Edge states in semi-materials

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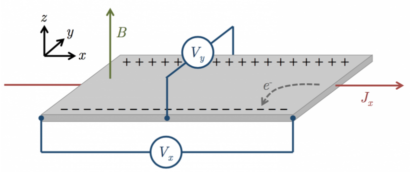
Some historical remarks.

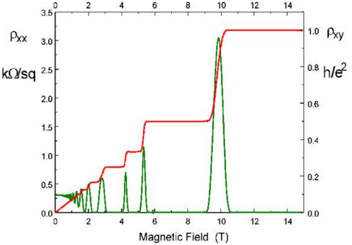
May 20, 2019: New definition of the kg by the *Bureau International des Poids et Mesures* (BIPM)[1] :
"Le kilogramme, symbole kg, est l'unité de masse du SI. Il est défini en prenant la valeur numérique fixée de la constante de Planck, h, égale à $6,626\,070\,15 \times 10^{-34}$ *J.s."*

Question: How do you measure h? How do you measure h with 10^{-9} accuracy?

Comments by von Klitzing[2]: *"The discovery of the QHE led to a new type of electrical resistor [...]. This resistor is universal for all 2D electron systems in strong magnetic fields with an uncertainty of less than one part in* 10^{10}*."*

QHE = Quantum Hall Effect[3] (von Klitzing got Nobel prize in 1985 for discovery of Quantum Hall Effect).





[1] https://www.bipm.org/fr/measurement-units/
[2] von Klitzing, Nature Physics 13, 2017
[3] K. von Klitzing; G. Dorda; M. Pepper, Phys. Rev. Lett. 45 (6): 494–497, 1980.

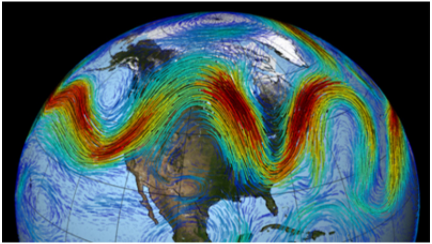
Modern interpretation: The plateaus correspond to different *topological phases of matter*[4], and the QHE is a manifestation of *bulk-edge correspondence:*

"For some systems, one can associate an edge index $I^\sharp \in \mathbb{Z}$, and a bulk index $I \in \mathbb{Z}$, and one has

$$\boxed{I^\sharp = I} \qquad \textit{(bulk-edge correspondence).}$$

These indices are «topological», hence are stable with respect to temperature, noise, deformation, ..."

The Planck constant h is related to I, while the electrical resistor by von Klitzing measures $I^\sharp$.



The Rossby Waves (wind) might be a manifestation of bulk-edge correspondence (Tauber/Delplace/Venaille, J. Fluid Mech. Vol 868 (2019).)
In this talk: Simple 1d model where bulk-edge correspondence happens.

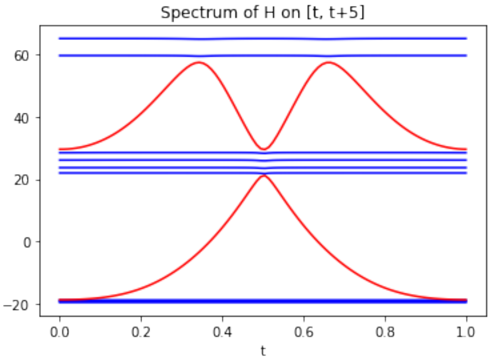
[4] D.J. Thouless, F.D.M. Haldane and J.M. Kosterlitz got Nobel prize in 2016 for the discovery of topological phases of matter

Another motivation: spectral pollution

We want to compute the spectrum of the (simple) operator

$$H := -\partial_{xx}^2 + V(x), \quad \text{with} \quad V(x) = 50 \cdot \cos(2\pi x) + 10 \cdot \cos(4\pi x).$$

The potential V is 1-periodic. Assume we study H in a box $[t, t+L]$ with Dirichlet boundary conditions.



Depending on where we fix the origin t, the spectrum differs...
There are branches of spurious eigenvalues = spectral pollution.

Goal: (simple) introduction to *bulk-edge correspondence.*

Motivation

Let $V : \mathbb{R} \to \mathbb{R}$ be a 1-periodic smooth potential, and let $V_t(x) := V(x - t)$. We consider

- The periodic (bulk) operator

$$H(t) := -\partial_{xx}^2 + V_t \quad \text{acting on } L^2(\mathbb{R})$$

- The edge operator

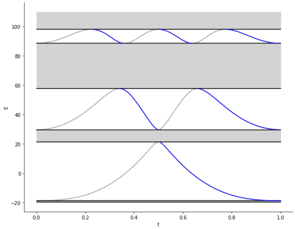
$$H_D^\sharp(t) := -\partial_{xx}^2 + V_t \quad \text{acting on } L^2(\mathbb{R}^+), \text{ with Dirichlet boundary conditions}$$

Theorem (Korotyaev 2000, Hempel Kohlmann 2011, DG 2020)

In the n-th essential gap, there is a flow of n eigenvalues going downwards as t goes from 0 to 1. In addition, these eigenvalues are simple, and their associated eigenvectors are exponentially localised.

= edge states

We provide here a simple topological proof, which will prove *bulk-edge correspondence* in this case.



Periodic operators

Preliminaries.

Potential: Let $V \in C^1(\mathbb{R}, \mathbb{R})$ be any potential (not necessarily 1-periodic).

Hamiltonian: $H := -\partial_{xx}^2 + V$ as an operator on $L^2(\mathbb{R})$.
Associated ODE: $-u'' + V(x)u = Eu, \quad \text{on} \quad \mathbb{R}.$
Vector space of solutions: Let $\mathcal{L}_V(E)$ denote the vectorial space of solutions of the ODE. Since it is a second order ODE, $\dim \mathcal{L}_V(E) = 2$, and

$$\mathcal{L}_V(E) = \mathrm{Ran}\left\{c_E, s_E\right\}, \quad \begin{cases} -c_E'' + Vc_E = Ec_E \\ c_E(0) = 1, \ c_E'(0) = 0 \end{cases}, \quad \begin{cases} -s_E'' + Vs_E = Es_E \\ s_E(0) = 0, \ s_E'(0) = 1 \end{cases}.$$

Lemma (definition?)

$E \in \mathbb{R}$ is an eigenvalue of H iff $\mathcal{L}_V(E) \cap L^2(\mathbb{R}) \neq \emptyset$.

Transfer matrix

$$T_E(x) := \begin{pmatrix} c_E(x) & c_E'(x) \\ s_E(x) & s_E'(x) \end{pmatrix}.$$

Lemma

For all $x \in \mathbb{R}$, we have $\det T_E(x) = 1$

Indeed, $\det T_E$ is the Wronskian of the ODE. At $x = 0$, we have $T_E(0) = \mathbb{I}_2$, and

$$(\det T_E)' = \left(c_E s_E' - s_E c_E'\right)' = c_E s_E'' - s_E c_E'' = c_E(V - E)s_E - s_E(V - E)c_E = 0.$$

Case of periodic potentials.

We now assume that V is 1-periodic.

If $u(x)$ is solution to the ODE, then so is $u(\cdot + 1)$. In particular there are constants $\alpha, \beta, \gamma, \delta$ such that

$$\begin{cases} c_E(x+1) = \alpha c_E(x) + \beta s_E(x) \\ s_E(x+1) = \gamma c_E(x) + \delta s_E(x). \end{cases} \quad \text{or equivalently} \quad T_E(x+1) = \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} T_E(x).$$

At $x = 0$, we recognise $T_E(x = 1)$, so $\boxed{T_E(x+1) = T_E(1) T_E(x)}$.

So for any solution $u \in \mathcal{L}_E$, we have

$$\begin{pmatrix} u(x+n) \\ u'(x+n) \end{pmatrix} = [T_E(1)]^n \begin{pmatrix} u(x) \\ u'(x) \end{pmatrix}.$$

$\Longrightarrow$ **The behaviour of solutions at infinity is given by the singular values of $T_E(1)$.**

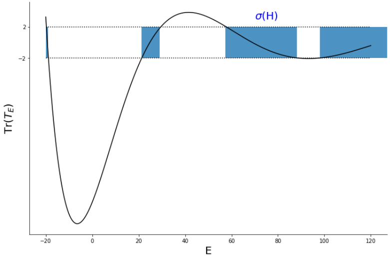
Recall that if λ_1 and λ_2 are the singular values of $T_E(1)$, then $\lambda_1 \lambda_2 = \det T_E(1) = 1$.
Also, $\lambda_1 + \lambda_2 = \mathrm{Tr}(T_E) \in \mathbb{R}$.

Two cases.

- if $|\lambda_1| > 1$, then $|\lambda_2| < 1$. Then $\lambda_1, \lambda_2 \in \mathbb{R}$ and $\boxed{|\mathrm{Tr}(T_E)| > 2}$.
  There is one mode exponentially increasing at $+\infty$ and exponentially decreasing at $-\infty$.
  There is one mode exponentially increasing at $-\infty$ and exponentially decreasing at $+\infty$.
  The elements of $\mathcal{L}_E$ cannot be approximated in L^2, which implies $E \notin \sigma(H)$.
- if $|\lambda_1| = 1$, the $|\lambda_2| = 1$. Then $|\lambda_1| = 1$, $\lambda_2 = \overline{\lambda_1}$ and $\boxed{|\mathrm{Tr}(T_E)| \leq 2}$.
  All solutions in $\mathcal{L}_E$ are bounded (quasi-periodic).
  All solutions in $\mathcal{L}_E$ can be approximated in L^2, which implies $E \in \sigma_{\mathrm{ess}}(H)$.

The spectrum of H can be read from the (continuous) map $E \mapsto \mathrm{Tr}(T_E)$.

Example: for $V(x) := 50 \cdot \cos(2\pi x) + 10 \cdot \cos(4\pi x)$,



Theorem (Spectrum of 1-dimensional periodic operators)

If V is 1-periodic, the spectrum $H := -\partial_{xx}^2 + V(x)$ is purely essential (no eigenvalues). It is composed of bands:

$$\sigma(H) = \sigma_{\text{ess}}(H) = \bigcup_{n \geq 1} [E_n^-, E_n^+].$$

Essential gap: The interval $g_n := (E_n^+, E_{n+1}^-)$ is called the n-th essential gap of the operator H.

Physical interpretation:

- If $E \in \sigma(H)$, waves with energy E can travel through the medium (quasi-periodic solutions);
- If $E \notin \sigma(H)$, waves cannot propagate: they are exponentially attenuated in the medium. In scattering theory, we would say that the wave is totally reflected.

Example: If $V = 0$, then $H = -\partial_{xx}^2$. We have $-u'' = Eu$ if $u = \alpha e^{i\sqrt{E}} + \beta e^{-i\sqrt{E}}$.

- If $E \geq 0$, $\sqrt{E} \in \mathbb{R}$, and we have *travelling waves*;
- If $E < 0$, $\sqrt{E} \in i\mathbb{R}$, and we have *exponential waves*.
- The spectrum of $-\partial_{xx}^2$ is $[0, \infty)$.

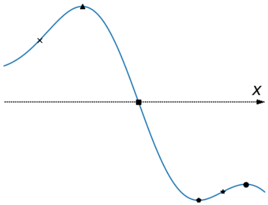
Bulk index

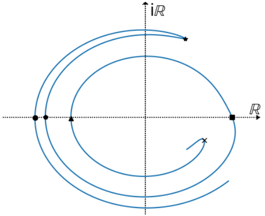
A basic remark

If $-\partial_{xx}^2 u + (V-E)u = 0$ is a non null *real-valued* solution, then $u(x)$ and $u'(x)$ cannot vanish at the same time (Cauchy-Lipschitz).

We can therefore define the discrete set $\mathcal{Z}[u] := u^{-1}(\{0\})$, and the map

$$x \mapsto \theta[u,x] := \frac{u'(x) - \mathrm{i}u(x)}{u'(x) + \mathrm{i}u(x)} \quad \text{from } \mathbb{R} \text{ to } \mathbb{S}^1 := \{z \in \mathbb{C}, |z| = 1\}.$$





Lemma

$\mathcal{Z}[u]$ and $\theta[u,x]$ only depends on $\mathrm{Vect}\{u\}$: $\theta[u,x_0] = \theta[v,x_0]$ iff $u = \lambda v$.

In the sequel, we fix x_0, consider a periodic family of solutions u_t for H_t, and compute the winding number of $t \mapsto \theta[u_t, x_0]$.

The Maslov[5] bulk index.

Translated Hamiltonian: We now fix $V \in C^1$ a 1-periodic potential, and we set:

$$V_t(x) := V(x-t), \quad \mathcal{L}_t(E) := \mathcal{L}_{V_t}(E), \quad \text{and} \quad H_t := -\partial_{xx}^2 + V_t.$$

Translations: If $\tau_t f(x) := f(x-t)$, we have $H_t = \tau_t H_0 \tau_t^*$, so H_t is unitary equivalent to H_0.
$\implies \sigma(H_t) = \sigma(H)$. In particular, the gaps g_n are independent of $t \in \mathbb{R}$.

We fix $E \in g_n$ in a common open gap.

Splitting of $\mathcal{L}_V(E)$. Since $E \notin \sigma(H_t)$, there is a natural splitting $\mathcal{L}_t(E) = \mathcal{L}_t^+(E) \oplus \mathcal{L}_t^-(E)$, where

$$\mathcal{L}_t^\pm(E) = \mathrm{Vect}\{\text{modes exp. decreasing at } \pm\infty\}, \quad \dim \mathcal{L}_t^\pm(E) = 1, \quad \mathcal{L}_t^+(E) \cap \mathcal{L}_t^-(E) = \{\mathbf{0}\}.$$

Remark: The map $t \mapsto \mathcal{L}_t^\pm(E)$ is 1-periodic, so the map $t \mapsto \theta\left[\mathcal{L}_t^\pm(E), x\right]$ is also 1-periodic on $\mathbb{S}^1$.
Winding number: We denote by $\mathcal{M}^\pm$ the corresponding winding numbers. By continuity, they are independent of $E \in g_n$ and of $x \in \mathbb{R}$.

Lemma

$\mathcal{M}^+ = \mathcal{M}^-$. The common number is our bulk index (it is a Maslov index).

Proof. Since $\mathcal{L}^+ \neq \mathcal{L}^-$, we have $\theta_t^+ \neq \theta_t^-$, so $\dfrac{\theta_t^+}{\theta_t^-} \in \mathbb{S}^1$ never touches 1, hence has null winding number.

This gives $\mathcal{M}^+ - \mathcal{M}^- = 0$.

[5] Maslov, *Théorie des perturbations et méthodes asymptotiques.* 1972

Lemma

$\mathcal{M}$ counts the flow of the discrete set $\mathcal{Z}_t$ across any $x_0 \in \mathbb{R}$.

Proof. Fix $x_0 \in \mathbb{R}$.
Step 1. We can compute the winding number of $\theta_t(x_0) := \theta[\mathcal{L}_t^+(x_0)]$ by counting the number of times it crosses the value $1 \in \mathbb{S}^1$ (with orientation).

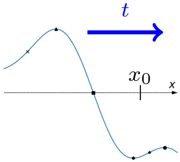
Step 2. We have $\theta_{t^*}(x_0) = 1$ iff $u(t^*, x_0) = 0$ iff $x_0 \in \mathcal{Z}_{t^*}$.
Let $x(t) \in \mathcal{Z}_t$ be the branch of zeros of $u(t, \cdot)$ such that $x(t^*) = x_0$, that is $u(t, x(t)) = 0$.
By the implicit theorem,

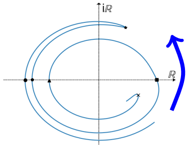
$$x'(t^*) = -\frac{\partial_t u(t^*, x_0)}{\partial_x u(t^*, x_0)}.$$

On the other hand, a computation shows that

$$\partial_t \theta(t^*, x_0) = -2\mathrm{i}\frac{\partial_t u(t^*, x_0)}{\partial_x u(t^*, x_0)} = 2\mathrm{i}x'(t^*).$$

At $t = t^*$, $\theta(t, x_0)$ is locally turning positively iff $x'(t^*)$ is crossing x_0 from the left to the right!





Bonus, in the dislocated case.

Lemma

In the case $V_t(x) := V(x-t)$, we have $\mathcal{M} = n$ in the n-th gap.

Proof.

Step 1. In this case, we have $\mathcal{Z}_t := \mathcal{Z}_0 + t$. By periodicity, we have $\mathcal{Z}_1 = \mathcal{Z}_0 + 1 = \mathcal{Z}_0$.
If $x_0 \in \mathcal{Z}_0$, then $x_0 + 1 \in \mathcal{Z}_0$. In particular, $(E, u_{t=0}|_{[x_0, x_0+1]})$ is an eigenpair of the Dirichlet problem

$$\begin{cases} \left(-\partial_{xx}^2 + V(x)\right) u = Eu, \quad \text{on} \quad (x_0, x_0+1) \\ u(x_0) = u(x_0+1) = 0. \end{cases}$$

The flow $\mathcal{M}$ corresponds to the number of zeros of u in the interval $[x_0, x_0+1)$.

Step 2 (deformation). For $0 \le s \le 1$, we introduce $(E(s), \widetilde{u_s})$ the Dirichlet eigenpair of

$$\begin{cases} \left(-\partial_{xx}^2 + sV(x)\right) \widetilde{u_s} = E_s \widetilde{u_s}, \quad \text{on} \quad (x_0, x_0+1) \\ \widetilde{u_s}(x_0) = \widetilde{u_s}(x_0+1) = 0. \end{cases}$$

which is a continuation of (E, u) at $s = 1$, and by $\mathcal{M}_s$ the number of zeros of $\widetilde{u_s}$ in the interval $[x_0, x_0+1)$.

By continuity, $E(s)$ cannot cross the essential spectrum, so $E(s)$ is always in the n-th gap.
By Cauchy-Lipschitz, two zeros cannot merge, so $\mathcal{M}_s$ is independent of s, and $\mathcal{M} = \mathcal{M}_{s=1}$.
At $s = 0$, we recover the usual Laplacian.

We deduce that $E(s)$ is the branch of n-th eigenvalues, and that $\mathcal{M} = n$.

Edge index and edge modes

The half-line Dirichlet Hamiltonian.

$$\boxed{H_D^\sharp(t) := -\partial_{xx}^2 + V(x-t),} \quad \text{on } \mathbb{R}^+ \quad \text{with Dirichlet boundary conditions at } x = 0.$$

Essential spectrum: We have $\sigma_{\rm ess}(H_D^\sharp(t)) = \sigma_{\rm ess}(H_0)$ independent of t. So g_n is well-defined.

Key remark: E is an eigenvalue of $H_D^\sharp(t)$ iff $0 \in \mathcal{Z}_t^+(E)$.

Lemma

If $E \in g_n$ is in the n-th gap, there are exactly n values $0 \le t_1 < t_2 \cdots < t_n < 1$ such that E is an eigenvalue of $H_D^\sharp(t_k)$.
The corresponding eigenfunctions (= edge modes) are exponentially localised near $x = 0$.

Theorem (Bulk-edge correspondence)

The branches of eigenvalues are decreasing function of t.
In particular, in the n-th gap, the decreasing spectral flow of $H_D^\sharp(\cdot)$ is $\mathcal{S}_{D,n}^\sharp = n$.

Idea of the proof.

If $\left(\widetilde{E}(t), \widetilde{u}(t)\right)$ is a branch of eigenpair for $H(t)$ with $\|\widetilde{u}_t\|^2 = 1$. We have $H(t)\widetilde{u}(t) = \widetilde{E}(t)$, and $\widetilde{E}(t) = \langle \widetilde{u}(t), H(t)\widetilde{u}(t)\rangle$. Differentiating in t gives (Hellman-Feynman)

$$\begin{aligned}\widetilde{E}'(t) &= \langle \widetilde{u}_t, \partial_t H_t \widetilde{u}_t\rangle + \langle \partial_t \widetilde{u}_t, H_t \widetilde{u}_t\rangle + \langle \widetilde{u}_t, H_t \partial_t \widetilde{u}_t\rangle \\ &= \langle \widetilde{u}_t, (\partial_t V_t)\, \widetilde{u}_t\rangle + \widetilde{E}(t) \underbrace{\left(\langle \partial_t \widetilde{u}_t, \widetilde{u}_t\rangle + \langle \widetilde{u}_t, \partial_t \widetilde{u}_t\rangle\right)}_{=\partial_t \|\widetilde{u_t}\|^2 = 0} = \int_0^\infty (\partial_t V_t)\, |\widetilde{u}_t|^2 \mathrm{d}x.\end{aligned}$$

On the other hand, if $u(t)$ is a branch of functions in $\mathcal{L}_t^+(E)$ (E is fixed now), then

$$(-\partial_{xx}^2 + V_t - E)u_t = 0.$$

These functions do not satisfy Dirichlet in general! Differentiating in t gives

$$(-\partial_{xx}^2 + V_t - E)\partial_t u_t + (\partial_t V_t)\, u_t = 0.$$

We multiply by u_t and integrate on $\mathbb{R}^+$. We integrate by part and obtain (now we have boundary terms)

$$\int_0^\infty (\partial_t V_t)\, |u_t|^2 = \partial_x u_t(0) \partial_t u_t(0).$$

At the point t, we have $u_t = \widetilde{u}_t$. In the special case where $V_t(x) = V(x-t)$ so that $u_t(x) = u(x-t)$, we obtain

$$\widetilde{E}'(t) = -|\partial_t u_t|^2(0) < 0.$$

The proof relies on integration by parts.
In some sense, this is a form of *bulk-edge correspondence*.

Extensions

The previous arguments can be used to extend the result to many other cases:

- Any boundary conditions;
- Different models (one-dimensional Dirac equation);
- Operators on $\mathbb{C}^n$, of the form $H = (-\partial_{xx}^2)\mathbb{I}_n + V_t(x)$, with $V_t(x)$ a $n \times n$ hermitian matrix.

In the latter case, the map $\theta[u_t, x]$ becomes a unitary $\theta[\mathcal{L}, x] \in \mathrm{U}(n)$.

Two-dimensional case

Let $V \in C^1(\mathbb{R}^2, \mathbb{R})$ be a $\mathbb{Z}^2$-periodic function. We consider (no t-parameter)

- The periodic bulk operator

$$H := -\Delta + V(\mathbf{x}), \quad \text{acting on } L^2(\mathbb{R}^2);$$

- The edge operator

$$H_D^\sharp := -\Delta + V(\mathbf{x}) \quad \text{acting on } L^2(\mathbb{R}^+ \times \mathbb{R}) + \text{Dirichlet boundary conditions.}$$

Both models are periodic in the x_2-direction. We can perform partial-Bloch transformation:

- Bloch bulk operator

$$H(t) := (-\mathrm{i}\partial_y + t)^2 - \partial_{xx}^2 + V \quad \text{acting on } L^2(\mathbb{R} \times [0,1]);$$

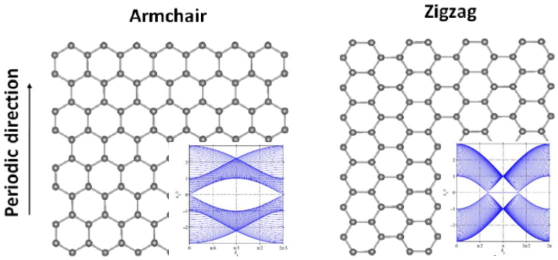
- Bloch edge operator

$$H_D^\sharp(t) := (-\mathrm{i}\partial_y + t)^2 - \partial_{xx}^2 + V \quad \text{acting on } L^2(\mathbb{R}^+ \times [0,1]);$$

It is the $n = \infty$ version of the previous case. The map θ becomes a unitary of $L^2([0,1])$.

Depending on the model, edge can (must) exist, or not.

Example: Graphene (a bit special... no spectral gap...).
Depending on the direction of the cut, edge can/must appear.



References:

- *Edge states in Ordinary Differential Equations for dislocations*, D.G., J. Math. Phys. 61, 2020 (arXiv 1908.01377).
- *Edge states for second order elliptic operators*, D.G., soon on arXiv.

Thank you for your attention.