Edge states in ordinary differential equations for dislocations

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Séminaire *EDP et physique mathématique* Paris 13
April 24th 2020

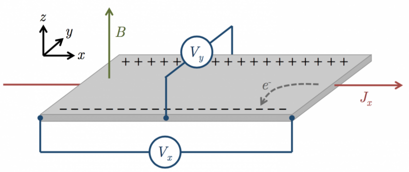
Some historical remarks.

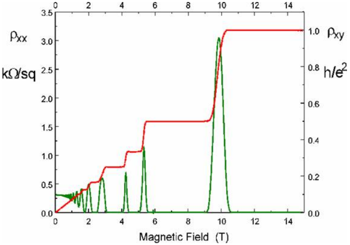
May 20, 2019: New definition of the kg by the *Bureau International des Poids et Mesures* (BIPM)[1] :
"Le kilogramme, symbole kg, est l'unité de masse du SI. Il est défini en prenant la valeur numérique fixée de la constante de Planck, h, égale à $6,626\,070\,15 \times 10^{-34}$ *J.s."*

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.

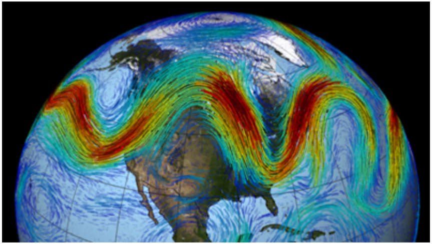
Modern interpretation: The plateaus correspond to different *topological phases of matter*[4], and the QHE is a manifestation of *bulk-edge correspondence:*

"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: not about QH/$2d$. Here, a simple 1d model where bulk-edge correspondence happens.

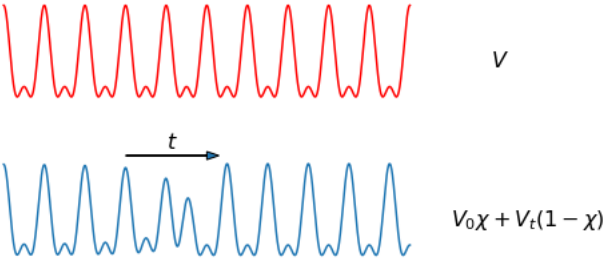
[4] D.J. Thouless, F.D.M. Haldane and J.M. Kosterlitz got Nobel prize in 2016 for the discovery of topological phases of matter

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
$$H(t) := -\partial_{xx}^2 + V_t.$$
- The dislocated operator
$$H_\chi^\sharp(t) := -\partial_{xx}^2 + [V_0\chi + V_t(1-\chi)],$$
where χ is a cut-off with $\chi(x) = 1$ if $x < -L$ and $\chi(x) = 0$ if $x > L$.



Question: How does the spectrum of $H_\chi^\sharp(t)$ vary with t?
Remark: Everything is 1-periodic in t.

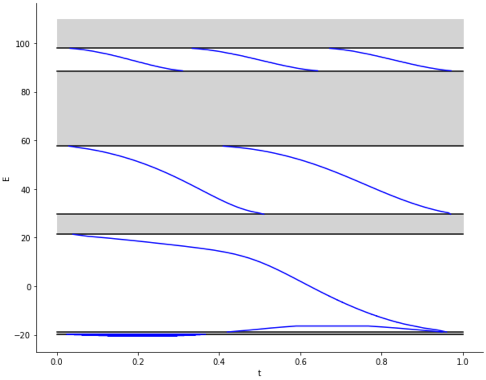


Figure: Spectrum of $H^\sharp_\chi(t)$ for $t \in [0, 1]$.

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.

E. Korotyaev, Commun. Math. Phys., 213(2):471–489, 2000.

R. Hempel and M. Kohlmann., J. Math. Anal. Appl., 381(1):166–178, 2011.

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 $\mathcal{L}_V(E) \cap L^2 \neq \emptyset$.

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 $T_E(1)$.**

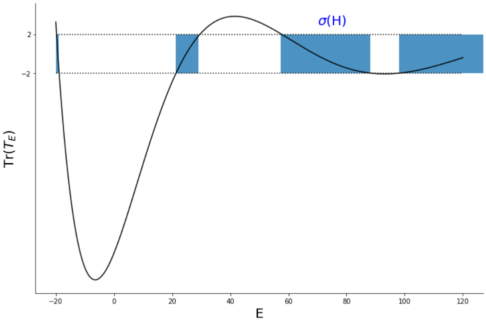
Recall that if λ_1 and λ_2 are the singular values of $T_E(1)$, then $\lambda_1 \lambda_2 = \det T_E(1) = 1$.
Also, $\lambda_1 + \lambda_2 = \mathrm{Tr}(T_E) \in \mathbb{R}$.

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:

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

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 $u = \alpha {\rm e}^{{\rm i}\sqrt{E}} + \beta {\rm e}^{-{\rm i}\sqrt{E}}$.

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

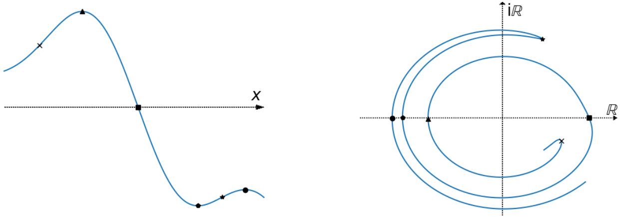
Bulk index

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

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

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).

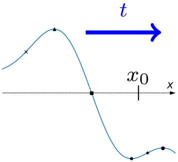
Step 2. We have $\theta_{t^*}(x_0) = 1$ iff $u(t^*, x_0) = 0$ iff $x_0 \in \mathcal{Z}_{t^*}$.
Let $x(t) \in \mathcal{Z}_t$ be the branch of zeros of $u(t, \cdot)$ such that $x(t^*) = x_0$, that is $u(t, x(t)) = 0$.
By the implicit theorem,

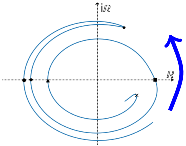
$$x'(t^*) = -\frac{\partial_t u(t^*, x_0)}{\partial_x u(t^*, x_0)}.$$

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

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

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

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

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 $x = 0$.

Corollary: spectral pollution
If one numerically studies the periodic Hamiltonian $H(0)$ on a large box with Dirichlet boundary conditions, spurious eigenvalues will appear.
On a box $[t, L+t]$ with L large, there will be flows of spurious eigenvalues in all essential gaps, corresponding to the localised edge modes near the boundaries t and $L+t$.

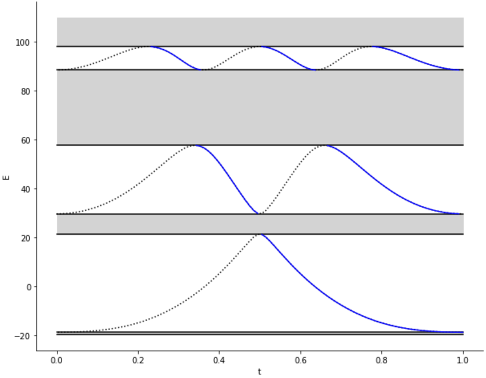


Figure: Spectrum of $H_D^\sharp(t)$ as a function of t (the dotted lines represent resonances).

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 argument)

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

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)

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

Of course, 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

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

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

The case of dislocation.

$$\boxed{H_\chi^\sharp(t) := -\partial_{xx}^2 + \chi(x)V_0(x) + [1-\chi(x)]\, V_t(x) =: -\partial_{xx}^2 + V_\chi^\sharp(t).}$$

Here, χ is a *switch function*: $\chi(x) = 1$ if $x < -L$ and $\chi(x) = 0$ if $x > L$.

Remarks:
- At $t = 0$, we recover H_0, which has purely essential spectrum.
- $t \mapsto H(t)$ is 1-periodic in t.

Fact:
- $\sigma_{\rm ess}\left(H_\chi^\sharp(t)\right)$ is independent of t, so the essential gaps g_n are well-defined.

Theorem

The decreasing spectral flow of $H_\chi^\sharp(\cdot)$ is $\mathcal{S}_{\chi,n}^\sharp = n$ in the n-th gap g_n.
It is independent of the switch function χ.

Idea of the proof.
Let $\mathcal{L}_t^{\sharp,\pm}(E)$ be the vectorial space of solutions which are square integrable at $\pm\infty$.
Key remark: E is an eigenvalue for $H_\chi^\sharp(t)$ iff $\mathcal{L}_t^{\sharp,+}(E) \cap \mathcal{L}_t^{\sharp,-}(E) \neq \{\mathbf{0}\}$, iff $\theta^{\sharp,+}(x_0,t) = \theta^{\sharp,-}(x_0,t)$.
Looking at $x \gg L$, we see that $\mathcal{L}_t^{\sharp,+}(E) \approx \mathcal{L}_t^{+}(E)$, so $\mathcal{M}^{\sharp,+} = \mathcal{M}^+$.
Looking at $x \ll L$, we see that $\mathcal{L}_t^{\sharp,-}(E) \approx \mathcal{L}_0^{-}(E)$, so $\mathcal{M}^{\sharp,-} = 0$ (independent of t).

We deduce that the winding is $\dfrac{\theta^{\sharp,+}(x_0,t)}{\theta^{\sharp,-}(x_0,t)}$ is

$$\mathcal{M}^{\sharp,+} - \mathcal{M}^{\sharp,-} = \mathcal{M}^+ - 0 = n.$$

Hence it crosses the value $1 \in \mathbb{S}^1$ exactly n times (with orientation).

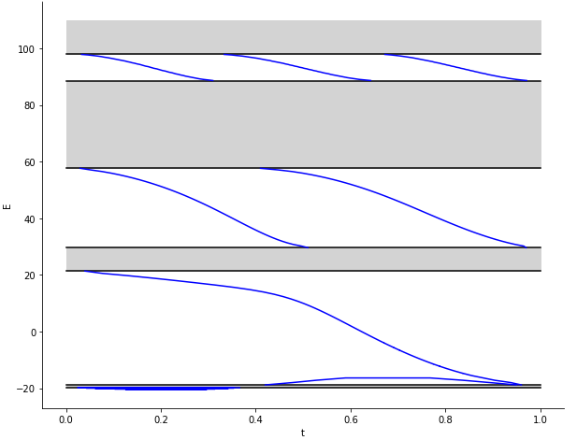


Figure: Spectrum of $H_\chi^\sharp(t)$ for $t \in [0, 1]$.

Remark: The spectral flow is independent of χ, but the form of the eigenvalue branches depends on χ.

Extensions

The Dirac case.

The Dirac equation is an ODE with values in $\mathbb{C}^2$ (spins), of the form

$$\mathrm{i} \begin{pmatrix} \psi^{\uparrow} \\ -\psi^{\downarrow} \end{pmatrix}' = \begin{pmatrix} 0 & V(x) \\ V(x) & 0 \end{pmatrix} \begin{pmatrix} \psi^{\uparrow} \\ \psi^{\downarrow} \end{pmatrix} + E \begin{pmatrix} \psi^{\uparrow} \\ \psi^{\downarrow} \end{pmatrix}.$$

Lemma (Fefferman/Lee-Thorp/Weinstein, AMS Vol. 247 (2017).**)**

If V switches from $V_{\rm per}$ at $x \le -L$ to $-V_{\rm per}$ at $x \ge L$, then 0 is in the spectrum of the Dirac operator.
= «Topologically protected state».

Idea: embed the 0 eigenvalue in a *spectral flow*!
Replace the group of translations with the group of spin rotations: family of operators $\mathcal{D}_\chi^\sharp(t)$:

$$\text{Consider} \quad V_\chi^\sharp(t,x) = \chi(x) V_{\rm per}(x) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + (1-\chi(x)) V_{\rm per}(x) \begin{pmatrix} \sin(2\pi t) & \cos(2\pi t) \\ \cos(2\pi t) & -\sin(2\pi t) \end{pmatrix}.$$

Remark: at $t = \frac{1}{2}$, this is a transition from $V_{\rm per}$ to $-V_{\rm per}$.

Lemma (DG, 2020)

*The decreasing spectral flow is 1 in each essential gap, and $\mathcal{D}^\sharp_\chi(\frac{1}{2} - t) = -\mathcal{D}^\sharp_\chi(\frac{1}{2} + t)$.
In particular, 0 is an eigenvalue at $t = 1/2$ (= previous result).*

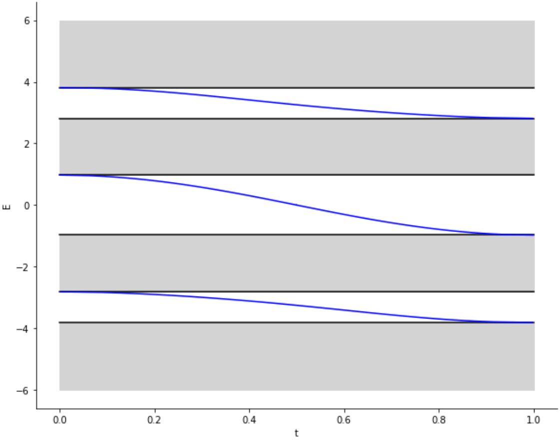


Figure: Spectrum of the Dirac operator $\mathcal{D}^\sharp_\chi(t)$ as a function of t

Future work: the 2d case

- Study dislocations in $2d$. Similar results, but in infinite dimensions.
- Study dislocations + rotations in $2d$.

Reference:

Edge states in Ordinary Differential Equations for dislocations, D.G., accepted in J. Math. Phys. (arXiv 1908.01377).

Thank you for your attention!