bounded and have bounded derivatives of all orders.

For $\varepsilon > 0$ let

$$W^\varepsilon(x) := W(\varepsilon x) \qquad \text{and} \qquad A^\varepsilon(x) = A(\varepsilon x)$$

be the scaled potentials. For $\varepsilon \ll 1$ they are slowly varying on the scale of the lattice and give rise to small fields.

3. Peierls substitution for magnetic subbands

Theorem (Freund, T. '13)

Let $\{E_n(k) \,|\, n \in I\}$ be a gapped group of bands with projection P_I. Then there exist an orthogonal projection $\Pi_I^\varepsilon \in \mathcal{L}(L^2(\mathbb{T}^2; \mathcal{H}_{\mathrm{f}}))$ such that

$$\left\| [\widetilde{H}_\Gamma, \Pi_I^\varepsilon] \right\| = \mathcal{O}(\varepsilon^\infty) \,.$$

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$$\left\| [\widetilde{H}_\Gamma, \Pi_I^\varepsilon] \right\| = \mathcal{O}(\varepsilon^\infty)\,.$$

Moreover, Π_I^ε is close to a pseudodifferential operator $\mathrm{Op}(P_I^\varepsilon)$,

$$\|\Pi_I^\varepsilon - \mathrm{Op}(P_I^\varepsilon)\| = \mathcal{O}(\varepsilon^\infty)\,, \qquad (*)$$

with principal symbol equal to $P_I(k - A(r))$.

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If $\|W\|_\infty$ is small enough, the spectral gaps remain open for $\varepsilon \in (0, \varepsilon_0]$ and $(*)$ holds for Π_I^ε being the corresponding spectral projection of H^ε.

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The construction is based on methods developed by *Helffer and Sjöstrand* in '89 that were applied in similar ways by *Martinez, Nenciu, Sordoni* '03, *Panati, Spohn, T.* '03, and many others.

3. Peierls substitution for magnetic subbands

To prove Peierls substitution, we need to show that $\Pi_j^\varepsilon H^\varepsilon \Pi_j^\varepsilon$ is unitarily equivalent to an operator of the form

$$H_j^{\mathrm{eff}} = E_j\big(k + A(\mathrm{i}\varepsilon\nabla_k)\big) + W(\mathrm{i}\varepsilon\nabla_k) + \mathcal{O}(\varepsilon)$$

acting on some suitable space of "scalar functions" of k.

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The first step is the construction of a unitary

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As discussed before, a unitary map from $\mathrm{ran}P_j$ to scalar functions over the torus can be obtained from a trivialising section of this bundle.

However, magnetic Bloch bundles in the Hofstadter model are never trivialisable, i.e. such a trivialising section does not exist.

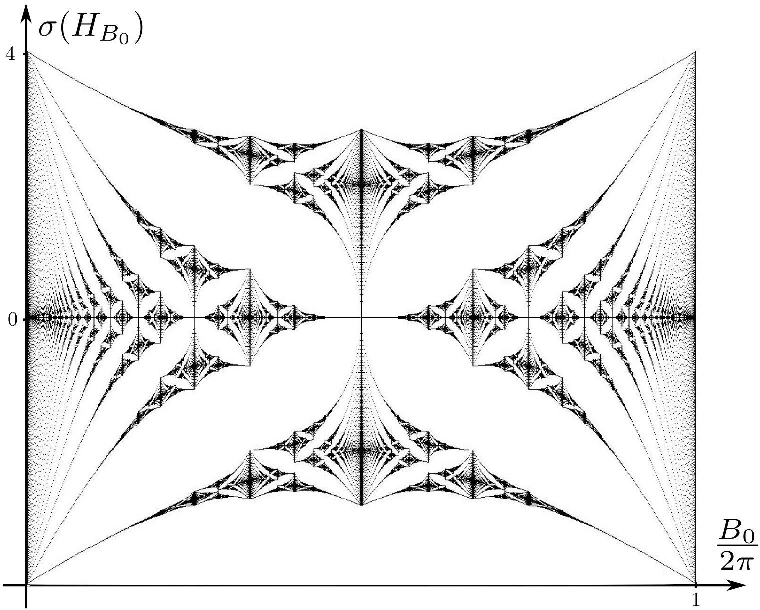
3. Peierls substitution for magnetic subbands

This can be seen by computing the *Chern number* θ_j of the jth Bloch bundle. Coloring the nth gap in the spectrum by the sum $\tilde{\theta}_n$ of the underlying Chern numbers,

$$\tilde{\theta}_n = \sum_{j=1}^{n} \theta_j \,,$$

yields a colored version of the Hofstadter butterfly.

3. Peierls substitution for magnetic subbands



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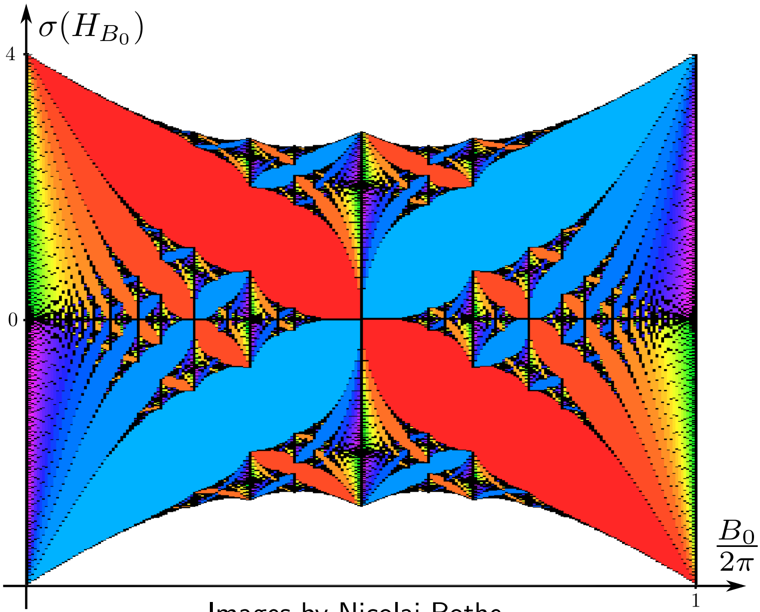

Images by Nicolai Rothe.

3. Peierls substitution for magnetic subbands

Theorem (Freund, T. '13)

Let $\{E_n(k)\,|\,n \in I\}$ be a gapped group of bands with projection P_I. Then there exists a unitary

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such that $H_I^{\mathrm{eff}} := U_I^\varepsilon \Pi_I^\varepsilon \widetilde{H}_\Gamma \Pi_I^\varepsilon U_I^{\varepsilon *}$ satisfies

$$H_I^{\mathrm{eff}} = E_I\big(k + A(\mathrm{i}\varepsilon\nabla_k^{\theta_I})\big) + W(\mathrm{i}\varepsilon\nabla_k^{\theta_I}) + \mathcal{O}(\varepsilon)\,.$$

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Here $\mathcal{H}_{\theta_I}$ is a space of L^2-section of a rank m vector bundle with connection ∇^{θ_I}. In the case of a single band $I = \{j\}$ of the Hofstadter model at $B_0 = \frac{p}{q}2\pi$ they are given by

$$\mathcal{H}_{\theta_I} := \left\{ f \in L^2_{\mathrm{loc}}(\mathbb{R}^2) \,\middle|\, f(k-n) = \mathrm{e}^{\frac{\mathrm{i}\theta_j k_2 q n_1}{2\pi}} f(k) \;\text{ for all } n \in \Gamma_q^* \right\}$$

and $\nabla^{\theta_j} = (\partial_{k_1}, \partial_{k_2} + \mathrm{i}\frac{q\theta_j k_1}{2\pi})$.

3. Peierls substitution for magnetic subbands

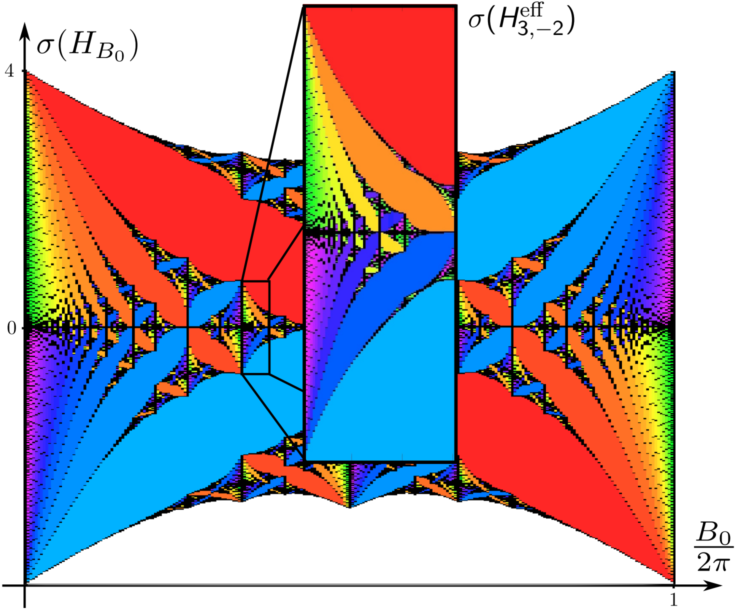
For the case of a perturbation by a constant magnetic field $B = \frac{2\pi}{q^2}\frac{\tilde{p}}{\tilde{q}}$, $W = 0$, and $E_j(k) = 2\cos(qk_1) + 2\cos(qk_2)$, one can represent H_j^{eff} again as a Hofstadter-type matrix

$$H^{\mathrm{eff}}_{q,\theta,B}(k) =$$

$$\begin{pmatrix} 2\cos(qk_2) & \mathrm{e}^{\mathrm{i}q(k_1-\theta\frac{\tilde{p}}{\tilde{q}})} & 0 & \cdots & \mathrm{e}^{-\mathrm{i}q(k_1-\theta\frac{\tilde{p}}{\tilde{q}})} \\ \mathrm{e}^{-\mathrm{i}q(k_1-\theta\frac{\tilde{p}}{\tilde{q}})} & 2\cos(q(k_2+qB)) & \mathrm{e}^{\mathrm{i}q(k_1-\theta\frac{\tilde{p}}{\tilde{q}})} & \cdots & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}q(k_1-\theta\frac{\tilde{p}}{\tilde{q}})} & 2\cos(q(k_2+2qB)) & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & & & & \mathrm{e}^{\mathrm{i}q(k_1-\theta\frac{\tilde{p}}{\tilde{q}})} \\ \mathrm{e}^{\mathrm{i}q(k_1-\theta\frac{\tilde{p}}{\tilde{q}})} & 0 & \cdots & \mathrm{e}^{-\mathrm{i}q(k_1-\theta\frac{\tilde{p}}{\tilde{q}})} & 2\cos(q(k_2+(\tilde{q}-1)qB)) \end{pmatrix}.$$

Here θ is the Chern number of the perturbed band and q the denominator in q the denominator in $B_0 = 2\pi\frac{p}{q}$.

3. Peierls substitution for magnetic subbands



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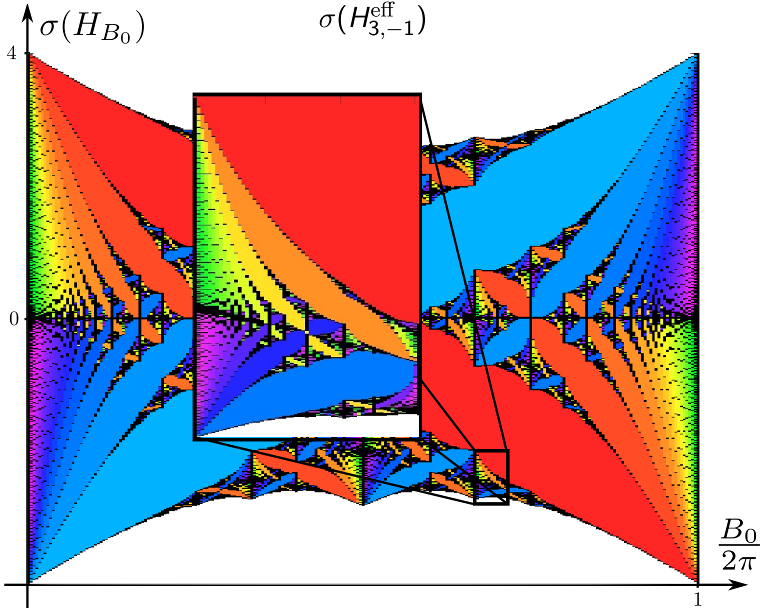

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5. Thanks and congratulations!

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Konrad Knopp, Mathematics Professor in Tübingen 1926–1950, and Herbert's grandfather

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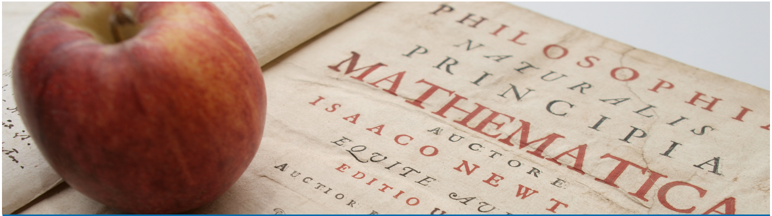
UNIVERSITÄT
TÜBINGEN

Faculty of Science
Departments of Mathematics and Physics



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