PDE METHODS IN CONDENSED MATTER PHYSICS

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Contents

1. Introduction

This are the notes taken by Zhongkai Tao from the topics course taught by Maciej Zworski in Fall 2022 at Berkeley, on mathematics of condensed matter physics.

We will cover the following topics:

- Magnetic Hamiltonian of the free electron; Landau levels, derivation of de Haas–van Alphen oscillations in that case.
- Spectral theory of periodic structures; band theory.
- Berry phase, curvature and Chern numbers.
- 2D crystals in magnetic fields and the Peierls substitution; semiclassical study of the de Haas–van Alphen effect.
- Semiclassical derivation of the tight binding model.
- Introduction to many-body interactions and the language (if nothing more) of second quantization.

2. Preliminaries

We discuss some preliminaries which will be useful later. A brief account of geometric preliminaries can be found at `https://math.berkeley.edu/~zworski/symple.pdf`. For tempered distributions ($\mathscr{S}'$) and Fourier transform an in depth presentation is provided in [Ho03, Chapter 7] (see also [Zw12, Chapter 3] for a more light-hearted treatment). References for pseudodifferential calculus (going beyond what is needed here) are [DS99] and [Zw12, Chapter 4]. For unbounded operators, a detailed account can be found in [Sch12] and for brief reviews see [DS99, Chapter 2] and [Zw12, Appendix C.2].

2.1. **Symplectic geometry.** A *symplectic manifold* is a smooth manifold M with a non-degenerate closed 2-form σ on M, called the *symplectic form*. On a cotangent bundle T^*M, there is a canonical symplectic structure given by

$$\sigma = \sum d\xi_j \wedge dx_j = d(\sum \xi_j \wedge dx_j).$$

In the case of $M = \mathbb{R}^n$, we can think of σ as a non-degenerate quadratic form on $\mathbb{R}^n \times \mathbb{R}^n$:

$$\sigma(X, \Xi, X', \Xi') = \langle \Xi, X' \rangle - \langle X, \Xi' \rangle. \tag{2.1}$$

Given a smooth real-valued function $p : T^*M \to \mathbb{R}$, we may define the *Hamiltonian vector field* H_p by

$$\sigma(\cdot, H_p) = dp.$$

In local coordinates, it is given by

$$H_p = \sum_j \frac{\partial p}{\partial \xi_j}\frac{\partial}{\partial x_j} - \frac{\partial p}{\partial x_j}\frac{\partial}{\partial \xi_j}. \tag{2.2}$$

The flow $\varphi_t = \exp tH_p$ under the Hamiltonian vector field is called the *Hamiltonian flow*. It is straightforward to verify that φ_t preserves the symplectic form and the function p. In particular, it preserves the volume form $d\,\mathrm{Vol} = \sigma^n/n!$ (Liouville theorem).

Example 1. Let $p(x,\xi) = \frac{1}{2}\xi^2 + V(x) : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, then the Hamiltonian flow is given by

$$\dot{x} = \xi, \quad \dot{\xi} = -\nabla V(x).$$

That is, $\ddot{x} = -\nabla V(x)$. We think of $V(x)$ as a potential and $\vec{F}(x) = -\nabla V(x)$ as the force, then this is Newton's law of motion.

Example 2. Suppose there is a charged particle in an electromagnetic field. By Maxwell equation

$$\nabla \cdot \vec{B} = \vec{0}, \quad \nabla \times \vec{E} = \vec{0}.$$

So there is a potential $V(x)$ and a vector potential $\vec{A}(x)$ such that

$$\vec{E} = -\nabla V(x), \quad \vec{B} = \nabla \times \vec{A}(x).$$

The force on the particle is then given by

$$\vec{F} = -\nabla V(x) + \dot{x} \times \vec{B}.$$

Now we have an equivalent Hamiltonian formulation. Let

$$p(x,\xi) = \frac{1}{2}\sum_j (\xi_j - A_j(x))^2 + V(x).$$

The Hamiltonian flow is given by

$$\dot{x}_j = \xi_j - A_j(x), \quad \dot{\xi}_j = \sum_k \partial_j A_k(x)(\xi_k - A_k(x)) - \partial_j V(x).$$

That is,

$$\ddot{x}_j = -\sum_k \partial_k A_j(x)\dot{x}_k + \dot{\xi}_j = \sum_k (\partial_j A_k(x) - \partial_k A_j(x))\dot{x}_k - \partial_j V(x) = (\dot{x} \times \vec{B} - \nabla V)_j.$$

The quantization of this Hamiltonian in the case of a constant magnetic field is the Landau Hamiltonian which we will study in §3.

A classical observable is a function a on $T^*\mathbb{R}^n$. Under the Hamiltonian flow $\varphi_t = \exp tH_p$, the evolution of the observable is given by $\varphi_t^* a(x,\xi) = a(\varphi_t(x,\xi))$. In other words,

$$\frac{d}{dt}\varphi_t^* a = \varphi_t^* H_p a = \varphi_t^*\{p,a\}. \tag{2.3}$$

2.2. **Analysis on $\mathbb{R}^n$.** The space of *Schwartz functions* is defined as

$$\mathscr{S}(\mathbb{R}^n) = \{u \in C^\infty(\mathbb{R}^n) : x^\alpha \partial_x^\beta u \in L^\infty, \forall \alpha, \beta \in \mathbb{N}^n\}.$$

The seminorms $\|u\|_{\alpha,\beta} = \|x^\alpha \partial_x^\beta u\|_{L^\infty}$ give $\mathscr{S}$ a structure of Fréchet spaces. The space of *Schwartz/tempered distributions* is the dual of $\mathscr{S}$, or equivalently,

$$\mathscr{S}'(\mathbb{R}^n) = \{u : \mathscr{S} \to \mathbb{C} : \exists N \in \mathbb{N}, C_N > 0, \text{ such that } |u(\varphi)| \le C_N \sum_{|\alpha|,|\beta|\le N} \|\varphi\|_{\alpha,\beta}, \forall \varphi \in \mathscr{S}\}.$$

We note that $L^p(\mathbb{R}^n) \subset \mathscr{S}'(\mathbb{R}^n)$, with the definition

$$u(\varphi) := \int u(x)\varphi(x)dx.$$

The main advantage of distributions, and in particular of tempered distributions, is the fact that the derivative is always defined using formal differentiation by parts:

$$(\partial_{x_j} u)(\varphi) := -u(\partial_{x_j}\varphi), \quad u \in \mathscr{S}'(\mathbb{R}^n), \quad \varphi \in \mathscr{S}(\mathbb{R}^n). \tag{2.4}$$

The *Fourier transform* of a Schwartz function $u \in \mathscr{S}$ is defined by

$$\mathcal{F}u(\xi) = \hat{u}(\xi) = \int_{\mathbb{R}^n} u(x) e^{-ix\cdot\xi} dx$$

and $\mathcal{F} : \mathscr{S} \to \mathscr{S}$ gives an automorphism of the Schwartz space. The *inverse Fourier transform* is given by

$$\mathcal{F}^{-1}u(x) = \check{u}(x) = \frac{1}{(2\pi)^n}\int_{\mathbb{R}^n} u(\xi) e^{ix\cdot\xi} d\xi. \tag{2.5}$$

We recall the basic properties of Fourier transform without proof.

Proposition 2.1. *The Fourier transform $\mathcal{F} : \mathscr{S} \to \mathscr{S}$ extend to a continuous linear isomorphism $\mathcal{F} : \mathscr{S}' \to \mathscr{S}'$, with the following properties.*

- *(Plancherel theorem) Up to a normalization constant, $\mathcal{F}$ is an isometry on $L^2(\mathbb{R}^n)$:*

$$\|\mathcal{F}u\|_{L^2}^2 = (2\pi)^n \|u\|_{L^2}^2.$$

- $\mathcal{F}\partial_{x_j} = i\xi_j \mathcal{F}$, $\mathcal{F}x_j = i\partial_{\xi_j}\mathcal{F}$.

Using Fourier transform, we can define the Weyl quantization for $a \in \mathscr{S}(\mathbb{R}^{2n})$ by

$$\mathrm{Op}^w(a)u(x) = a^w(x,D)u(x) = \frac{1}{(2\pi)^n}\int e^{i(x-y)\cdot\xi} a\left(\frac{x+y}{2},\xi\right)u(y)dyd\xi, \quad u \in \mathscr{S}(\mathbb{R}^n). \tag{2.6}$$

For $u \in \mathscr{S}$ you can check that $a^w(x,D)u \in \mathscr{S}$ as well.

Here

$$D_{x_j} = \frac{1}{i}\frac{\partial}{\partial x_j}.$$

This definition can be extended to a more general class of symbols such that $\mathrm{Op}^w(x_j)$ is multiplication by x_j and $\mathrm{Op}^w(\xi_j) = D_{x_j}$. In this class we will only need the case when $a \in \mathscr{S}$ or when $a(x,\xi)$ is a polynomial in ξ.

Example 3. The quantization of Landau's Hamiltonian is given by

$$P = \frac{1}{2}\sum_j (D_{x_j} - A_j(x))^2 + V(x).$$

This is called the magnetic Schrödinger operator.

2.3. **Unbounded operators.** The quantization of a classical observable is ususally an unbounded operator on a Hilbert space. We recall some results for unbounded operators.

Definition 2.2. *Let H_1, H_2 be Banach spaces. An unbounded operator $P : H_1 \to H_2$ means a linear subspace $D(P) \subset H_1$ along with a linear map $P : D(P) \to H_2$. P is called densely defined if $D(P)$ is dense in H_1.*

Definition 2.3. *The graph of an unbounded operator $P : H_1 \to H_2$ is*

$$G(P) = \{(x, Px) : x \in D(P)\} \subset H_1 \times H_2.$$

P is closed if the graph is closed. P is closeable if $\overline{G(P)}$ is the graph of an operator $\overline{P}$, called the closure of P. We say $P \subset Q$ if $G(P) \subset G(Q)$.

We will say a densely defined operator $P : H \to H$ on a Hilbert space H to be *formally self-adjoint* or *symmetric* if

$$\langle Pu, v\rangle = \langle u, Pv\rangle, \quad u, v \in D(P).$$

Given a densely defined operator $P : H_1 \to H_2$ between Hilbert spaces, the adjoint P^* is defined as

$$D(P^*) = \{u \in H_2 : \exists C = C(u), \text{ such that } |\langle u, Pv\rangle_{H_2}| \le C\|v\|_{H_1}, \forall v \in D(P)\}$$

and $P^* : D(P^*) \to H_1$ satisfying

$$\langle P^*u, v\rangle = \langle u, Pv\rangle, \quad u \in D(P^*), v \in D(P).$$

The adjoint is well-defined by Riesz representation theorem. We recall some facts of the adjoint operator without proof

Proposition 2.4. *The operator P^* is closed. Also, if P^* is densely defined, then P is closeable and $\overline{P} = P^{**}$.*

Now we can define *self-adjoint* operators.

Definition 2.5. *Let $P : H \to H$ be a symmetric operator on a Hilbert space H. We say P is self-adjoint if $P = P^*$. P is called essentially self-adjoint if $\overline{P}$ is self-adjoint, that is $\overline{P} = P^*$.*

Example 4. One way to obtain self-adjoint extensions of symmetric semibounded operators is via Friedrich's extension: suppose that P is a densely defined operator with a domain $D_0(P)$ and that

$$c_0 := \inf_{\|u\|=1, u\in D_0(P)} \langle Pu, u\rangle > -\infty.$$

Then there exists a self-adjoint extension of P with domain $D(P)$ such that

$$\langle Pu, u\rangle \geq c_0\|u\|^2, \quad u \in D(P).$$

For the proof see for instance [Ho88, Theorem 3.2.10].

Example 5. Suppose $A_j(x)$ are linear, $V(x) = 0$. Then Landau's Hamiltonian

$$\frac{1}{2}\sum_j (D_{x_j} - A_j(x))^2,$$

defined with the domain given by $\mathscr{S}(\mathbb{R}^n)$ is an essentially self-adjoint operator. This follows from a more general case of operator of the form

$$P = \frac{1}{2}\langle Ax, x\rangle + \frac{1}{2}\langle Bx, D_x\rangle + \frac{1}{2}\langle D_x, Bx\rangle + \frac{1}{2}\langle CD_x, D_x\rangle$$

where $A = A^T$, $C = C^T$ are two symmetric matrices. Let

$$p(x,\xi) = \frac{1}{2}\langle Ax, x\rangle + \langle Bx, \xi\rangle + \frac{1}{2}\langle C\xi, \xi\rangle,$$

be the symbol of P in the sense that for $u \in \mathscr{S}$,

$$Pu = p^w(x, D)u.$$

Let N_p be the operator P with domain $D(N_p) = \mathscr{S}(\mathbb{R}^n)$ and M_p be the operator P with domain

$$D(M_p) = \{u \in L^2(\mathbb{R}^n) : Pu \in L^2(\mathbb{R}^n)\}.$$

The proof of the following properties can be found in [Zw12, Appendix C.2]

- M_p is closed;
- $\overline{N}_p = M_p$;

- $N_p^* = M_p^* = M_{\bar{p}}$.

Those properties imply that if p is real-valued, then M_p is a self-adjoint operator and N_p is essentially self-adjoint.

The importance of self-adjointness is due to the following spectral theorem.

Theorem 1. *Let $P : H \to H$ be a self-adjoint operator on a Hilbert space. Then there exists a measure space $(X, \mathcal{M}, \mu)$, a measuable function $f : X \to \mathbb{R}$ and a unitary operator $U : H \to L^2(X, \mu)$ such that*

- *$x \in D(P)$ if and only if $f \cdot Ux \in L^2(X, \mu)$;*
- *$U(Px) = f \cdot Ux$ for any $x \in D(P)$.*

Remark 1. *The spectrum of an arbitrary operator P is defined as*

$$\mathrm{Spec}(P) = \{z \in \mathbb{C} : P - z \textit{ is not invertible } \}.$$

In the case of self-adjoint operators, we can apply Theorem 1 so that it is given by $\overline{f(X)}$. In particular in that case the spectrum is real.

Using spectral theorem, we can define the unitary evolution by

$$U(t) = e^{-itP} : H \to H, \quad U(t) = U^* M_{\exp(-itf)} U, \quad e^{-itf} \in L^\infty(X, \mu).$$

One then checks (again using the spectral theorem) that for $u \in D(P)$,

$$\|(U(t+h) - U(t))u/h + iPU(t)u\|_H \to 0, \quad h \to 0.$$

(Convert P to multiplication by f and use dominated convergence theorem based on $fu \in L^2$.)

A quantum observable is a linear operator $A : H \to H$, the evolution of a quantum system is described by (Heisenberg picture)

$$A(t) = U(t)^* A U(t).$$

In other words,

$$\frac{d}{dt} A(t) = i[P, A(t)]. \tag{2.7}$$

Comparing the quantum evolution (2.7) with the classical evolution (2.3), we obtain a similarity between them. The Poisson bracket corresponds to the commutator after quantization. This is explained in the following example.

Example 6. We have $\{\xi_k, x_j\} = \delta_{jk}$ and $[\xi_k^w, x_j^w] = [D_{x_k}, x_j] = \frac{1}{i}\delta_{jk}$.

The ideal generalization of this would be

$$[p^w, q^w] = -i\{p, q\}^w,$$

for the quantization (2.6) or another form of quantization. However the Groenewold–Van Hove theorem showed that it is impossible. However, it remains true up to "lower order terms" – see Proposition 2.7.

2.4. **Properties of pseudodifferential operators.** The Weyl quantization has many good properties.

Proposition 2.6.
- *Formally, $(a^w)^* = (\overline{a})^w$. In particular, if a is real, then a^w is formally self-adjoint.*
- *(Calderon–Vaillancourt theorem* [Zw12, Theorem 4.23]*) If $\partial^\alpha_{x,\xi} a \in L^\infty$, then $a^w(x,D) : L^2 \to L^2$ is bounded.*
- *(Beals theorem* [Zw12, Theorem 8.3]*) If $A : L^2 \to L^2$ is bounded and $\operatorname{ad}_{x_j} \operatorname{ad}_{\xi_k} \cdots A : L^2 \to L^2$ is also bounded, then there exists $a : \mathbb{R}^{2n} \to \mathbb{C}$ with $\partial^\alpha_{x,\xi} a \in L^\infty$ such that $A = a^w(x,D)$.*

The first property is straightforward calculation. The next two are deeper. We will not prove those properties here but just indicate the L^2 boundedness is easy if we assume $a \in \mathscr{S}$. In fact, when $a \in \mathscr{S}$, we write

$$a^w\widehat{(x,D)}u(\eta) = \frac{1}{(2\pi)^n}\int\int\int a\left(\frac{x+y}{2},\xi\right)e^{i(x-y)\cdot\xi}u(y)e^{-ix\cdot\eta}dyd\xi dx.$$

We write the phase as follows

$$\langle x-y,\xi\rangle - \langle x,\eta\rangle = -2\langle \tfrac{x+y}{2}, \eta-\xi\rangle - \langle y, 2\xi-\eta\rangle.$$

We then put

$$\hat{a}_1(\zeta,\xi) := \int a(z,\xi)e^{-iz\cdot\zeta}dz.$$

Hence,

$$\begin{aligned} a^w\widehat{(x,D)}u(\eta) &= \frac{2^n}{(2\pi)^n}\int \hat{a}_1(2\eta-2\xi,\xi)\hat{u}(2\xi-\eta)d\xi \\ &= \frac{1}{(2\pi)^n}\int \hat{a}_1(\eta-\zeta,\tfrac{\eta+\zeta}{2})\hat{u}(\zeta)d\zeta := [K\hat{u}](\eta). \end{aligned}$$

Because of Parseval's identity ($\|u\|_{L^2} = (2\pi)^{-n/2}\|\hat{u}\|_{L^2}$) it is enough to prove

$$\|Kv\|_{L^2} \le C\|v\|_{L^2}. \tag{2.8}$$

We now recall Schur's criterion for boundedness on L^2: if

$$Kv(\eta) = \int K(\eta,\zeta)v(\zeta)d\zeta$$

and

$$\int |K(\eta,\zeta)|d\eta \le C, \quad \int |K(\eta,\zeta)|d\zeta \le C, \tag{2.9}$$

then (2.8) holds with the same C. In fact, using Cauchy–Schwarz inequality we see that

$$\|Kv\|_{L^2}^2 = \int \left| \int K(\eta,\zeta) v(\zeta) d\zeta \right|^2 d\eta \leq \int \left(\int |K(\eta,\zeta)| d\zeta \right) \left(\int |K(\eta,\zeta)| |v(\zeta)|^2 d\zeta \right) d\eta$$
$$\leq \left(\sup_\eta \int |K(\eta,\zeta)| d\zeta \right) \left(\sup_\zeta \int |K(\eta,\zeta)| d\eta \right) \left(\int |v(\zeta)|^2 d\zeta \right) \leq C^2 \|v\|_{L^2}^2, \tag{2.10}$$

which proves (2.8).

In our specific case

$$K(\eta,\zeta) := \frac{1}{(2\pi)^n} \hat{a}_1(\eta - \zeta, \tfrac{\eta+\zeta}{2}),$$

and (2.9) holds as $a \in \mathscr{S}$ so that $a_1 \in \mathscr{S}$ as well.

We note that we can use a weaker condition:

$$|\hat{a}_1(\zeta,\xi)| \leq (1 + |\zeta|)^{-n-\varepsilon}, \quad \varepsilon > 0,$$

as that also implies (2.9).

The composition properties for quantizations are also interesting. We recall the following result without proof. In principle, it could be shown without general theory since it involves only differential operators.

Proposition 2.7. *Suppose $a_j = \sum_{|\alpha| \leq m_j} a_{j,\alpha}(x) \xi^\alpha$, $j = 1, 2$. Then $a_1^w \circ a_2^w = a_3^w$ with*

$$a_3 \sim \sum_{k=0}^\infty \frac{1}{k!} \left(\frac{i}{2} \sigma(D_x, D_\xi, D_y, D_\eta) \right)^k a_1(x,\xi) a_2(y,\eta)|_{x=y,\xi=\eta}, \tag{2.11}$$

where σ is the symplectic form given in (2.1). In particular,

$$[a_1^w(x,D), a_2^w(x,D)] = \frac{1}{i} \{a_1, a_2\}^w(x,D) + r^w(x,D),$$

where $\xi \mapsto r(x,\xi)$ is a polynomial of degree less than the degree of $\{a_1, a_2\}$ (which is less than or equal to $m_1 + m_2 - 1$.)

We refer to [Zw12, Theorem 4.12] for the proof and the sense in which the asymptotic expansion (2.11) is valid.

2.5. **Trace class operators.** In this section we recall basic properties of trace class operators.

Let H be a Hilbert space and $A : H \to H$ be a compact operator. Then $\mathrm{Spec}(A) = \{\lambda_i\}$ is discrete and can be ordered as

$$|\lambda_0| \geq |\lambda_1| \geq \cdots \geq |\lambda_j| \to 0. \tag{2.12}$$

If A is self-adjoint, then λ_j's are real. Moreover, there exists an orthonormal basis $\{e_j\}$ consisting of eigenvectors of A, such that

$$Au = \sum_j \lambda_j \langle u, e_j \rangle e_j.$$

In the non-self-adjoint case, there is a similar form using *singular value decomposition* (SVD).

Proposition 2.8. *Let H_1, H_2 be Hilbert spaces and $A : H_1 \to H_2$ be a compact operator. Then there exists*

$$s_0 \geq s_1 \geq \cdots \geq s_j \to 0, \tag{2.13}$$

and orthonormal sets $\{e_j\} \subset H_1$, $\{f_j\} \subset H_2$, such that

$$Au = \sum_j s_j \langle u, e_j \rangle f_j.$$

In fact $\{s_j\} \setminus \{0\} = \mathrm{Spec}((A^*A)^{1/2}) \setminus \{0\} = \mathrm{Spec}((AA^*)^{1/2}) \setminus \{0\}$.

Proof. Observe that $A^*A : H_1 \to H_1$ is a non-negative self-adjoint operator. Let $\{e_j\}$ be the eigenvectors corresponding to the eigenvalues $s_j^2 = \lambda_j(A^*A)$. Let

$$f_j = \begin{cases} s_j^{-1} A e_j, & s_j \neq 0 \\ 0, & s_j = 0. \end{cases}$$

Then it is direct to check f_j's are orthonormal and

$$Au = \sum_j s_j \langle u, e_j \rangle f_j.$$

$\square$

The set $\{s_j\}$ are called *singular values* of A. We list some properties without proof.

- $s_n(A) = \min\{\|A - K\|_{H_1 \to H_2} : \mathrm{rank}\, K \leq n\}$.
- $s_{j+k}(A + B) \leq s_j(A) + s_k(B)$.
- $s_{j+k}(AB) \leq s_j(A) s_k(B)$. In particular, $s_k(AB) \leq \|A\| s_k(B)$.

Here is an example of how to use those inequalities.

Example 7. Let $s > 0$ and $A : L^2(\mathbb{T}^n) \to H^s(\mathbb{T}^n) \subset L^2(\mathbb{T}^n)$ be a bounded operator, then $s_j(A) \leq C j^{-s/n}$. This is because

$$\begin{aligned} s_j(A) &= s_j((-\Delta + 1)^{-s/2} (-\Delta + 1)^{s/2} A) \\ &\leq \|(-\Delta + 1)^{s/2} A\|_{L^2 \to L^2} s_j((-\Delta + 1)^{-s/2}) \\ &\leq C j^{-s/n}. \end{aligned}$$

The claim $s_j((-\Delta+1)^{-s/2}) \leq Cj^{-s/n}$ is proved by lattice point counting:

$$\#\{s_j : |s_j| \geq r\} \lesssim \#\{m \in \mathbb{Z}^n : (m^2+1)^{-s/2} \geq r\} \lesssim r^{-n/s}.$$

Now we can give the definition of trace class operators.

Definition 2.9. *Let H be a Hilbert space, the family of trace class operators is*

$$\mathcal{L}_1(H) = \{A : H \to H : A \text{ is compact and } \sum_j s_j(A) < \infty\}.$$

The norm for $\mathcal{L}_1(H)$ is defined as

$$\|A\|_1 = \sum_j s_j(A).$$

It makes $\mathcal{L}_1(H)$ a Banach space with a continuous functional called trace:

$$\operatorname{tr}(A) = \sum_j \langle Ae_j, e_j\rangle$$

where e_j is any orthonormal basis.

The trace norm can also be written as

$$\|A\|_1 = \sum_j \langle |A|e_j, e_j\rangle$$

where $|A| = (A^*A)^{1/2}$ and $\{e_j\}$ is any orthonormal basis. This is because for two orthonormal bases $\{e_j\}$ and $\{f_j\}$ we have

$$\sum_j \langle |A|e_j, e_j\rangle = \sum_{j,k,k'} \langle |A|f_k, f_{k'}\rangle \langle e_j, f_k\rangle \overline{\langle e_j, f_{k'}\rangle} = \sum_k \langle |A|f_k, f_k\rangle. \tag{2.14}$$

If $A \in \mathcal{L}_1(H)$, then $A = U|A|$ for some unitary operator U. Thus

$$\begin{aligned}\sum_j |\langle Ae_j, e_j\rangle| = \sum_j |\langle U|A|e_j, e_j\rangle| &\leq \sum_j \||A|^{1/2}e_j\|\||A|^{1/2}U^*e_j\| \\ &\leq \left(\sum_j \langle |A|e_j, e_j\rangle \sum_k \langle |A|U^*e_k, U^*e_k\rangle\right)^{1/2} = \sum_j s_j = \|A\|_{\mathcal{L}_1}.\end{aligned}$$

So the trace is well defined and bounded by the trace norm. For the same reason as (2.14), the definition of trace does not depend on the choice of orthonormal bases.

We recall some properties of trace class operators without proof.

- (Lidskii's theorem) If $A \in \mathcal{L}(H)$ has eigenvalues λ_j ordered as (2.12), then $\operatorname{tr}(A) = \sum_j \lambda_j$.

- (Weyl inequalities) Let $A \in \mathcal{L}_1(H)$ with eigenvalues λ_j and singular values s_j ordered as in (2.12) and (2.13), then
$$\sum_{j=0}^{n} |\lambda_j| \le \sum_{j=0}^{n} s_j, \quad \forall n,$$
$$\prod_{j=0}^{n} (1+|\lambda_j|) \le \prod_{j=0}^{n} (1+s_j), \quad \forall n.$$
- If $A : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is in $\mathcal{L}_1(L^2(\mathbb{R}^n))$, with integration kernel $K_A(x,y)$, then $K_A(x,x) \in L^1(\mathbb{R}^n)$ and
$$\operatorname{tr}(A) = \int_{\mathbb{R}^n} K_A(x,x)dx.$$
This is easily verified by $K_A(x,y) = \sum s_j(A) f_j(x)\overline{e_j(y)}$.

We remark that the trace class condition is much stronger than the condition that $K_A(x,x)$ can be integrated. For example, for any $a \neq 1$, $Au(x) = u(ax)$ gives a bounded operator with $K_A(x,y) = \delta(y-ax)$. Then $K_A(x,x) = \delta((1-a)x) = |1-a|^{-1}\delta(x)$ and
$$\int K_A(x,x)dx = |1-a|^{-1}.$$
But A is far from being in the trace class.

2.6. **Grushin problems.** In this section we review Schur's complement formula and its application to spectral theory. Schur's complement formula is a direct lemma in linear algebra:

Lemma 2.10. *Suppose*
$$\begin{pmatrix} P & R_- \\ R_+ & R_{+-} \end{pmatrix} = \begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix}^{-1} : X_1 \times X_- \to X_2 \times X_+ \tag{2.15}$$
are bounded operators on Banach spaces, then P is invertible if and only if E_{-+} is invertible. Moreover, in such case we have
$$P^{-1} = E - E_+ E_{-+}^{-1} E_-, \quad E_{-+}^{-1} = R_{+-} - R_+ P^{-1} R_-. \tag{2.16}$$

Proof. The proof is direct. If E_{-+} is invertible, then from
$$PE + R_-E_- = I, \quad PE_+ + R_-E_{-+} = 0,$$
we get $PE - PE_+E_{-+}^{-1}E_- = I$. Similarly, since
$$EP + E_+R_+ = I, \quad E_-P + E_{-+}R_+ = 0,$$
we get $EP - E_+E_{-+}^{-1}E_-P = I$. We conclude that P is invertible and $P^{-1} = E - E_+E_{-+}^{-1}E_-$. The proof for the other direction is similar. □

If $R_{+-} = 0$, we have the following observation.

Proposition 2.11. *If $R_{+-} = 0$ in (2.15), then R_+ and E_- are surjective, and R_- and E_+ are injective.*

Proof. This is because we have

$$R_+E_+ = I, \quad E_-R_- = I.$$

∎

We will call the $R_{+-} = 0$ case a Grushin problem, that is

$$\begin{pmatrix} P & R_- \\ R_+ & 0 \end{pmatrix} = \begin{pmatrix} E & E_+ \\ E_- & E_{-+} \end{pmatrix}^{-1} : X_1 \times X_- \to X_2 \times X_+ \tag{2.17}$$

Perturbation of Grushin problems are stable due to the Neumann series argument.

Proposition 2.12. *Suppose (2.17) is true, and suppose $A : X_1 \to X_2$ satisfies*

$$\|EA\|_{X_1\to X_1}, \|AE\|_{X_2\to X_2} < 1,$$

then the Grushin problem

$$\mathcal{P}_A = \begin{pmatrix} P + A & R_- \\ R_+ & 0 \end{pmatrix}$$

is still well-posed with inverse

$$\begin{pmatrix} F & F_+ \\ F_- & F_{-+} \end{pmatrix}$$

where

$$F_{-+} = E_{-+} + \sum_{k=1}^{\infty} (-1)^k E_- A (EA)^{k-1} E_+.$$

Proof. Let

$$\mathcal{P} = \mathcal{E}^{-1} = \begin{pmatrix} P & R_- \\ R_+ & 0 \end{pmatrix}$$

then

$$\mathcal{P}_A = \mathcal{P}\left(1 + \mathcal{E}\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}\right)$$

and

$$\begin{aligned}\mathcal{P}_A^{-1} &= \left(1 + \mathcal{E}\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}\right)^{-1} \mathcal{P}^{-1} = \sum_{k=0}^{\infty} (-1)^k \left(\mathcal{E}\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}\right)^k \mathcal{E} \\ &= \mathcal{E} + \sum_{k=1}^{\infty} (-1)^k \begin{pmatrix} (EA)^k & 0 \\ E_-A(EA)^{k-1} & 0 \end{pmatrix} \mathcal{E}.\end{aligned}$$

□

We will usually study the Grushin problem for Fredholm operators. For more details, see [DyZw2, Appendix C].

Definition 2.13. *A bounded linear operator $P : X_1 \to X_2$ between two Banach spaces is called a Fredholm operator if the kernel and cokernel of P are both finite dimensional. The index of a Fredholm operator is defined as*

$$\mathrm{ind} P = \dim \ker P - \dim \operatorname{coker} P.$$

Proposition 2.14. *(i) Suppose $P : X_1 \to X_2$ is a Fredholm operator. Then there exists finite dimensional spaces $X_\pm$ and operators $R_- : X_- \to X_2$ and $R_+ : X_1 \to X_+$ such that the Grushin problem (2.17) is well-posed. In particular, the image of P is closed.*

(ii) Suppose the Grushin problem (2.17) is well-posed, then P is a Fredholm operator if and only if E_{-+} is a Fredholm operator, and

$$\mathrm{ind} P = \mathrm{ind} E_{-+}.$$

Proof. (i) Let $n_+ = \dim \ker P$ and $n_- = \dim \operatorname{coker} P$. Let $X_\pm = \mathbb{C}^{n_\pm}$. Suppose $\ker P$ is spanned by $x_1, \cdots, x_{n_+}$, by Hahn-Banach theorem there exists $x_j^* : X_1 \to \mathbb{R}$ such that $x_j^*(x_i) = \delta_{ij}$. We then define

$$R_+ : X_1 \to \mathbb{C}^{n_+}, \quad x \mapsto (x_1^*(x), \cdots, x_{n_+}^*(x)).$$

On the other hand, choose a representative $y_1, \cdots, y_{n_-}$ of $\operatorname{coker} P$ and define

$$R_- : \mathbb{C}^{n_-} \to X_2, \quad (a_1, \cdots, a_{n_-}) \mapsto \sum_{j=1}^{n_-} a_j y_j.$$

We claim the operator

$$\begin{pmatrix} P & R_- \\ R_+ & 0 \end{pmatrix}$$

is bijective. First, if

$$\begin{pmatrix} P & R_- \\ R_+ & 0 \end{pmatrix} \begin{pmatrix} u \\ u_- \end{pmatrix} = 0,$$

then since the intersection of the range of P and R_- is zero, we have $Pu = R_- u_- = 0$, so $u_- = 0$ and $u \in \ker P$. By $R_+ u = 0$ we conclude $u = 0$. We conclude injectiveness. On the other hand, $(R, R_-) : X_1 \times X_- \to X_2$ is surjective by definition. Since modifying $u \in \ker P$ does not affect value of Pu, we conclude the whole matix is also surjective.

Finally, PX_1 can be viewed as the image of the closed subspace $(X_1, 0)$ under the invertible map (P, R_+) $(\mathrm{mod} \ker P)$. So the image of P is closed.

(ii) Take $u_- = 0$, we observe that

$$Pu = v \quad \Longleftrightarrow \quad u = Ev + E_+ v_+,\ 0 = E_- v + E_{-+} v_+. \tag{2.18}$$

So $E_- : PX_1 \to E_{-+}X_+$ and induces

$$E_-^{\#} : X_2/PX_1 \to X_-/E_{-+}X_+.$$

By Proposition 2.11, E_- is surjective, so $E_-^{\#}$ is surjective. On the other hand, $E_- v \in E_{-+}X_+$ will give us $v \in PX_1$ by (2.18), so $E_-^{\#}$ is also injective. We conclude

$$\dim \operatorname{coker} P = \dim \operatorname{coker} E_{-+}.$$

Now we look at

$$E_+ : \ker E_{-+} \to \ker P.$$

It is injective by Proposition 2.11. Moreover, if $u \in \ker P$, then by (2.18) we get $v_+ \in \ker E_{-+}$ such that $E_+ v_+ = u$, so E_+ is also surjective. We conclude

$$\dim \ker P = \dim \ker E_{-+}.$$

This finishes the proof of (ii). □

Corollary 2.15.
- *The family of Fredholm operators is open and the index map is locally constant, that is*

$$\operatorname{ind} : \pi_0(\operatorname{Fred}(\mathcal{H}_1, \mathcal{H}_2)) \to \mathbb{Z}.$$

- *If K is a compact operator, then* $\operatorname{ind}(I + K) = 0$.
- *A Fredholm operator has closed image.*

2.7. **Vector bundles.** Let E, X be topological spaces, $\pi : E \to X$ is called a (complex) *vector bundle* of rank r if for any $x \in X$, $\pi^{-1}(x)$ is a (complex) vector space of dimension r, and there exists a covering $\{U_i\}$ of X such that we have an isomorphism which is linear on each fiber

$$\begin{tikzcd} \pi^{-1}(U_i) \arrow[r, "\cong"] \arrow[d, "\pi"'] & U_i \times \mathbb{C}^r \arrow[dl, "\mathrm{pr}_1"] \\ U_i & \end{tikzcd}$$

A vector bundle of rank 1 is called a *line bundle*. We will only consider complex vector bundles.

Let E, F be two vector bundles over X. A vector bundle morphism $f : E \to F$ is a continuous map preserving each fiber and linear on each fiber:

$$\begin{tikzcd} E \arrow[r, "f"] \arrow[d] & F \arrow[dl] \\ X & \end{tikzcd}$$

A bijective morphism is called an isomorphism. Let $g : Y \to X$ be a continuous map between topological spaces, $\pi : E \to X$ be a vector bundle on X, then the pullback bundle $\pi_{g^*E} : g^*E \to Y$ is defined as

$$g^*E := \{(y,p) : y \in Y, p \in E, \pi(p) = g(y)\}, \quad \pi_{g^*E}(y,p) := y.$$

If $Y \to X$ is an inclusion, then pullback bundle can be thought of as the restriction of the bundle E to Y and we denote it by $E|_Y$.

A vector bundle isomorphic to $X \times \mathbb{C}^r$ is called a trivial bundle. In general, a vector bundle can be nontrivial, and we are interested in criteria guaranteeing triviality. One is provided by the following proposition from Bott–Tu [BoTu82, Section 6].

Proposition 2.16. *Let X be a compact Hausdorff space, and $E \to X \times [0,1]$ be a vector bundle. Let $p_1 : X \times [0,1] \to X$ be the projection to X and $i_0 : X = X \times \{0\} \to X \times [0,1]$ be the inclusion, then $E \cong p_1^* i_0^* E$. In particular, if $i_0^* E$ is trivial, then E is trivial.*

Proof. Let $F = i_0^* E$. It suffices to construct an isomorphism between E and $p_1^* F$. We call the variable $t \in [0,1]$, then at $t = 0$, $E|_{t=0} = F$ by definition. We can then find a finite cover U_i of X, such that over each U_i, there exists $\varepsilon_i > 0$ such that the isomorphism extends to $U_i \times [0, \varepsilon_i]$. Using a partition of unity, we get a map $E \to p_1^* F$ in a neighbourhood $X \times [0, \varepsilon]$ for some $\varepsilon > 0$. By choosing ε small, we may assume it is an isomorphism since isomorphism is an open condition. By connectedness of $[0,1]$, we can extend this isomorphic to the whole $X \times [0,1]$. □

Corollary 2.17. *Any vector bundle over a compact contractible Hausdorff space is trivial.*

Proof. By definition, X is contractible if there exist (with $*$ denoting a point space) $i : * \to X$, $p : X \to *$ and $H : X \times [0,1] \to X$ such that $H_0 = \mathrm{id}_X$ and $H_1 = i \circ p$. By Proposition 2.16, $E = H_0^* E \cong H_1^* E = p^* i^* E$. So E is a trivial bundle. □

For paracompact spaces, this remains true but the proof becomes a bit more subtle. We provide a direct proof for the case we will need.

Corollary 2.18. *Any vector bundle over $\mathbb{R}^n$ is trivial.*

Proof. Let E be a vector bundle over $\mathbb{R}^n$. Then E is trivial over $\overline{B}(0,\varepsilon)$ for some $\varepsilon > 0$. Since $\overline{B}(0,R) \setminus B(0,\varepsilon)$ is homeomorphic to $S^{n-1} \times [0,1]$, we conclude from Proposition 2.16 that E is trivial over $B(0,R)$ for any $R > 0$. Then it is easy to glue those trivializations to get a global trivialization of E over $\mathbb{R}^n$. ☐

3. Spectra of magnetic Schrödinger operators

Let $B > 0$ be a constant and suppose we have a constant magnetic field $\vec{B} = (0,0,B)$. Let the vector potential be $A = (0, Bx_1, 0)$. We are interested in the spectrum of the magnetic Schrödinger operator

$$P_B = D_{x_1}^2 + (D_{x_2} + Bx_1)^2 + D_{x_3}^2 \tag{3.1}$$

with symbol $p_B = \xi_1^2 + (\xi_2 + Bx_1)^2 + \xi_3^2$. We have proved in Example 5 that P_B is self-adjoint with domain

$$D(P_B) = \{u \in L^2(\mathbb{R}^3) : P_B u \in L^2(\mathbb{R}^3)\}.$$

Before studying P_B, we first look at two simpler examples.

3.1. **Spectrum of the Laplace operator.**

Let $P = -\Delta$ be the Laplace operator on $\mathbb{R}^n$, with domain $D(P) = \{u \in L^2(\mathbb{R}^n) : Pu \in L^2\} = H^2(\mathbb{R}^n)$. Then we may use Fourier transform to conjugate and explicitly diagonalize it. Let

$$Uu(\xi) = \frac{1}{(2\pi)^{n/2}} \int u(x) e^{-ix\cdot\xi} dx,$$

then $U : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is unitary, and

$$UPU^* = |\xi|^2.$$

In particular, $\mathrm{Spec}(P) = [0, \infty)$.

The propagation equation

$$(i\partial_t - P)u = 0, \quad u|_{t=0} = u_0$$

can be explicitly solved by

$$\hat{u}(\xi) = e^{-it|\xi|^2} \hat{u}_0.$$

We call $\lambda = |\xi|^2$ the dispersion relation.

There is a similar operator $P_0 = \sqrt{-\Delta}$. We can also diagonalize it by $UP_0U^* = |\xi|$. The dispersion relation for the corresponding half wave equation $(i\partial_t - P_0)u = 0$ will then be $\lambda = |\xi|$.

3.2. **Spectrum of the harmonic oscillator.** Let $P_\omega = -\Delta + \sum_{j=1}^d \omega_j^2 x_j^2$, $\omega_j > 0$. This is called the harmonic oscillator. For each j, we can do a change of variable $y_j = \sqrt{\omega_j} x_j$ and get

$$D_{x_j}^2 + \omega_j^2 x_j^2 = \omega_j (D_y^2 + y^2).$$

Without loss of generality, we study the operator $P = D_x^2 + x^2$ on $\mathbb{R}$. We define the "annihilation operator" $A = D_x - ix$ and the "creation operator" $A^* = D_x + ix$. We notice

- $A^*A = D_x^2 + x^2 - 1 = P - 1$;
- $AA^* = D_x^2 + x^2 + 1 = P + 1$;
- $[A, A^*] = 2$.

Let $v_0 = e^{-x^2/2}$, then it is easy to verify that $Av_0 = 0$, thus $Pv_0 = v_0$. We notice $PA^*v_0 = (A^*A+1)A^*v_0 = 3A^*v_0$, so we will let $v_1 = A^*v_0$ and we have $Pv_1 = 3v_1$. In general, let

$$v_n = (A^*)^n v_0$$

then

$$Pv_n = (2n+1)v_n.$$

So A^* "creates" higher and higher excited states of P. Since v_n are eigenvectors of P with distinct eigenvalues, we have

$$\langle v_n, v_m \rangle = 0, \quad n \neq m.$$

Let $u_n = \dfrac{v_n}{\|v_n\|_{L^2}} = H_n(x)e^{-x^2/2}$, it is easy to verify inductively that $H_n(x)$ are polynomials of degree n, with nonvanishing leading coefficients. Moreover, $H_n(-x) = (-1)^n H_n(x)$. Those polynomials $H_n(x)$ are called Hermite polynomials.

We now claim the sequence $\{u_n\}$ is an orthonormal basis of $L^2(\mathbb{R})$. It suffices to prove $\operatorname{span}\{u_n\}$ is dense. We prove by contradiction: suppose there is $0 \neq g \in L^2(\mathbb{R})$ such that

$$0 = \int g(x)\overline{u_n(x)}dx, \quad \forall n \in \mathbb{N},$$

then we know

$$\int g(x)x^n e^{-x^2/2}dx = 0, \quad \forall n \in \mathbb{N}.$$

By Taylor expansion of $e^{-ix\xi}$ we know

$$\int g(x)e^{-ix\xi - x^2/2}dx = 0, \quad \forall \xi \in \mathbb{R}.$$

This implies that $g(x) = 0$, a contradiction.

So if we define

$$U : L^2(\mathbb{R}) \to \ell^2(\mathbb{N}), \quad Uu(n) = \int u(x)\overline{u_n(x)}dx.$$

Then $UPU^*u(n) = (2n+1)u(n)$. In particular,

$$\mathrm{Spec}(P) = \{2n+1 : n \in \mathbb{N}\}.$$

For $P_\omega = -\Delta + \sum_{j=1}^d \omega_j^2 x_j^2$, it follows that

$$\mathrm{Spec}(P_\omega) = \left\{ \sum_{j=1}^d \omega_j (2n_j + 1) : n_j \in \mathbb{N} \right\}.$$

3.3. **Spectrum of the magnetic Schrödinger operator.** Now we come back to the magnetic Schrödinger operator (3.1). We can first use

$$U_1 u(x_1, \xi_2, \xi_3) = \frac{1}{2\pi} \int u(x_1, x_2, x_3) e^{-ix_2\xi_2 - ix_3\xi_3} dx_2 dx_3$$

and get

$$U_1 P U_1^* = D_{x_1}^2 + (\xi_2 + Bx_1)^2 + \xi_3^2.$$

Then it looks very much like the harmonic oscillator: we put

$$x_1 = B^{-\frac{1}{2}} y_1 - B^{-1}\xi_2, \quad y_1 = B^{\frac{1}{2}} x_1 + B^{-\frac{1}{2}}\xi_2,$$

so that

$$D_{x_1}^2 + (\xi_2 + Bx_1)^2 = B(D_{y_1}^2 + y_1^2).$$

This motivates the introduction of the following unitary operator:

$$U_2 v(y_1, \xi_2, \xi_3) = B^{-1/4} v(B^{-1/2} y_1 - B^{-1}\xi_2, \xi_2, \xi_3),$$

for which we have

$$U_2 U_1 P U_1^* U_2^* = B(D_{y_1}^2 + y_1^2) + \xi_3^2.$$

We then use

$$U_3 u(n, \xi_2, \xi_3) = \int u(y_1, \xi_2, \xi_3) \overline{u_n(y_1)} dy_1$$

and let $U = U_3 U_2 U_1$. Then

$$UPU^* u(n, \xi_2, \xi_3) = (B(2n+1) + \xi_3^2) u(n, \xi_2, \xi_3).$$

So we explicitly diagonalize (3.1) and conclude

$$\mathrm{Spec}(P_B) = \{B(2n+1) + \xi_3^2 : n \in \mathbb{N}, \xi_2, \xi_3 \in \mathbb{R}\} = [B, \infty).$$

3.4. **A different gauge.** We could also consider a two dimensional version of P_B:

$$P_B = D_{x_1}^2 + (D_{x_2} + Bx_1)^2. \tag{3.2}$$

In that case

$$\mathrm{Spec}(P_B) = \{B(2n+1) : n \in \mathbb{N}\}.$$

The eigenspaces have infinite multiplicity and are given by

$$H_n := \left\{ u(x) = B^{\frac{1}{4}} \int_{\mathbb{R}} u_n(B^{\frac{1}{2}}x_1 + B^{-\frac{1}{2}}\xi_2) f(\xi_2) e^{ix_2\xi_2} d\xi_2 : f \in L^2(\mathbb{R}) \right\}.$$

It is interesting to compare this to the eigenfunctions in the *symmetric gauge*:

$$P_B = (D_{x_1} - Bx_2/2)^2 + (D_{x_2} + Bx_1/2)^2.$$

In this case, let $w = x_1 + ix_2$, we have

$$\begin{aligned} P_B &= -\Delta + \tfrac{1}{4}B^2|x|^2 - iB(x_1\partial_{x_2} - x_2\partial_{x_1}) \\ &= -4\partial_w\partial_{\bar{w}} + \tfrac{1}{4}B^2|w|^2 - B(w\partial_w - \bar{w}\partial_{\bar{w}}) \\ &= \left(-2\partial_w + \tfrac{1}{2}B\bar{w}\right)\left(2\partial_{\bar{w}} + \tfrac{1}{2}Bw\right) + B \end{aligned}$$

So one ground state is given by $u_0 = \exp(-\frac{Bw\bar{w}}{4})$ and the other ground states can be written as

$$u(w, \bar{w}) = f(w)e^{-\frac{B|w|^2}{4}}$$

where $f(w)$ is a holomorphic function such that

$$\int |f(w)|^2 e^{-\frac{B|w|^2}{2}} dm(w) < \infty.$$

4. Magnetic oscillations for the free electron

In this section we study the magnetic oscillations for the free electron. The mathematical tool to study it is the *density of states*.

4.1. **Motivation.** Suppose A is a self-adjoint matrix acting on $\mathbb{C}^N$. We can then think of

$$d\rho(\lambda) := \sum_{\mu \in \mathrm{Spec}(A)} \delta(\lambda - \mu) d\lambda = \rho(\lambda) d\lambda$$

as measuring *density of states*: we count the number of states per unit of energy:

$$|\mathrm{Spec}(A) \cap [a,b]| = \int_a^b d\rho(\lambda).$$

More generally, we have

$$\sum_{\mu \in \mathrm{Spec}(A)} f(\mu) = \int f(\lambda) d\rho(\lambda), \quad f \in C(\mathbb{R}).$$

Another way to think about this is to order the eigenvalues ("states" in physics) from the smallest one ("ground state") onwards and to consider

$$\omega(\lambda) := |\mathrm{Spec}(A) \cap (-\infty, \lambda]|, \quad \rho(\lambda) = \frac{d\omega(\lambda)}{d\lambda}.$$

We can then think of the measure $d\rho(\lambda)$ as a distribution $\rho \in \mathscr{S}'(\mathbb{R})$ (see §2.2).

These definition is applicable for any operator with discrete spectrum but already care is needed to guarantee that $\rho \in \mathscr{S}'$.

Example 8. Let $P = -\Delta + \sum_{j=1}^n \omega_j^2 x_j^2$, $\omega_j > 0$, be the harmonic oscillator in $\mathbb{R}^n$. Show that for $f \in \mathscr{S}$, $f(P) \in \mathcal{L}_1(L^2(\mathbb{R}^n))$ and that $\mathrm{tr} f(P) = \int f(\lambda)\rho(\lambda)d\lambda$ where $\rho \in \mathscr{S}'(\mathbb{R})$.

This definition of density of states is not applicable to operators appearing in condensed matter physics: already for $P = -\Delta$ we see that $f(P)$ is not of trace class. The same is true for magnetic Schrödinger operators considered in §3. We have then consider *density of states* per unit of energy (as above) per unit volume. That is done by renormalizing the trace and introducing

$$\widetilde{\mathrm{tr}} f(P) := \lim_{L \to \infty} \frac{\mathrm{tr}(\mathbb{1}_{[-L,L]^n} f(P))}{(2L)^n},$$

provided that the traces and the limit exist: we are restricting $f(P)$ to a box of size L, taking the trace and then dividing by the volume of the box and letting $L \to \infty$.

Density of states plays an important role in the *kinetic theory of solids* as it allows calculations of such quantities as the internal energy, specific heat capacity and thermal conductivity. In this section, we will be interested in the internal energy and magnetization. That corresponds to choosing the function f in $\widetilde{\mathrm{tr}} f(P_B)$ using the *Dirac–Fermi* distribution (see [Ka03, §D.1.2]): for chemical potential z_0 and temperature T we take

$$f(\lambda) := f_{T,z_0}(\lambda) := T \log\left(1 + \exp\left(\frac{z_0 - \lambda}{T}\right)\right). \tag{4.1}$$

From the mathematical point of view we will be interested in asymptotic behaviour of free energy, Ω and magnetization m,

$$\Omega(B) = \Omega(B, T, z_0, N) := N z_0 - \widetilde{\mathrm{tr}} f_{z_0,T}(P_B), \quad m(B) = \partial_B \Omega(B, T, z_0, N). \tag{4.2}$$

as $T \to 0$ and $B \to 0$. The chemical potential and the number of particles are related by the condition that $\partial_{z_0}\Omega = 0$ but we will make a simplifying assumption and fix N and z_0 (the simplified relation between them can be derived by putting $T = B = 0$ – see [HS90b, §2] for a finer analysis explaining why this approximation is justified). The goal will be to see the oscillations in $m(B)$ as a function of $1/B$ – see Figures 1, 2 and 3. For the fascinating story of theoretical and experimental discoveries related to these oscillations we refer to [Sh84, Chapter 1].

4.2. **Density of states.** Suppose we have a self-adjoint operator P, then for a bounded measurable function f on $\mathbb{R}$, it makes sense to define $f(P) : H \to H$ thanks to spectral theorem. If for any $f \in C_c(\mathbb{R})$, $f(P)$ is in trace class (defined in section 2.5), then we can define $\mathrm{tr} f(P)$ and get a measure μ supported on the spectrum of P, defined via Riesz representation theorem:

$$\mathrm{tr} f(P) = \int f(\lambda) d\rho(\lambda).$$

This measure μ is called the density of states for P. In general, however, we may not have $f(P) \in \mathcal{L}_1$ even for $f \in C_c(\mathbb{R})$, so we will study the regularized trace. In our example, when $H = L^2(\mathbb{R}^n)$, we will study

$$\widetilde{\mathrm{tr}} f(P) = \lim_{L\to\infty} \frac{\mathrm{tr}(\mathbb{1}_{[-L,L]^n} f(P))}{(2L)^n}. \tag{4.3}$$

Let us first look at the example of $P = -\Delta$. In this case

$$f(-\Delta) = \mathcal{F}^{-1} f(|\xi|^2)\mathcal{F}$$

and the integration kernel of $f(-\Delta)$ is given by

$$K_{f(-\Delta)}(x, y) = \frac{1}{(2\pi)^n} \int e^{i(x-y)\cdot\xi} f(|\xi|^2) d\xi.$$

When restricting to the diagonal, $K_{f(-\Delta)}(x, x) = \frac{1}{(2\pi)^n} \int f(|\xi|^2) d\xi$ is a constant and is not integrable. However, when we multiply by a cutoff function $\chi(x) \in C_0^\infty(\mathbb{R}^n)$, the integration kernel of $A = \chi(x) f(-\Delta)$ is

$$K_A(x, y) = \frac{\chi(x)}{(2\pi)^n} \int e^{i(x-y)\cdot\xi} f(|\xi|^2) d\xi \in \mathscr{S}(\mathbb{R}^n \times \mathbb{R}^n).$$

If we fix a torus $\mathbb{T}^n$ containing the support of χ, then

$$A : L^2(\mathbb{R}^n) \to C_0^\infty((B(0, R)) \subset H^s(\mathbb{T}^n), \quad \forall s > 0.$$

Choose $s > n$ and use Example 7, we see $A \in \mathcal{L}_1$ and

$$\mathbb{1}_{[-L,L]^n} f(-\Delta) = \mathbb{1}_{[-L,L]^n} \chi(x) f(-\Delta) \in \mathcal{L}_1.$$

Thus

$$K_{\mathbb{1}_{[-L,L]^n} f(-\Delta)}(x, x) = \frac{\mathbb{1}_{[-L,L]^n}}{(2\pi)^n} \int f(|\xi|^2) d\xi$$

and

$$\mathrm{tr}(\mathbb{1}_{[-L,L]^n} f(-\Delta)) = \frac{(2L)^n}{(2\pi)^n} \int f(|\xi|^2) d\xi.$$

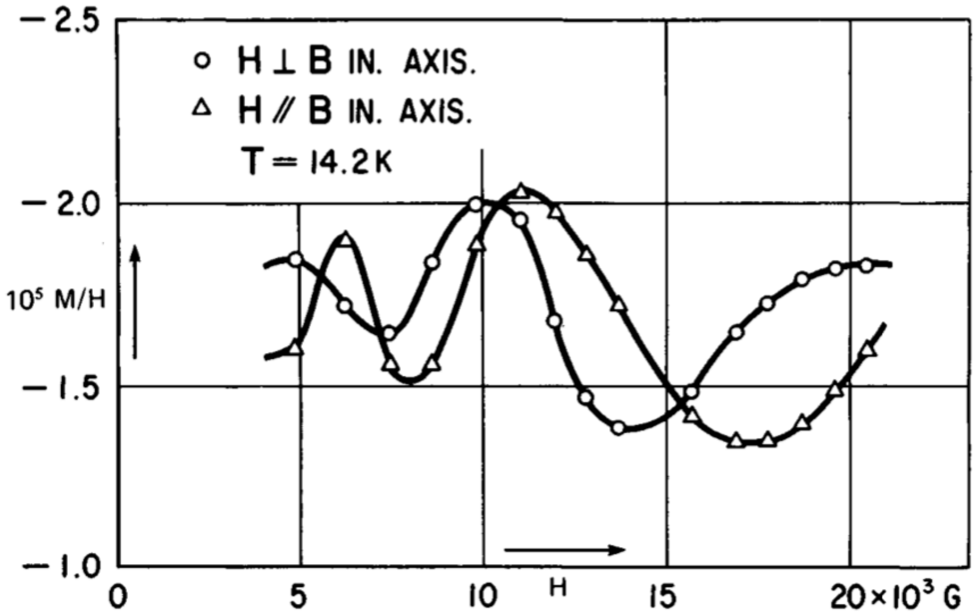


FIGURE 1. The first experimental observation of magnetic oscillations: the de Haas–van Alphen experiment of putting bismuth in magnetic field. Reproduced from [Sh84].

So the regularized trace is given by

$$\begin{aligned}\widetilde{\operatorname{tr}}(f(-\Delta)) &= \frac{1}{(2\pi)^n}\int f(|\xi|^2)d\xi = \frac{1}{(2\pi)^n}\int_{\mathbb{R}}\int_{\mathbb{R}^n}\delta(s-|\xi|^2)d\xi f(s)ds \\ &= \frac{\operatorname{vol}(S^{n-1})}{(2\pi)^n}\int_{\mathbb{R}}\int_0^\infty \delta(s-r^2)r^{n-1}dr f(s)ds \\ &= \int_{\mathbb{R}} c_n s_+^{\frac{n-2}{2}} f(s)ds =: \rho(f), \quad c_n := \frac{\operatorname{vol}(S^{n-1})}{2(2\pi)^n}\end{aligned} \tag{4.4}$$

so the *density of states* is the distribution $c_n s_+^{\frac{n-2}{2}}$, where for $\gamma > -1$,

$$s_+^\gamma := \begin{cases} s^\gamma, & s > 0, \\ 0 & s \le 0. \end{cases} \tag{4.5}$$

4.3. **Two dimensions.** We study the desity of states for the 2-dimensional magnetic Schrödinger operator

$$P_B = D_{x_1}^2 + (D_{x_2} + Bx_1)^2 = U^*(B(2n+1))U$$

where $U : L^2(\mathbb{R}^2) \to \ell^2(\mathbb{N}, L^2(\mathbb{R}))$ is given by

$$Uu(n,\xi_2) = \frac{B^{1/4}}{\sqrt{2\pi}} \int u(x_1,x_2)\overline{u_n(B^{1/2}x_1 + B^{-1/2}\xi_2)} e^{-ix_2\xi_2} dx_1 dx_2$$

and

$$U^* v(x_1,x_2) = \frac{B^{1/4}}{\sqrt{2\pi}} \sum_n \int u_n(B^{1/2}x_1 + B^{-1/2}\xi_2) v(n,\xi_2) e^{ix_2\xi_2} d\xi_2.$$

For $f \in \mathscr{S}(\mathbb{R})$, the integration kernel of $f(P_B)$ is

$$K(x,x') = \frac{B^{1/2}}{2\pi} \sum_n \int u_n(B^{1/2}x_1 + B^{-1/2}\xi_2)\overline{u_n(B^{1/2}x_1' + B^{-1/2}\xi_2)} f(B(2n+1)) e^{i(x_2-x_2')\xi_2} d\xi_2.$$

Restricting to the diagonal we get

$$K(x,x) = \frac{B^{1/2}}{2\pi} \sum_n \int |u_n(B^{1/2}x_1 + B^{-1/2}\xi_2)|^2 f(B(2n+1)) d\xi_2 = \frac{B}{2\pi} \sum_n f(B(2n+1)).$$

As before we conclude the regularized trace is

$$\widetilde{\operatorname{tr}} f(P_B) = \frac{B}{2\pi} \sum_n f(B(2n+1)). \tag{4.6}$$

As discussed in §4.1 the free energy per volume is given by

$$\Omega(B,T,z_0,N) = Nz_0 - \widetilde{\operatorname{tr}} f_{z_0,T}(P_B)$$

where $f_{z_0,T}(x) = T\log(1+\exp(\frac{z_0-x}{T}))$ and z_0 is determined by $\frac{\partial\Omega}{\partial z_0} = 0$. In the $T \to 0$ limit,

$$f_{z_0,T} \to (z_0 - x)_+^1, \quad f'_{z_0,T} \to -(z_0-x)_+^0, \quad f''_{z_0,T} \to \delta_{z_0}(x)$$

where

$$x_+^\gamma = x^\gamma \mathbb{1}_{x>0}, \quad \operatorname{Re}\gamma > -1. \tag{4.7}$$

From (4.6) we get

$$\Omega = Nz_0 - \frac{B}{2\pi} \sum_n f_{z_0,T}(B(2n+1))$$

and

$$m(B) = \partial_B \Omega(B) = -\frac{1}{2\pi} \sum_n f_{z_0,T}(B(2n+1)) - \frac{B}{2\pi} \sum_n (2n+1) f'_{z_0,T}(B(2n+1)).$$

In the $T \to 0$ limit we have

$$m(B) = \frac{1}{2\pi} \sum_{z_0 - B(2n+1) \geq 0} (-z_0 + 2B(2n+1))$$

and

$$m(B) = \partial_B \Omega(B) = \frac{M+1}{2\pi} \left(2B(M+1) - z_0\right), \quad M := \left[\frac{z_0 - B}{2B}\right]. \tag{4.8}$$

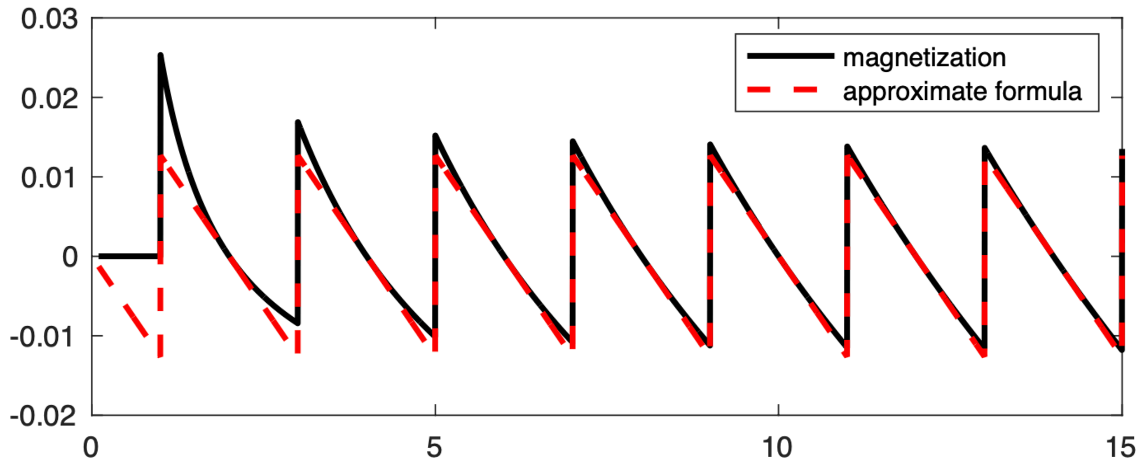


FIGURE 2. The plot of $\partial_B \Omega$ as a function of $1/B$ for the two dimensional Hamiltonian. It is given by (4.8) where we put $z_0 = 0$. It is compared to the approximation (4.9).

One can show without much trouble (see proof of [BeZw19, Theorem 3] for a slightly more complicated case of relativistic Landau levels) that

$$m(B) = \frac{1}{2\pi} z_0 \sigma(z_0 B^{-1} - 1) + \mathcal{O}(B), \quad \sigma(t) := [t/2] - t/2 + 1/2. \tag{4.9}$$

4.4. **Three dimensions.** The 3-dimensional case is similar to 2-dimensional case and we get

$$\widetilde{\operatorname{tr}} f(P_B) = \frac{B}{(2\pi)^2} \sum_n \int f(B(2n+1) + \xi_3^2) d\xi_3. \tag{4.10}$$

As a sanity check we verify that $\widetilde{\operatorname{tr}} f(P_B) \to \widetilde{\operatorname{tr}} f(-\Delta)$ as $B \to 0$. Observe as $B \to 0$, (4.10) is a Riemann sum and converges to

$$\begin{aligned}\frac{1}{2(2\pi)^2} \int f(s + \xi_3^2) ds d\xi_3 = \frac{1}{2(2\pi)^2} \int f(\rho^2 + \xi_3^2) 2\rho d\rho d\xi_3 = \frac{1}{(2\pi)^3} \int f(\rho^2 + \xi_3^2) \rho d\rho d\theta d\xi_3 \\ = \frac{1}{(2\pi)^3} \int f(|\xi|^2) d\xi.\end{aligned}$$

As in (4.4) we obtain a formula for the density of states:

$$\widetilde{\operatorname{tr}} f(P_B) = \int f(\lambda) \rho_B(\lambda) d\lambda, \quad \rho_B(\lambda) = \frac{B}{(2\pi)^2} \sum_{n=0}^{\infty} (\lambda - (2n+1)B)_+^{-\frac{1}{2}}. \tag{4.11}$$

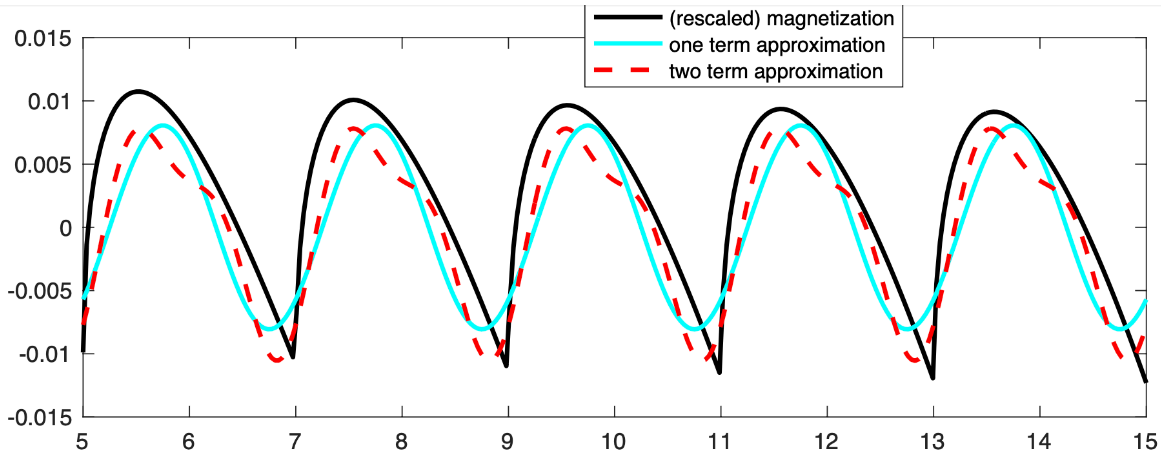


FIGURE 3. The plot of $\partial_B\Omega/\sqrt{B}$ as a function of $1/B$ ($m := \partial_B\Omega$ is the "magnetization") for the three dimensional Hamiltonian – see §§3.3,4.4. We also show one term and two terms approximation using Fourier series/Poisson summation formula. Oscillations are smoother in 3D when a potential is present, that is, when we are dealing with metals.

We will follow [HS90b, §2] (which in turn follows presentations in the physics literature such as [Ca64]) and describe asymptotics of $m(B) = \partial_B\Omega(B)$, $\Omega(B) := \Omega(B, 0, N, z_0)$ – see (4.2). That means using a specific $f = f_{T,z_0}$ and considering $T \to 0$.

4.4.1. *Formula for m_B and statement of the result.* We proceed as in §4.3 to we obtain from (4.11) a formula for m_B. (Strictly speaking, we need to differentiate Ω with respect to B for $T > 0$ and then take the limit $T \to 0+$.) This gives

$$m(B) = \frac{1}{(2\pi)^2}\sum_{n=0}^{\infty}\left(2z_0(z_0-(2n+1)B)_+^{\frac{1}{2}} - (10/3)(z_0-(2n+1)B)_+^{\frac{3}{2}}\right). \tag{4.12}$$

The sum in (4.12) can be expressed using the *Riesz means* of the harmonic oscillator,

$$r_\gamma(s) := \sum_{n=0}^{\infty}(s-(2n+1))_+^{\gamma}, \quad \gamma > 0, \tag{4.13}$$

as follows

$$m(B) = \frac{1}{(2\pi)^2}\sum_{n=0}^{\infty}\left(-(10/3)B^{\frac{3}{2}}r_{\frac{3}{2}}\left(\frac{z_0}{B}\right) + 2z_0B^{\frac{1}{2}}r_{\frac{1}{2}}\left(\frac{z_0}{B}\right)\right). \tag{4.14}$$

The asymptotics of r_γ presented in the next section will give

Theorem 2. *For $m(B)$ given by (4.12) with $z_0 > 0$ we have, as $B \to 0$,*

$$B^{-\frac{1}{2}} m(B) = \frac{2z_0}{(2\pi)^2} \Gamma\left(\tfrac{3}{2}\right) \sum_{k=1}^{\infty} (-1)^k (\pi k)^{-\frac{3}{2}} \cos\left(\frac{k\pi z_0}{B} - \frac{3\pi}{4}\right) + \mathcal{O}(B^{\frac{1}{2}}). \tag{4.15}$$

This result is illustrated in Figure 3. The asymptotics of the next section provide an expansion of the error term in (4.15) as well. However, when the constant z_0 is replaced by $z_0(B)$ (determined by $\partial_{z_0}\Omega = 0$) additional terms appear – see [HS89, Proposition 2.2].

4.4.2. *Asymptotics of Riesz means.* This is a nice exercise in classical analysis which is a good illustration of various asymptotic methods.

We start with the following application of the Fourier inversion formula (2.5):

Lemma 4.1. *In the notation of (4.7) and for* $\operatorname{Re}\gamma > 0$,

$$\sigma_+^\gamma = \frac{\Gamma(\gamma+1)}{2\pi i} \int_{c-i\infty}^{c+i\infty} u^{-\gamma-1} e^{\sigma u} du, \tag{4.16}$$

for any $c > 0$, and $u \mapsto u^{-\gamma-1}$ defined on $\mathbb{C} \setminus (-\infty, 0]$.

Proof. For $c > 0$, $f(\sigma) := \sigma_+^\gamma e^{-c\sigma}$ is integrable and

$$\begin{aligned}\hat{f}(s) &= \int_0^\infty \sigma^\gamma e^{-\sigma(c+is)} d\sigma = (c+is)^{-\gamma-1} \int_0^\infty ((c+is)\sigma)^\gamma e^{-\sigma(c+is)} d(\sigma(c+is)) \\ &= (c+is)^{-\gamma-1} \int_{\mathscr{C}} \tau^\gamma e^{-\tau} d\tau = \Gamma(\gamma+1)(c+is)^{-\gamma-1}.\end{aligned}$$

where $\mathscr{C}$ is the contour $[0,\infty) \ni \sigma \mapsto \tau = \sigma(c+is)$, which we deform to $[0,\infty)$ and apply the definition of the Γ-function.

Since $s \mapsto (c+is)^{-\gamma-1}$ in integrable, the Fourier inversion formula ((2.5) with $n = 1$) now gives

$$\sigma_+^\gamma e^{-c\sigma} = \frac{\Gamma(\gamma+1)}{2\pi} \int_{-\infty}^\infty (c+is)^{-\gamma-1} e^{\sigma(is+c)} e^{-\sigma c} ds,$$

where the integral converges since $-\operatorname{Re}\gamma - 1 < -1$. Cancelling $e^{-\sigma c}$ on each side and putting $u = c + is$ (with $du = ids$) gives (4.16). □

Remark 2. *By putting $\sigma = 1$, (4.16) gives the following formula for the reciprocal of the Γ function:*

$$\frac{1}{\Gamma(z+1)} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} u^{-z-1} e^u du, \quad \operatorname{Re} z > 0.$$

To obtain a formula valid for all $z \in \mathbb{C}$ we need to take advantage of exponential decay of e^u when $\operatorname{Re} u \to -\infty$. For that we deform the contour to a Hankel *contour,* $\mathscr{C}$

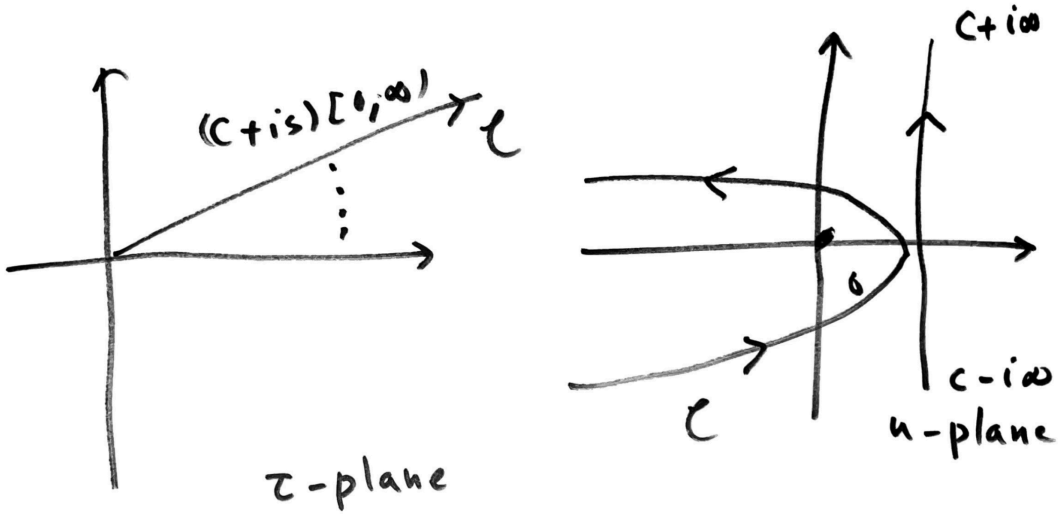


FIGURE 4. On the left the contour used for the evaluation of the Fourier transform of $\sigma \mapsto \sigma_+^\gamma e^{-\sigma s}$ in the proof of Lemma 4.1. On the right the contours in (4.16) and the Hankel contour in (4.17).

shown in Figure 4. The contour deformation is easily justified when $\operatorname{Re} z > 0$ *and, by analytic continuation, we obtain a formula valid for all* $z \in \mathbb{C}$*:*

$$\frac{1}{\Gamma(z+1)} = \frac{1}{2\pi i} \int_{\mathscr{C}} u^{-z-1} e^u du, \quad z \in \mathbb{C}. \tag{4.17}$$

We can now obtain asymptotics of the Riesz means:

Lemma 4.2. *For* $r_\gamma(s)$ *defined by* (4.13) *for* $\gamma > 0$ *we have, for every* M*,*

$$r_\gamma(s) = \Gamma(\gamma+1) \left(\sum_{k=1}^{\infty} (-1)^k (\pi k)^{-\gamma-1} \cos\left(k\pi s - \tfrac{(\gamma+1)\pi}{2}\right) + \tfrac{1}{2} \sum_{j=0}^{M} \frac{\gamma_j}{\Gamma(\gamma+2-2j)} s^{\gamma+1-2j} \right) + \mathcal{O}(s^{\gamma-1-2M}),$$

where γ_j *come from the Taylor expansion* $t/\sinh t = \sum_{j=0}^{\infty} \gamma_j t^{2j}$, $|t| < \pi/2$, $\gamma_0 = 1$.

Proof. Using Lemma 4.1 and the fact that $\sum_{n=0}^{\infty} e^{t(s-2n-1)} = e^{ts}/(2\sinh t)$, we rewrite r_γ as

$$r_\gamma(s) = \frac{\Gamma(\gamma+1)}{4\pi i} \int_{c-i\infty}^{c+\infty} e^{st} (\sinh t)^{-1} t^{-\gamma-1} dt.$$

The residue theorem and contour deformation show that

$$r_\gamma(s) = \Gamma(\gamma+1) \sum_{k=1}^{\infty} (-1)^k (\pi k)^{-\gamma-1} \cos\left(k\pi s - \tfrac{(\gamma+1)\pi}{2}\right) + I_\gamma(s),$$

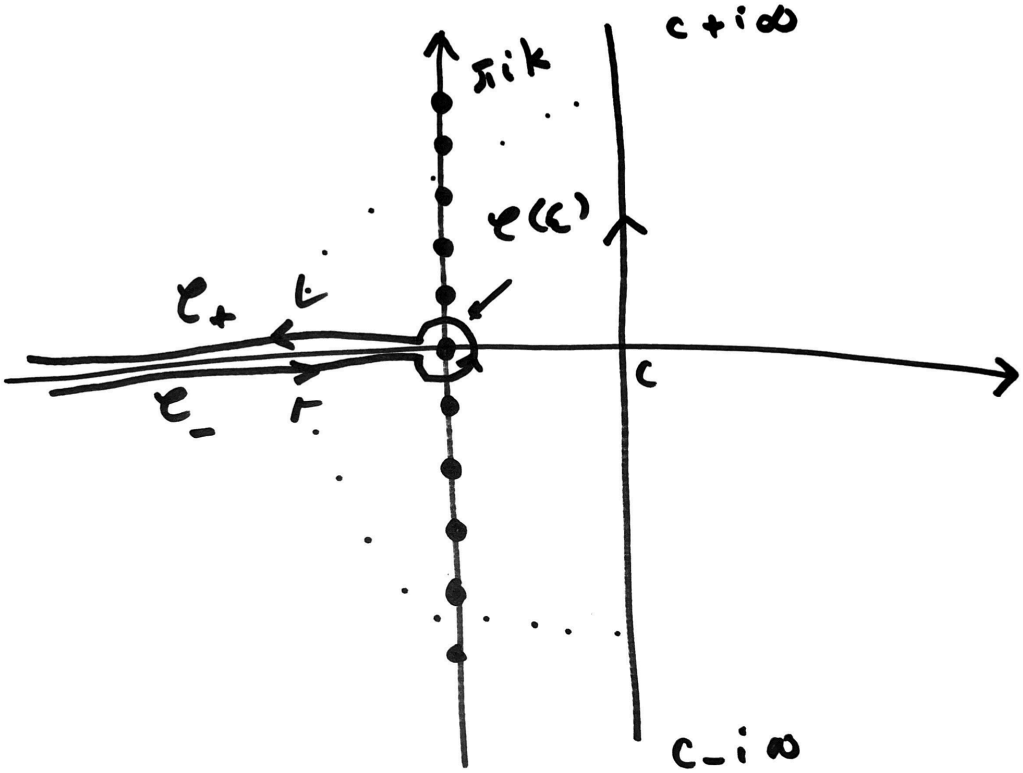


FIGURE 5. Contour deformation used in the proof of Lemma 4.2

where, with the Hankel contour $\mathscr{C}$ of Remark 2,

$$I_\gamma(s) := \frac{\Gamma(\gamma+1)}{4\pi i}\int_{\mathscr{C}} e^{st}(\sinh t)^{-1} t^{-\gamma-1} dt.$$

This we deform to

$$\widetilde{\mathscr{C}}(\varepsilon) := \mathscr{C}_+(\varepsilon) + \mathscr{C}_-(\varepsilon) + \mathscr{C}(\varepsilon),$$

where $\mathscr{C}_\pm = (-\infty, -\varepsilon] \pm i0$ with positive $(-)$ and negative $(+)$ orientations and $\mathscr{C}(\varepsilon)$ is the circle of radius ε centered at 0 with positive orientation – see Figure 5.

Using exponential decay of e^{st} on $\mathscr{C}_\pm(\varepsilon)$ we see that

$$I_\gamma(s) = I_\gamma(s,\varepsilon) + \mathcal{O}(e^{-\varepsilon s}\varepsilon^{-\gamma-1}), \quad I_\gamma(s,\varepsilon) := \frac{\Gamma(\gamma+1)}{4\pi i}\int_{\mathscr{C}(\varepsilon)} e^{st}(\sinh t)^{-1} t^{-\gamma-1} dt. \tag{4.18}$$

We now expand $t/\sinh t$ in Taylor series at 0 so that in the notation of the lemma,

$$I_\gamma(s,\varepsilon) = \frac{\Gamma(\gamma+1)}{2}\sum_{j=0}^{M} \gamma_j \frac{1}{2\pi i}\int_{\mathscr{C}(\varepsilon)} e^{st} t^{2j-\gamma-2} dt + \mathcal{O}(\varepsilon^{2M-\gamma-1} e^{\varepsilon s}).$$

We now use (4.17) by inserting the "missing" contours $\mathscr{C}_\pm(\varepsilon)$, estimating their contributions as in (4.18) and changing variables $u = ts$:

$$\begin{aligned}\frac{1}{2\pi i}\int_{\mathscr{C}(\varepsilon)} e^{ts}t^{2j-\gamma-2}dt &= \frac{1}{2\pi i}\int_{\widetilde{\mathscr{C}}(\varepsilon)} e^{ts}t^{2j-\gamma-2}dt + \mathcal{O}(e^{-\varepsilon s}\varepsilon^{-\gamma-2}) \\ &= s^{\gamma+1-2j}\Gamma(\gamma+2-2j)^{-1} + \mathcal{O}(e^{-\varepsilon s}\varepsilon^{-\gamma-2}).\end{aligned}$$

Inserting this in (4.18) gives an expansion for $r_\gamma(s)$ with an error

$$\mathcal{O}(e^{\varepsilon s}\varepsilon^{2M-\gamma-1} + e^{-\varepsilon s}\varepsilon^{-\gamma-2}).$$

This can be optimized by choosing $\varepsilon = \varepsilon(s)$ so that $e^{-2\varepsilon s} = \varepsilon^{2M}$ and gives an error estimate $\mathcal{O}(\varepsilon(s)^{M-\gamma-2}) = \mathcal{O}(s^{-M/2})$, $M \gg 1$ (we note that $s^{-1} = \varepsilon(s)/M|\log(\varepsilon(s))| \gtrsim_M \varepsilon(s)^{1-\delta}$, for any $\delta > 0$). By changing M this concludes the proof. $\square$

Proof of Theorem 2. We need to show the cancellation of the leading non-oscillatory contributions in (4.14):

$$-\frac{\Gamma(\frac{5}{2})}{\Gamma(\frac{7}{2})}\frac{10}{3}B^{\frac{3}{2}}(z_0/B)^{\frac{3}{2}+1} + 2\frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{5}{2})}z_0B^{\frac{1}{2}}(z_0/B)^{\frac{1}{2}+1} = z_0^{\frac{5}{2}}B^{-1}(-\tfrac{2}{5}\tfrac{10}{3} + \tfrac{4}{3}) = 0,$$

where we used $\Gamma(z+1) = z\Gamma(z)$. The next term in the expansion of r_γ, $\gamma = \frac{1}{2}, \frac{3}{2}$ provides the $\mathcal{O}(B^{\frac{1}{2}})$ error in (4.15). $\square$

5. Bloch–Floquet theory

5.1. **Motivation.** We will now consider electrons in a periodic structure such as a crystal or a metal. In this case, electrons are interacting with each other and are subjected to forces from the atoms forming the periodic structure (which we assume do not move or interact with each other).

An extremely successful model for that is given by a periodic Schrödinger operator

$$P = -\Delta + V(x), \quad V \in C^\infty(\mathbb{R}^n;\mathbb{R}), \quad V(x+\gamma) = V(x), \quad \gamma \in \Gamma, \tag{5.1}$$

where $\Gamma = \bigoplus_{j=1}^n \gamma_j\mathbb{Z}$, $\{\gamma_j\}_{j=1}^n$ linearly independent vectors in $\mathbb{R}^n$, is a lattice in $\mathbb{R}^n$ (we will concentrate on $n = 2$). This is a Hamiltonian in which there is no interaction between electrons and it corresponds to a *pseudo-particle* rather than the actual electrons in the metal. We will indicate why this approximation is acceptable in §5.2.

We will then diagonalize operators such as (5.1) and develop *band theory*.

5.2. **Hohenberg-Kohn theorem and the passage to non-interacting pseudoparticles.** The transition to non-interacting pseudo-particles modelling of the actual quantum mechanical system is now most frequently done using the density functional theory. It is an approach to studying the Schrödinger equation by writing quantities of interest, such as energies, in terms of the particle density, instead of in terms of the wave function. This can simplify computations considerably, especially when the number of particles is large.

In an N-body system we are primarily interested in the *ground state* that is an N-body wave function ψ (see Theorem 3) which is a function of N (2D or 3D) variables, for which

$$\langle \psi | \hat{H} | \psi \rangle = \min_{\|\varphi\|=1} \langle \varphi | \hat{H} | \varphi \rangle.$$

In the non-interacting system (especially when considering electrons which are fermions – we will neglect such issues here), a composite ψ can be build of non-interacting particles at different energy levels (not the ground state of the full Hamiltonian). The game here is to replace the actual ground state by a ground state of a non-interactive system with the same density.

To explain this we present here an extract from the notes by `https://www.math.purdue.edu/~kdatchev/dftintro.pdf`, see also [Cr*23]. They can be consulted for a more detailed discussion and references.

A very general Hamiltonian describing an N-electron system is given by

$$\hat{H} = \hat{T} + \hat{V}_{ee} + \hat{V},$$

where

$$\hat{T} = -\frac{1}{2}\sum_{j=1}^{N} \nabla_j^2, \qquad \hat{V}_{ee} = \sum_{1 \le i < j \le N} \frac{1}{|\vec{r}_i - \vec{r}_j|}, \qquad \hat{V} = \sum_{i=1}^{N} v(\vec{r}_i) = \sum_{i=1}^{N} \int d^3r\, \delta(\vec{r} - \vec{r}_i) v(\vec{r}),$$

and where v is the potential coming from the external forces on the electrons. Here $\hat{T}$ is the kinetic energy term, $\hat{V}_{ee}$ is the repulsive Coulomb potential energy between the electrons, and $\hat{V}$ is the potential energy due to external forces. We are ignoring the sizes of the nuclei, the movements of the nuclei, spin, and relativistic effects.

For example, consider a system of N electrons in a molecule made up of M atoms. Then v is the attractive Coulomb potential energy arising from the M atomic nuclei, given by

$$v(\vec{r}) = \sum_{k=1}^{M} \frac{-Z_k}{|\vec{r} - \vec{R}_k|}, \tag{5.2}$$

where $\vec{R}_k$ is the position of the kth nucleus and Z_k is the number of protons it has.

The density is defined by

$$n(\vec{r}) = \langle \psi | \hat{n}(\vec{r}) | \psi \rangle = \int d^3r_1 \int d^3r_2 \cdots \int d^3r_N\, \psi^*(\vec{r}_1, \ldots, \vec{r}_N) \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i) \psi(\vec{r}_1, \ldots, \vec{r}_N).$$

Note that $\int d^3r\, n(\vec{r}) = N$, and, for any region U, the quantity $\int_U d^3r\, n(\vec{r})$ gives the expected value of the number of electrons to be found in U.

The basic case is the hydrogen atom, where $N = M = Z_1 = 1$. The ground state energy of the electron is precisely -0.5 Hartrees, the corresponding wavefunction is $\psi(r) = e^{-r}/\sqrt{\pi}$, the density is $n(r) = e^{-2r}/\pi$, and the probability density of the electron being at distance r from the nucleus is $4\pi r^2 n(r)$ and it achieves its maximum at precisely $r = 1$ Bohr radius.

The point of density functional theory is, instead of writing and computing in terms of ψ, to write and compute in terms of n. The basic result is the Hohenberg–Kohn Theorem which says that if $n(\vec{r})$ is a ground state density, then no information is lost by doing this.

5.2.1. *The Hohenberg–Kohn Theorem.* Consider two N-electron systems, with Hamiltonians $\hat{H}_1$ and $\hat{H}_2$ defined by:

$$\hat{H}_k = \hat{T} + \hat{V}_{ee} + \hat{V}_k,$$

with

$$\hat{V}_k = \sum_{i=1}^{N} v_k(\vec{r}_i) = \sum_{i=1}^{N} \int d^3r\, \delta(\vec{r} - \vec{r}_i) v_k(\vec{r}),$$

and where each v_k is continuous except perhaps at some isolated points where it may go to infinity (the nuclei).

Theorem 3. *Suppose each Hamiltonian $\hat{H}_k$ has at least one normalizable ground state $|\psi_k\rangle$, and these ground states lead to identical densities*

$$n(\vec{r}) = \langle \psi_1 | \hat{n}(\vec{r}) | \psi_1 \rangle = \langle \psi_2 | \hat{n}(\vec{r}) | \psi_2 \rangle,$$

where

$$\langle \psi_k | \hat{n}(\vec{r}) | \psi_k \rangle = \int d^3r_1 \int d^3r_2 \cdots \int d^3r_N\, \psi_k^*(\vec{r}_1, \ldots, \vec{r}_N) \sum_{i=1}^{N} \delta(\vec{r} - \vec{r}_i) \psi_k(\vec{r}_1, \ldots, \vec{r}_N).$$

Then $v_1 - v_2$ is a constant.

Proof. By the variational principle,

$$\langle \psi_1 | \hat{H}_1 | \psi_1 \rangle \leq \langle \psi_2 | \hat{H}_1 | \psi_2 \rangle. \tag{5.3}$$

Since

$$\begin{aligned}\langle \psi_k | \hat{V}_1 | \psi_k \rangle &= \int d^3r_1 \int d^3r_2 \cdots \int d^3r_N\, \psi_k^*(\vec{r}_1, \ldots, \vec{r}_N) \sum_{i=1}^{N} \int d^3r\, \delta(\vec{r} - \vec{r}_i) v_1(\vec{r}) \psi_k(\vec{r}_1, \ldots, \vec{r}_N) \\ &= \int d^3r\, v_1(\vec{r}) n(\vec{r}),\end{aligned}$$

and the right hand side is independent of k, (5.3) simplifies to

$$\langle \psi_1 | \hat{T} + \hat{V}_{ee} | \psi_1 \rangle \leq \langle \psi_2 | \hat{T} + \hat{V}_{ee} | \psi_2 \rangle.$$

In the same way, starting from $\langle\psi_2|\hat{H}_2|\psi_2\rangle \le \langle\psi_1|\hat{H}_2|\psi_1\rangle$, we get

$$\langle\psi_2|\hat{T}+\hat{V}_{ee}|\psi_2\rangle \le \langle\psi_1|\hat{T}+\hat{V}_{ee}|\psi_1\rangle.$$

Hence both sides are equal and it follows that both $|\psi_1\rangle$ and $|\psi_2\rangle$ are ground states of both Hamiltonians. Then the result follows from the Lemma below. $\square$

Lemma 5.1. *If there exists a state $|\psi\rangle$ which is an eigenstate of both Hamiltonians $\hat{H}_1$ and $\hat{H}_2$, then $v_1 - v_2$ is a constant.*

Proof. We have

$$\hat{H}_1|\psi\rangle = E_1|\psi\rangle \quad \text{and} \quad \hat{H}_2|\psi\rangle = E_2|\psi\rangle,$$

for some E_1 and E_2. Subtracting, we get

$$(\hat{V}_1 - \hat{V}_2 - E_1 + E_2)|\psi\rangle = 0,$$

and hence

$$W(\vec{r}_1,\dots,\vec{r}_N)\psi(\vec{r}_1,\dots,\vec{r}_N) = 0, \quad \text{where} \quad W(\vec{r}_1,\dots,\vec{r}_N) = \sum_{i=1}^N (v_1(\vec{r}_i) - v_2(\vec{r}_i)) - E_1 + E_2. \tag{5.4}$$

From this we will conclude that $W(\vec{r}_1,\dots,\vec{r}_N) = 0$ for all points $(\vec{r}_1,\dots,\vec{r}_N)$. This will complete the proof because then $\sum_{i=1}^N (v_1(\vec{r}_i) - v_2(\vec{r}_i)) - E_1 + E_2 = 0$ which implies $v_1(\vec{r}_i) - v_2(\vec{r}_i)$ is independent of $\vec{r}_i$. The tricky part here is that we must rule out the possibility that $\psi = 0$ and $W \neq 0$. We will use the fact (due to quantum tunneling/unique continuation) that $\int_U |\psi|^2 > 0$ for any region U.

To carry this out, multiply (5.4) by $\psi^*(\vec{r}_1,\dots,\vec{r}_N)$ and integrate over an arbitrary region U to obtain

$$\int_U W|\psi|^2 = 0,$$

for any region U. We have

$$0 = \int_U W|\psi|^2 \le \max_U W \int_U |\psi|^2,$$

which implies $\max_U W \ge 0$, and similarly

$$0 = \int_U W|\psi|^2 \ge \min_U W \int_U |\psi|^2,$$

which implies $\min_U W \le 0$. Hence

$$\min_U W \le 0 \le \max_U W. \tag{5.5}$$

Fix any point $(\vec{r}_1,\dots,\vec{r}_N)$, and consider regions U containing that point and getting smaller and smaller. As the diameter of U goes to zero, both $\min_U W$ and $\max_U W$ converge to $W(\vec{r}_1,\dots,\vec{r}_N)$ because W is continuous. Hence, (5.5) becomes

$$W(\vec{r}_1,\dots,\vec{r}_N) \le 0 \le W(\vec{r}_1,\dots,\vec{r}_N),$$

which implies $W(\vec{r}_1, \ldots, \vec{r}_N) = 0$. Since the point $(\vec{r}_1, \ldots, \vec{r}_N)$ was arbitrary, it follows that $W = 0$ everywhere. $\square$

5.2.2. *The Kohn–Sham method.* The Kohn–Sham method computes densities and energies using a fictitious N-particle non-interacting system, designed so that its ground state density is the same as the ground state density for the N-particle interacting system $\hat{H}$.

More precisely, let $v_s(\vec{r})$ be the potential (called the *Kohn–Sham potential*) such that if $\varepsilon_1, \ldots, \varepsilon_N$ are the N lowest energies and $\varphi_1, \ldots, \varphi_N$ corresponding normalized states (called *Kohn–Sham orbitals*) for the single particle problem

$$\Big(-\frac{1}{2}\nabla^2 + v_s(\vec{r})\Big)\varphi_i(\vec{r}) = \varepsilon_i \varphi_i(\vec{r}),$$

then

$$n(\vec{r}) = \sum_{i=1}^{N} |\varphi_i(\vec{r})|^2,$$

where this n is the same as the one for the ground state of the problem we are studying. By the Hohenberg–Kohn theorem, this requirement determines the potential up to an overall constant.

5.3. **Periodic structure and the Bloch transform.** In this section we discuss the Bloch transform for periodic structures.

Let $\Gamma \subset \mathbb{R}^n$ be a lattice of rank n. The dual lattice Γ^* is defined as

$$\Gamma^* = \{k \in \mathbb{R}^n : k \cdot \gamma \in 2\pi\mathbb{Z}, \forall \gamma \in \Gamma\}.$$

For periodic functions $u \in C^\infty(\mathbb{R}^n/\Gamma)$, we can define the Fourier series as follows.

$$\hat{u}(k) = \frac{1}{|\mathbb{R}^n/\Gamma|^{1/2}} \int_{\mathbb{R}^n/\Gamma} u(x) e^{-ik\cdot x} dx, \quad k \in \Gamma^*.$$

We recall the properties of Fourier series.

- If $u \in C^\infty(\mathbb{R}^n/\Gamma)$, then for any $N \in \mathbb{N}$, there exists $C_N > 0$ such that $|\hat{u}(k)| \le C_N(1 + |k|)^{-N}$. In this case,

$$u(x) = \frac{1}{|\mathbb{R}^n/\Gamma|^{1/2}} \sum_{k\in\Gamma^*} \hat{u}(k) e^{ik\cdot x}. \tag{5.6}$$

- For $u \in C^\infty(\mathbb{R}^n/\Gamma)$, we have Plancherel identity $\|u\|_{L^2(\mathbb{R}^n/\Gamma)} = \|u\|_{\ell^2(\Gamma^*)}$. Thus the Fourier series extends to a unitary operator on L^2.

Here we just show a simple proof, due to Paul Chernoff, of the Fourier inversion formula for $n = 1$ and $\Gamma = 2\pi\mathbb{Z}$ case (it easily generalizes). First we note that it suffices to show $u(0)=0$ implies $\sum_{k\in\Gamma^*}\hat{u}(k)=0$. But $u(0)=0$ implies $u(x)=(e^{ix}-1)g(x)$ for some $g(x)\in C^\infty(\mathbb{R}/2\pi\mathbb{Z})$. Thus

$$\sum_{k\in\Gamma^*}\hat{u}(k)=\sum_{k\in\Gamma^*}(\hat{g}(k-1)-\hat{g}(k))=0.$$

Here we used the fact, that g is smooth so that $|\hat{g}(k)|\le C_N(1+|k|)^{-N}$.

Now for any $\theta\in\mathbb{R}^n/\Gamma^*$, let

$$\mathcal{H}_\theta=\{u\in L^2_{\mathrm{loc}}(\mathbb{R}^n):u(x-\gamma)=e^{i\gamma\cdot\theta}u(x),\forall\gamma\in\Gamma\}. \tag{5.7}$$

The inner product on $\mathcal{H}_\theta$ is given by

$$\langle u,v\rangle_{\mathcal{H}_\theta}:=\int_F u(x)\overline{v(x)}dx,$$

where $F\subset\mathbb{R}^n$ is a fundamental domain of Γ. need to define a fundamental domain?

We consider the space $L^2(\mathbb{R}^n/\Gamma^*;\mathcal{H}_\theta)$, that is measurable functions $g:\mathbb{R}^n/\Gamma^*\times\mathbb{R}^n\to\mathbb{C}$ such that

$$g(\theta,x-\gamma)=e^{i\gamma\cdot\theta}g(\theta,x),\quad \int_{\mathbb{R}^n/\Gamma^*}\int_{\mathbb{R}^n/\Gamma}|g(\theta,x)|^2dxd\theta<\infty.$$

Now we can state our theorem.

Theorem 4. *For $u\in\mathscr{S}(\mathbb{R}^n)$, let*

$$\mathcal{B}u(\theta,x)=\frac{1}{|\mathbb{R}^n/\Gamma^*|^{1/2}}\sum_{\gamma\in\Gamma}e^{-i\gamma\cdot\theta}u(x-\gamma). \tag{5.8}$$

Then $\mathcal{B}$ extends to a unitary operator

$$L^2(\mathbb{R}^n)\to L^2(\mathbb{R}^n/\Gamma^*;\mathcal{H}_\theta).$$

Moreover, $\mathcal{B}^*=\mathcal{B}^{-1}=\mathcal{C}$ where

$$\mathcal{C}g(x)=\frac{1}{|\mathbb{R}/\Gamma^*|^{1/2}}\int_{\mathbb{R}^n/\Gamma^*}g(\theta,x)d\theta. \tag{5.9}$$

Proof. For $u\in\mathscr{S}$, we check

$$\begin{aligned}\|\mathcal{B}u\|^2_{L^2}&=\sum_{\gamma,\gamma'\in\Gamma}\frac{1}{|\mathbb{R}^n/\Gamma^*|}\int_{\mathbb{R}^n/\Gamma^*}\int_{\mathbb{R}^n/\Gamma}e^{-i(\gamma-\gamma')\cdot\theta}u(x-\gamma)\overline{u(x-\gamma')}dxd\theta\\&=\sum_{\gamma\in\Gamma}\int_{\mathbb{R}^n/\Gamma}|u(x-\gamma)|^2dx=\int_{\mathbb{R}^n}|u(x)|^2dx=\|u\|^2_{L^2(\mathbb{R}^n)}.\end{aligned}$$

and hence $\mathcal{B}$ extends to an isometry from $L^2(\mathbb{R}^n)$ to $L^2(\mathbb{R}^n/\Gamma^*;\mathcal{H}_\theta)$, and $\mathcal{B}^*\mathcal{B}=I_{L^2(\mathbb{R}^n)}$.

We now check that $\mathcal{B}\mathcal{B}^* = I$ and we start with $g \in C^\infty(\mathbb{R}/\Gamma^*; \mathbb{H}_\theta)$. Using (5.9) we get,

$$\begin{aligned}\mathcal{B}\mathcal{C}g(\theta, x) &= \frac{1}{|\mathbb{R}^n/\Gamma^*|} \sum_{\gamma\in\Gamma} e^{-i\gamma\cdot\theta} \int_{\mathbb{R}^n/\Gamma^*} g(\tau, x-\gamma) d\tau \\ &= \frac{1}{|\mathbb{R}^n/\Gamma^*|} \sum_{\gamma\in\Gamma} \int_{\mathbb{R}^n/\Gamma^*} g(\tau, x) e^{i\gamma\cdot(\tau-\theta)} d\tau = g(\theta, x),\end{aligned}$$

where we used (5.6) (with the roles of Γ and Γ^* reversed. $\square$

Sometimes we also use the modified Bloch transform

$$\tilde{\mathcal{B}}u(\theta, x) = e^{ix\cdot\theta}\mathcal{B}u(\theta, x)$$

such that

$$\tilde{\mathcal{B}}u(\theta + k, x - \gamma) = e^{ik\cdot x}\tilde{\mathcal{B}}u(\theta, x), \quad k \in \Gamma^*.$$

5.4. **Bloch–Floquet spectrum: diagonalization of periodic Hamiltonians.** Now suppose we have a differential operator $P(x, D) = \sum_{|\alpha|\le 2} a_\alpha(x) D^\alpha$ such that $P(x + \gamma, D) = P(x, D)$ for any $\gamma \in \Gamma$. Then

$$\mathcal{B}P(x, D)\mathcal{B}^* v(\theta, x) = P(x, D_x) v(\theta, x)$$

and

$$\tilde{\mathcal{B}}P(x, D)\tilde{\mathcal{B}}^* v(\theta, x) = e^{ix\cdot\theta}P(x, D_x)e^{-ix\cdot\theta}v(\theta, x) = P(x, D_x - \theta)v(\theta, x).$$

Example 9. For $P = D_x$, we have $\tilde{\mathcal{B}}P\tilde{\mathcal{B}}^* = D_x - \theta$ acts on $H^1(\mathbb{R}/2\pi\mathbb{Z})$ for each θ. The spectrum is given by $-\theta + \mathbb{Z}$.

Let $U : L^2(\mathbb{R}) \to L^2(\mathbb{R}/\mathbb{Z}; \ell^2(\mathbb{Z}))$,

$$Uu(\theta, m) = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \tilde{\mathcal{B}}u(\theta, x) e^{-imx} dx.$$

If we let $P_\theta = UPU^* = m - \theta$, then

$$\operatorname{Spec}(P) = \bigcup_{\theta\in\mathbb{R}/\mathbb{Z}} \operatorname{Spec}(P_\theta) = \mathbb{R}.$$

Recall for $s \in \mathbb{R}$, the Sobolev space $H^s(\mathbb{R}^n/\Gamma)$ is defined as

$$H^s(\mathbb{R}^n/\Gamma) = \{u \in \mathscr{S}' : u(x-\gamma) = u(x), \ \forall\gamma \in \Gamma, \text{ and } \sum_{k\in\Gamma^*} (1 + |k|^2)^s |\hat{u}(k)|^2 < \infty\}.$$

The sum in the definition of H^s defines the square of the norm in H^s.

We leave an exercise for the reader to check that for $s \in \mathbb{N}$,

$$\begin{aligned}H^s(\mathbb{R}^n/\Gamma) &= \{u \in L^2(\mathbb{R}^n/\Gamma) : \partial_x^\alpha u \in L^2, \forall|\alpha| \le s\},\\ H^{2s}(\mathbb{R}^n/\Gamma) &= \{u \in L^2(\mathbb{R}^n/\Gamma) : \Delta^p u \in L^2, \forall p \le s\}.\end{aligned}$$

We recall the elliptic regularity lemma.

Lemma 5.2. *Let $P = -\Delta + \sum_{|\alpha|\leq 1} a_\alpha(x) D_x^\alpha$ be a periodic second order differential operator on $\mathbb{R}^n/\Gamma$, then there exists $C > 0$ such that for any $u \in C^\infty(\mathbb{R}^n/\Gamma)$,*

$$\|u\|_{H^2} \leq C\|Pu\|_{L^2} + C\|u\|_{L^2}, \quad L^2 = L^2(\mathbb{R}^n/\Gamma), \quad H^2 = H^2(\mathbb{R}^n/\Gamma).$$

Proof. First,

$$\begin{aligned}
\frac{1}{2}\|Pu\|_{L^2}^2 + \frac{1}{2}\|u\|_{L^2}^2 \geq |(Pu, u)| &\geq -\int_{\mathbb{R}^n/\Gamma} \Delta u \bar{u} dx - \left| \int_{\mathbb{R}^n/\Gamma} \sum_{|\alpha|\leq 1} a_\alpha(x) D_x^\alpha u \bar{u} dx \right| \\
&\geq \int_{\mathbb{R}^n/\Gamma} |Du|^2 dx - \frac{1}{2}\int_{\mathbb{R}^n/\Gamma} |Du|^2 dx - C\|u\|_{L^2}^2 \\
&\geq \frac{1}{2}\|Du\|_{L^2}^2 - C\|u\|_{L^2}^2.
\end{aligned}$$

Moreover, we also have

$$\|Pu\|_{L^2}^2 \geq \|\Delta u\|_{L^2}^2 - C\|Du\|_{L^2}^2 - C\|u\|_{L^2}^2.$$

Thus

$$\begin{aligned}
\|u\|_{H^2} = \|\Delta u\|_{L^2}^2 + \|u\|_{L^2}^2 &\leq \|Pu\|_{L^2}^2 + C\|Du\|_{L^2}^2 + C\|u\|_{L^2}^2 \\
&\leq (C+1)\|Pu\|_{L^2}^2 + 2C(C+1)\|u\|_{L^2}^2,
\end{aligned}$$

which concludes the proof. □

Now suppose the periodic elliptic operator in Lemma 5.2 gives self-adjoint operators $P(x, D_x - \theta) : H^2(\mathbb{R}^n/\Gamma) \to L^2(\mathbb{R}^n/\Gamma)$, then

$$(P(x, D_x - \theta) + i)^{-1} : L^2(\mathbb{R}^n/\Gamma) \to H^2(\mathbb{R}^n/\Gamma)$$

is compact, and thus has discrete spectrum, with eigenvalues converging to 0. So it is easy to see

$$\mathrm{Spec}_{L^2(\mathbb{R}^n/\Gamma)}(P(x, D_x - \theta)) = \{E_j(\theta)\}_{j=0}^\infty$$

where

$$E_0(\theta) \leq E_1(\theta) \leq \cdots$$

are real eigenvalues, going to ∞ as $j \to \infty$. We summarise this in

Theorem 5.

$$
\begin{aligned}
\operatorname{Spec}_{L^2(\mathbb{R}^n)}(P) &= \bigcup_{\theta\in\mathbb{R}^n/\Gamma^*} \operatorname{Spec}_{\mathcal{H}_\theta}(P_\theta) \\
&= \bigcup_{\theta\in\mathbb{R}^n/\Gamma^*} \operatorname{Spec}_{L^2(\mathbb{R}^n/\Gamma)}(P(x, D_x-\theta)) \\
&= \bigcup_{\theta\in\mathbb{R}^n/\Gamma^*} \{E_j(\theta)\}.
\end{aligned} \tag{5.10}
$$

Example 10. Let $P = -\Delta$ and $\Gamma = (2\pi\mathbb{Z})^n$. Then $P_\theta = (D_x-\theta)^2$ and $\operatorname{Spec}(P_\theta) = \{(-\theta+m)^2 : m\in\mathbb{Z}^n\}$. The picture for the bands is shown in Picture 6.

Let us look at two more interesting one dimensional examples.

Example 11. The Kronig–Penney model is an explicitly solvable model of a one dimensional periodic system (see [Wo78] for a brief account):

$$
P := D_x^2 + \sum_{m\in\mathbb{Z}} q\delta(x-m). \tag{5.11}
$$

We then consider Bloch eigenfunctions and eigenvalues as §5.4:

$$
Pw(\theta,x) = E(\theta)w(\theta,x), \quad w(\theta,x-1) = e^{i\theta}w(\theta,x).
$$

They are explicitly given as follows:

$$
w(\theta,x) = e^{-i\theta x}u(\theta,x), \quad u(\theta,x) := \sum_{m\in\mathbb{Z}} u_1(\theta,x-m),
$$

where

$$
\begin{gathered}
u_1(\theta,x) = c_1(\theta)(e^{i\theta x}\sin\alpha(\theta)x + e^{i\theta(1+x)}\sin(\alpha(\theta)(1-x)))\mathbb{1}_{[0,1]}, \\
q\sin\alpha(\theta) + 2\alpha(\theta)\cos\alpha(\theta) = 2\alpha(\theta)\cos\theta, \quad \operatorname{Im}\alpha(\theta)\geq 0, \quad E(\theta) = \alpha(\theta)^2,
\end{gathered} \tag{5.12}
$$

where $c_1(\theta)$ is the normalization constant guaranteeing $\|u_1(\theta,\bullet)\|_{L^2(\mathbb{R}/\mathbb{Z})} = 1$. The transcedental equation for $\alpha(\theta)$ in (5.12) has a discrete set of solutions (with imaginary values of α occurring when q is negative) – see Figure 7. We see that $u_1(\theta,0) = c_1(\theta)e^{i\theta}\sin\alpha(\theta) = u_1(\theta,1)$ which means that

$$
\begin{gathered}
u(\theta,x+m) = u(\theta,x), \quad u(\theta+2\pi\ell,x) = e^{2\pi i x\ell}u(\theta,x), \quad \ell\in\mathbb{Z}, \\
u(\bullet,\theta)\in C(\mathbb{R};\mathbb{C})\cap H^1_{\mathrm{loc}}(\mathbb{R};\mathbb{C}), \quad e^{i\theta x}u(x,\bullet)\in C^\infty(\mathbb{R};\mathbb{C}).
\end{gathered} \tag{5.13}
$$

The discontinuities of $x\to\partial_x u(x,\theta)$ are needed to produce the δ-function potential:

$$
P(\theta)u(\theta,x) := \left((D_x-\theta)^2 + \sum_{m\in\mathbb{Z}} q\delta(x-m)\right)u(\theta,x) = E(\theta)u(\theta,x). \tag{5.14}
$$

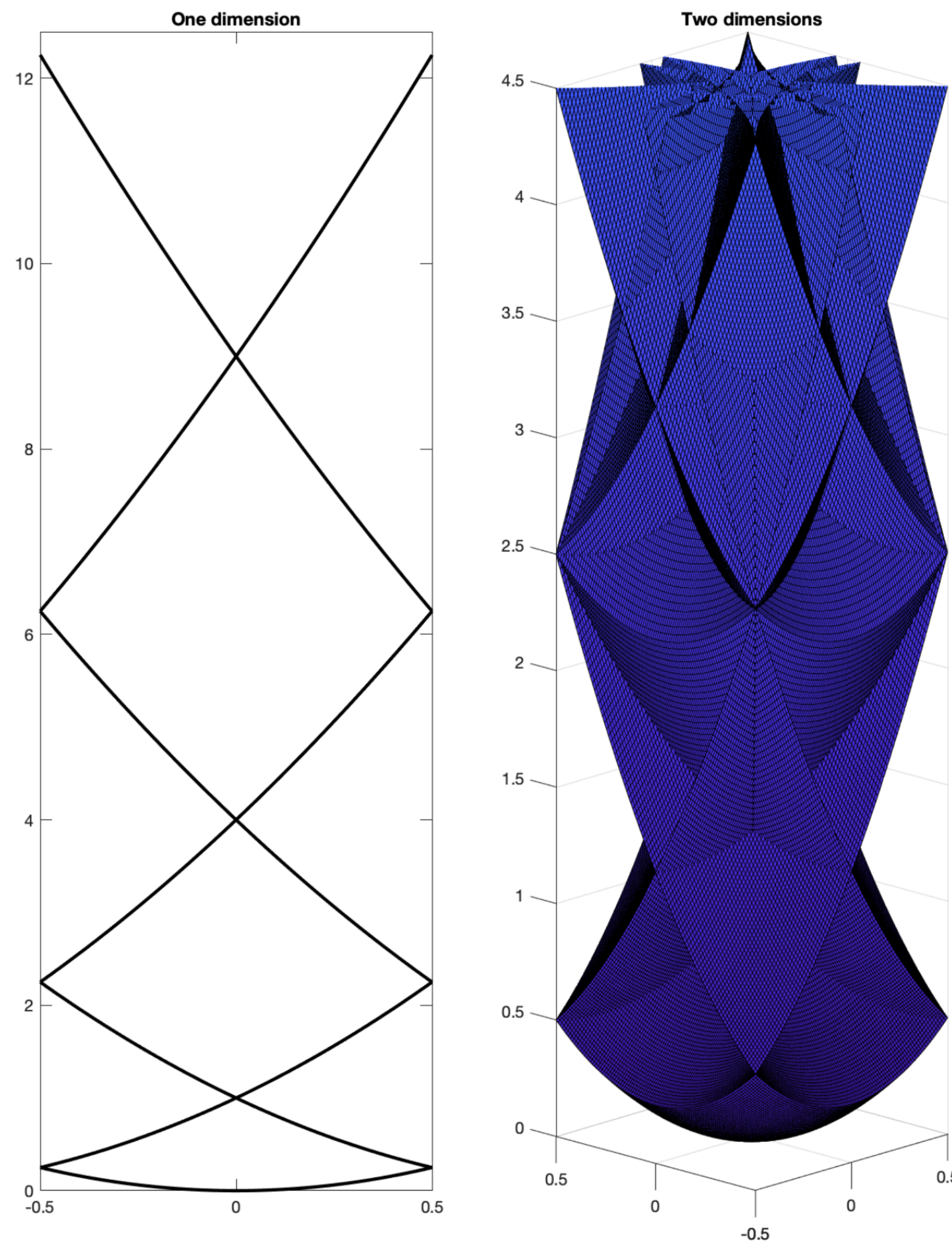


FIGURE 6. The band structure for the free Laplacian with $\Gamma = (2\pi\mathbb{Z})^n$, $n = 1, 2$. For θ in the fundamental domain of $\mathbb{R}^n/\Gamma^*$, $\Gamma^* = \mathbb{Z}^n$, we plot $|p - \theta|^2$, $p \in \mathbb{Z}^n$. That gives $0 \leq E_1(\theta) \leq E_2(\theta) \leq \cdots$. Note that $\theta \to E_j(\theta)$ are not smooth because of the lack of separation between the bands.

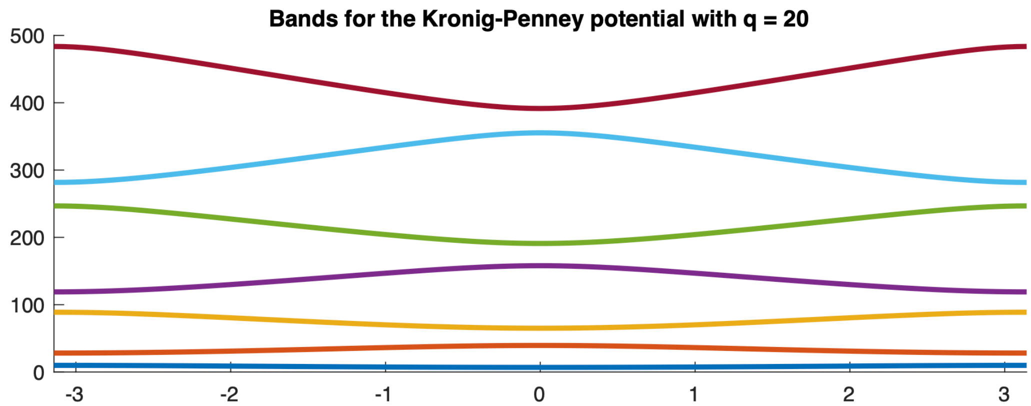


FIGURE 7. The first 7 bands for (5.11) with $q = 20$. They are computed using the transcendental equation in (5.12).

The next example uses perturbation theory to see band splitting when a periodic potential is turned on.

Example 12. Let $n = 1, \lambda \in \mathbb{R}$, $P_\lambda = D_x^2 + \lambda \cos x$. We are interested in the spectrum of P_λ when $\lambda > 0$. We will consider it as a perturbation problem and use the Grushin problem method to study the perturbation. See Section 2.6 for more details.

Let $P_\theta^\lambda = (D_x - \theta)^2 + \lambda \cos x$. We will consider the following Grushin problem.

$$\mathcal{P}_\theta^\lambda(z) = \begin{pmatrix} P_\theta^\lambda - z & R_- \\ R_+ & 0 \end{pmatrix} : H^2(\mathbb{R}^n/\Gamma) \times \mathbb{C}^k \to L^2(\mathbb{R}^n/\Gamma) \times \mathbb{C}^k. \tag{5.15}$$

First we consider the case when z_0 is a simple eigenvalue with eigenfunction u_0 ($\|u_0\|_{L^2} = 1$). Then as in Proposition 2.14, we may take $k = 1$ and

$$R_+ u = \langle u, u_0 \rangle, \quad R_- u_- = u_- u_0.$$

When $\lambda = 0$, this gives a well-posed Grushin problem. Let $\{u_j\}_{j=0}^\infty$ be an orthonormal basis such that $Pu_j = z_j u_j$, then

$$E(z)v = \sum_{j \neq 0} \frac{1}{z_j - z} \langle v, u_j \rangle u_j, \qquad E_+(z)v_+ = v_+ u_0,$$
$$E_-(z)v = \langle v, u_0 \rangle u_0, \qquad E_{-+}(z)v_+ = (z - z_0)v_+.$$

Now we consider a perturbation by $Q = \cos x$, via the Grushin problem

$$\begin{pmatrix} P - z + \lambda Q & R_- \\ R_+ & 0 \end{pmatrix}^{-1} = \begin{pmatrix} E^\lambda & E_+^\lambda \\ E_-^\lambda & E_{-+}^\lambda \end{pmatrix}.$$

By Proposition 2.12 we have

$$E_{-+}^\lambda(z) = z - z_0 + \sum_{k=1}^\infty (-\lambda)^k E_- Q(EQ)^{k-1} E_+. \tag{5.16}$$

So $z(\lambda) = z_0 + \lambda\langle Qu_0, u_0\rangle + \mathcal{O}(\lambda^2)$. As a corollary, we get the Feynman–Hellmann formula

$$z'(0) = \langle Qu_0, u_0\rangle.$$

It also has a direct proof assuming $z(\lambda)$ is smooth in λ: first write down the eigenvalue equation $P^\lambda u^\lambda = z(\lambda)u^\lambda$, then differentiate on λ. We get

$$Qu_0 + P\dot{u}_0 = z'(0)u_0 + z_0\dot{u}_0.$$

Moreover, $\langle P\dot{u}_0, u_0\rangle = \langle \dot{u}_0, Pu_0\rangle = z_0\langle \dot{u}_0, u_0\rangle$. Pairing with u_0 gives

$$z_0 = \langle Qu_0, u_0\rangle.$$

Now we want to study how the bands of $P_\theta = (D_x - \theta)^2 + \lambda\cos x$ split. There are two cases where we have a double eigenvalue for $\lambda = 0$:

- $\theta = 0$, $m_1 = m$, $m_2 = -m$, where $m \in \mathbb{N}_+$, $P_\theta^{\lambda=0}$ has eigenvalue $z_0 = m^2$;
- $\theta = \frac{1}{2}$, $m_1 = m$, $m_2 = -m+1$, $m \in \mathbb{N}_+$, $P_\theta^{\lambda=0}$has eigenvalue $(m-1/2)^2$.

In the first case, we consider the Grushin problem (5.15) with $k = 2$. Let $e_j(x) = \frac{1}{\sqrt{2\pi}}e^{ijx}$ be eigenfunctions of D_x, we let

$$u_- = \begin{pmatrix} u_{--} \\ u_{-+} \end{pmatrix}, \quad v_+ = \begin{pmatrix} v_{+-} \\ v_{++} \end{pmatrix},$$

and

$$R_-u_- = u_{--}e_{-m} + u_{-+}e_m, \quad R_+u = \begin{pmatrix} \langle u, e_{-m}\rangle \\ \langle u, e_m\rangle \end{pmatrix}.$$

This gives a well-posed Grushin problem with $E_- = R_+$, $E_+ = R_-$, and

$$E_{-+}^\theta = \begin{pmatrix} z - (-m-\theta)^2 & 0 \\ 0 & z - (m-\theta)^2 \end{pmatrix}.$$

By Proposition 2.12 we get

$$\begin{aligned} E_{-+}^{\theta,\lambda}(z) = &\begin{pmatrix} z - (-m-\theta)^2 & 0 \\ 0 & z - (m-\theta)^2 \end{pmatrix} \\ &+ \sum_{k=1}^{m} \lambda^{2k} \begin{pmatrix} \langle e_{-m}, Q(EQ)^{2k-1}e_{-m}\rangle & 0 \\ 0 & \langle e_m, Q(EQ)^{2k-1}e_m\rangle \end{pmatrix} \\ &+ \frac{\lambda^{2m}}{4^m} \prod_{j=-m+1}^{m-1} ((j-\theta)^2 - z)^{-1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \mathcal{O}(\lambda^{2m+2}). \end{aligned}$$

Note for $z \in \mathbb{R}$,

$$\begin{aligned} \langle e_{-m}, Q(EQ)^{2k-1}e_{-m}\rangle &= \langle \overline{e_{-m}}, \overline{Q(EQ)^{2k-1}e_{-m}}\rangle \\ &= \langle e_m, Q(EQ)^{2k-1}\overline{e_{-m}}\rangle = \langle e_m, Q(EQ)^{2k-1}e_m\rangle. \end{aligned}$$

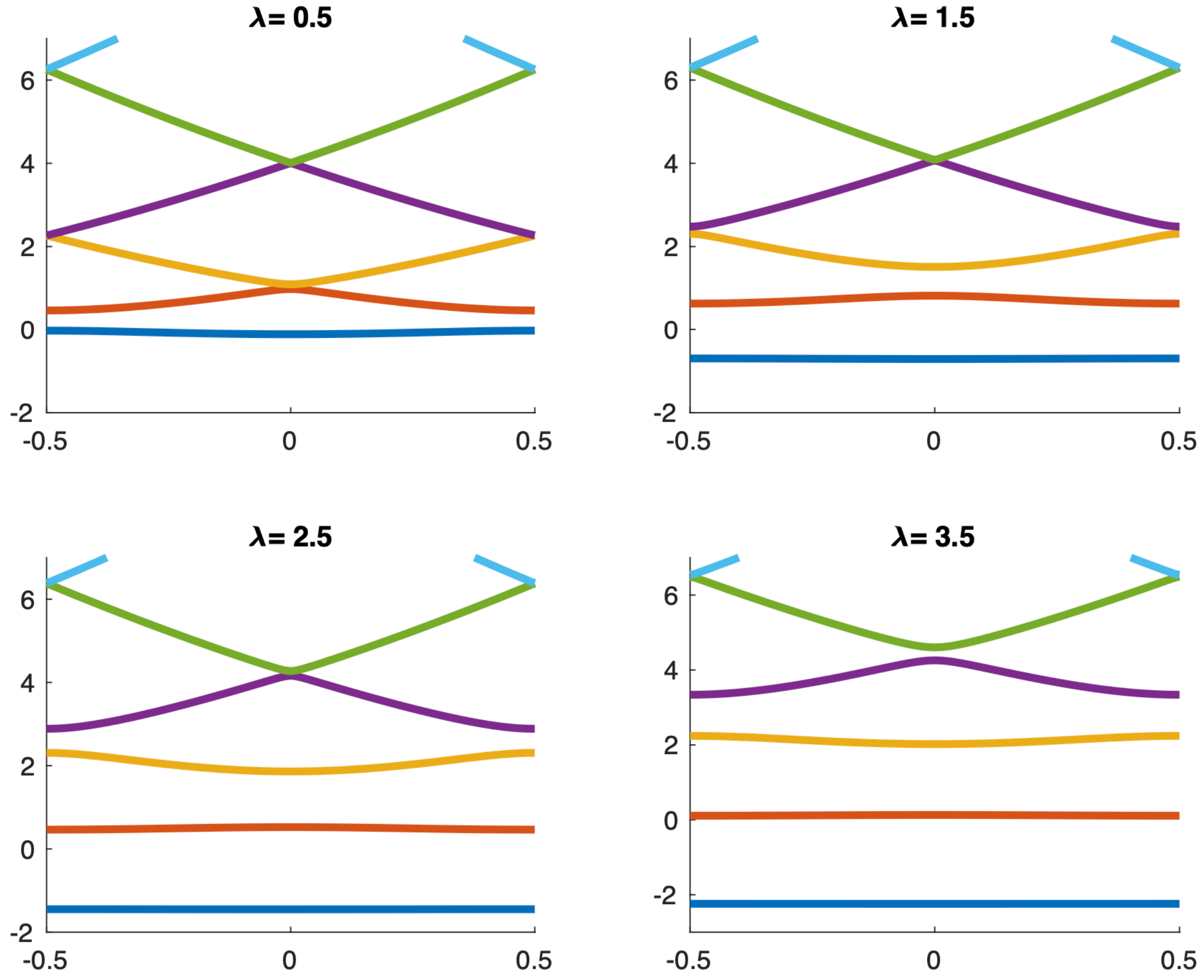


FIGURE 8. The band structure for $P = D_x^2 + \lambda \cos x$: we show $E_j(\theta)$, $-0.5 < \theta \leq 0.5$ for $j \leq 5$. Despite appearances there are gaps between all bands as soon as $\lambda > 0$. See the movie for an animated version with $0 \leq \lambda \leq 2$.

Thus we will see a splitting of the bands of size $\approx \lambda^{2m}$around $z_0 = m^2$.

In the second case, we still have $k = 2$, but eigenfunctions become e_{-m+1} and e_m, so

$$R_- u_- = u_{--} e_{-m+1} + u_{-+} e_m, \quad R_+ u = \begin{pmatrix} \langle u, e_{-m+1} \rangle \\ \langle u, e_m \rangle \end{pmatrix}.$$

This still gives a well-posed Grushin problem with $E_- = R_+$, $E_+ = R_-$, and

$$E^\theta_{-+} = \begin{pmatrix} z - (-m+1-\theta)^2 & 0 \\ 0 & z - (m-\theta)^2 \end{pmatrix}.$$

By Proposition 2.12 we get

$$\begin{aligned} E^{\theta,\lambda}_{-+}(z) &= \begin{pmatrix} z - (-m+1-\theta)^2 & 0 \\ 0 & z - (m-\theta)^2 \end{pmatrix} \\ &+ \sum_{k=1}^{m} \lambda^{2k} \begin{pmatrix} \langle e_{-m+1}, Q(EQ)^{2k-1} e_{-m+1}\rangle & 0 \\ 0 & \langle e_m, Q(EQ)^{2k-1} e_m \rangle \end{pmatrix} \\ &+ \frac{\lambda^{2m-1}}{2^{2m-1}} \prod_{j=-m+2}^{m-1} ((j-\theta)^2 - z)^{-1} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \mathcal{O}(\lambda^{2m+1}). \end{aligned}$$

Note for $z \in \mathbb{R}$,

$$\begin{aligned} \langle e_{-m+1}, Q(EQ)^{2k-1} e_{-m+1}\rangle &= \langle e^{ix}\overline{e_{-m+1}}, e^{ix}\overline{Q(EQ)^{2k-1}e_{-m+1}}\rangle \\ &= \langle e_m, Q(EQ)^{2k-1} e^{ix}\overline{e_{-m+1}}\rangle = \langle e_m, Q(EQ)^{2k-1} e_m\rangle. \end{aligned}$$

So we see a splitting of bands of size $\approx \lambda^{2m-1}$ around $z_0 = (m-1/2)^2$. In particular, when $m=1$, we have

$$E^{\theta,\lambda}_{-+}(z) = \begin{pmatrix} z - \theta^2 & 0 \\ 0 & z - (1-\theta)^2 \end{pmatrix} + \frac{\lambda}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \mathcal{O}(\lambda^2).$$

For $\theta = \frac{1}{2}$, one gets

$$z_\pm(\lambda) = \frac{1}{4} \pm \frac{\lambda}{2} + \mathcal{O}(\lambda^2).$$

See Figure 8 for the splitting of the bands (with a movie).

5.5. **Density of states for periodic Hamiltonians.** In §4.2 we provided motivating discussion of the density of states and considered it for constant magnetic field without an external potential. We now use the the explicit diagonalization given by the Bloch transform to describe it in terms of Bloch–Floquet spectrum. We recall,

$$\mathcal{B} : L^2(\mathbb{R}^n) \to L^n(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta), \quad u \mapsto \frac{1}{|\mathbb{R}^n/\Gamma^*|^{1/2}} \sum_{\gamma \in \Gamma} e^{-i\gamma\cdot\theta} u(x-\gamma)$$

and

$$U : L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta) \to L^2(\mathbb{R}^n/\Gamma^*; \ell^2(\mathbb{N})), \quad Uu(\theta,k) = \langle u(\theta,\bullet), \varphi_k(\theta,\bullet)\rangle_{\mathcal{H}_\theta}$$

where $\varphi_k(\theta,x)$ is the k-th eigenfunction of $P_\theta : \mathcal{H}_\theta \to \mathcal{H}_\theta$. That gives $U\mathcal{B}P(U\mathcal{B})^* v(\theta,k) = E_k(\theta) v(\theta,k)$ and hence

$$U\mathcal{B} f(P) (U\mathcal{B})^* v(\theta,k) = f(E_k(\theta)) v(\theta,k).$$

So

$$\begin{aligned}f(P)w(x) &= \sum_k \mathcal{B}^*(f(E_k(\theta))\varphi_k(\theta,x)\langle \mathcal{B}w(\theta,\bullet),\varphi_k(\theta,\bullet)\rangle_{\mathcal{H}_\theta}) \\ &= \frac{1}{|\mathbb{R}^n/\Gamma^*|}\sum_{k,\gamma}\int_{\mathbb{R}^n/\Gamma^*} f(E_k(\theta))\varphi_k(\theta,x)\int_{\mathbb{R}^n/\Gamma} e^{-i\gamma\cdot y}w(y-\gamma)\overline{\varphi_k(\theta,y)}dyd\theta \\ &= \frac{1}{|\mathbb{R}^n/\Gamma^*|}\sum_{k}\int_{\mathbb{R}^n/\Gamma^*} f(E_k(\theta))\varphi(\theta,x)\int_{\mathbb{R}^n} w(y)\overline{\varphi(\theta,y)}dyd\theta = \int_{\mathbb{R}^n} K(x,y)w(y)dy\end{aligned}$$

where

$$K(x,y) = \frac{1}{|\mathbb{R}^n/\Gamma^*|}\sum_k \int_{\mathbb{R}^n/\Gamma^*} f(E_k(\theta))\varphi_k(\theta,x)\overline{\varphi_k(\theta,y)}d\theta.$$

Note $K(x,x)$ is Γ-periodic, and thus the regularized trace (4.3) is given by

$$\begin{aligned}\widetilde{\operatorname{tr}} f(P) &= \frac{1}{|\mathbb{R}^n/\Gamma|}\int_{\mathbb{R}^n/\Gamma} K(x,x)dx = \frac{1}{|\mathbb{R}^n/\Gamma||\mathbb{R}^n/\Gamma^*|}\sum_k\int_{\mathbb{R}^n/\Gamma^*}\int_{\mathbb{R}^n/\Gamma} f(E_k(\theta))|\varphi(\theta,x)|^n dxd\theta \\ &= \frac{1}{(2\pi)^n}\sum_k\int_{\mathbb{R}^n/\Gamma^*} f(E_k(\theta))d\theta =: \int_{\mathbb{R}} f(\lambda)\rho(\lambda)d\lambda,\end{aligned}$$

where the last integral is meant as distributional pairing and it defines the *density of states*, $\rho \in \mathscr{S}'(\mathbb{R})$. It is given by

$$\rho(\lambda) = \frac{1}{(2\pi)^n}\sum_k\int_{\mathbb{R}^n/\Gamma^*}\delta(\lambda - E_k(\theta))d\theta = \frac{1}{(2\pi)^n}\frac{d}{d\lambda}\left(\sum_k\int_{\lambda_k(\theta)\le\lambda} d\theta\right)$$

In particular, if $E_N(\theta) < \lambda_0 < E_{N+1}(\theta)$ for all $\theta \in \mathbb{R}^n/\Gamma^*$, then

$$\int_{-\infty}^{\lambda_0}\rho(\lambda)d\lambda = \frac{N}{|\mathbb{R}^n/\Gamma|}$$

gives the number of of states per unit volume in agreement with the discussion in §4.2.

We also note that if λ is a regular value of $E(\theta)$, we can also write

$$\rho(\lambda) = \frac{1}{(2\pi)^n}\sum_k\int_{E_k(\theta)=\lambda}\frac{dS}{|\nabla E_k(\theta)|}.$$

Example 13. We can compute the density of states for the Kronig–Penney Hamiltonian in Example 11. That amounts to computing $d\theta/dE$ inside the spectrum and for that we can use the implicit formula (5.12):

$$\cos\theta = \frac{q\sin\sqrt{E}}{2\sqrt{E}} + \cos\sqrt{E}.$$

The spectral bands are defined by the condition that

$$-1 \le \frac{q\sin\sqrt{E}}{2\sqrt{E}} + \cos\sqrt{E} \le 1,$$

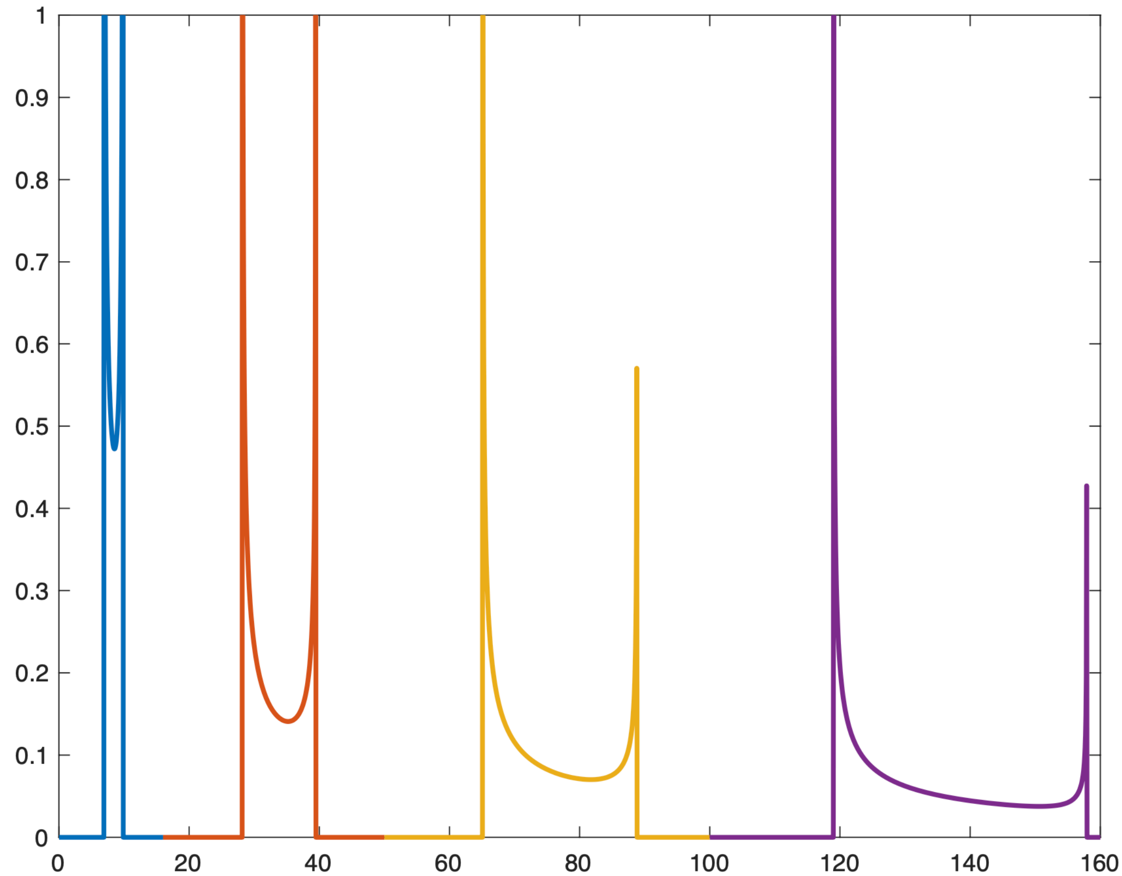


FIGURE 9. The plot of the density of states (up to a multiplicative constant) for the Konig–Penney potential. We see the singularities at the edges of the first 4 bands – see Figure 7.

(see Figure 7) in which case,

$$\frac{d\theta}{dE} = \frac{1}{4}(1-(q\sin\sqrt{E}/\sqrt{E}+\cos\sqrt{E})^2)^{-\frac{1}{2}}\left((q+2E)\sin\sqrt{E}/E^{\frac{3}{2}}-q\cos\sqrt{E}/E\right).$$

This is shown in Figure 9.

5.6. **Isolated bands for time reversible operators: trivial topology.** We first study the case when there is an isolated band, that is let $I_j = \{E_j(\theta) : \theta \in \mathbb{R}^n/\Gamma^*\}$, we assume

$$\begin{gathered} E_k(\theta) \text{ is a simple eigenvalue of } P \text{ on } \mathcal{H}_\theta, \\ I_k \cap I_j = \varnothing \text{ for any } j \neq k. \end{gathered} \tag{5.17}$$

Let $\Pi(\theta) : \mathcal{H}_\theta \to \ker(P|_{\mathcal{H}_\theta} - E_k(\theta)) \cong \mathbb{C}$ and $\tilde{\Pi}(\theta) = e^{ix\cdot\theta}\Pi(\theta)e^{-ix\cdot\theta} : L^2(\mathbb{R}^n/\Gamma^*) \to \ker(P(x, D_x - \theta) - E_k(\theta))$, we claim

Proposition 5.3.

$$\Pi(\theta) = \frac{1}{2\pi i} \oint_\gamma (z - P|_{\mathcal{H}_\theta})^{-1} dz \tag{5.18}$$

where γ is a positively oriented closed contour separating I_k from other bands.

Proof. For two functions f, g, define

$$f \otimes g := f\langle u, g\rangle.$$

Then the spectral theorem shows that

$$(z - P|_{\mathcal{H}_\theta})^{-1} = \sum_j \frac{\varphi_j(\cdot, \theta) \otimes \varphi_j(\cdot, \theta)}{z - E_j(\theta)}.$$

This implies that

$$\frac{1}{2\pi i} \oint_\gamma (z - P|_{\mathcal{H}_\theta})^{-1} dz = \varphi_k \otimes \varphi_k.$$

□

Remark 3. *In general, if we have any operator P and a simple closed curve γ such that $\gamma \cap \operatorname{Spec}(P) = \varnothing$, then*

$$\Pi = \frac{1}{2\pi i} \oint_\gamma (z - P)^{-1} dz$$

is a projection. We can take another curve $\tilde{\gamma}$ which is homotopic to γ inside $\mathbb{C} \setminus \operatorname{Spec}(P)$, and γ inside the interior of $\tilde{\gamma}$. Then

$$\begin{aligned}
\Pi^2 &= \frac{1}{(2\pi i)^2} \oint_{\tilde{\gamma}} \oint_\gamma (z - P)^{-1} (\zeta - P)^{-1} dz d\zeta \\
&= \frac{1}{(2\pi i)^2} \oint_{\tilde{\gamma}} \oint_\gamma (\zeta - z)^{-1} ((z - P)^{-1} - (\zeta - P)^{-1}) dz d\zeta \\
&= \frac{1}{(2\pi i)^2} \oint_{\tilde{\gamma}} \oint_\gamma (\zeta - z)^{-1} (z - P)^{-1} dz d\zeta \\
&= \frac{1}{2\pi i} \oint_\gamma (z - P)^{-1} dz d\zeta \\
&= \Pi.
\end{aligned}$$

If P is self-adjoint, then by functional calculus, Π is the spectral projector to the spectrum inside γ. This is because

$$f(x) = \frac{1}{2\pi i} \oint_\gamma (z - x)^{-1} dz = \begin{cases} 1, & x \text{ is inside } \gamma, \\ 0, & x \text{ is outside } \gamma. \end{cases}$$

We can think of Π as the spectral projector even for non-self-adjoint operators.

The family $\Pi(\theta)$ we defined is analytic in θ.

Lemma 5.4. *The map*

$$\theta \mapsto \Pi(\theta) : \mathbb{R}^n/\Gamma^* \to B(\mathcal{H}_\theta)$$

is a real analytic family of operators, that is there exists $\varepsilon > 0$ such that this map extends to a holomorphic map

$$\mathbb{R}^n/\Gamma^* + iB(0,\varepsilon) \ni \theta \mapsto \Pi(\theta).$$

Proof. It suffices to check for

$$\tilde{\Pi}(\theta) = \frac{1}{2\pi i}\oint_\gamma (z - P(x, D_x - \theta))^{-1} d\theta,$$

whose holomorphicity is clear from the definition. □

Remark 4. *Here we are talking about the holomorphicity in a Banach space, so we recall the following definition.*

Suppose we have two Hilbert spaces H_1, H_2, and a map $\theta \mapsto B(\theta)$ from $\mathbb{C}^n \to B(H_1, H_2)$. Then we say $B(\theta)$ is holomorphic if the following equivalent conditions are satisfied.

- *For any $\varphi \in H_1, \psi \in H_2$, the map $\theta \mapsto \langle B(\theta)\varphi, \psi\rangle$ is holomorphic;*
- *The derivative in the weak sense $\overline{\partial}_{\theta_j} B(\theta) = 0$;*
- $\dfrac{\partial B}{\partial \theta_j} := \lim_{z\to 0} \dfrac{B(\theta + ze_j) - B(\theta)}{z}$ *exists in the norm topology.*

The reader can check the equivalence using uniform boundedness principle.

The eigenspace $\mathcal{H}_\theta$ thus defines a complex line bundle over the torus $\mathbb{R}^n/\Gamma^*$. We refer to Section 2.7 for basic properties of line bundles.

The following theorem tells us when there is time reversal symmetry, the line bundle is actually trivial.

Theorem 6. *Suppose $\overline{P(x,D)u} = P(x,D)\overline{u}$, then there exists $\varphi \in C^\infty(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)$ such that*

- *$P\varphi(\theta) = E_k(\theta)\varphi(\theta)$, and $\|\varphi(\theta)\| = 1$, that is $\varphi(\theta)$ is a normalized eigenvector of P with eigenvalue $E_k(\theta)$.*
- *$\varphi(-\theta) = \overline{\varphi(\theta)}$.*
- *In addition, $\theta \mapsto \varphi(\theta)$ extends to a holomorphic map on $\mathbb{R}^n/\Gamma^* + iB(0,\varepsilon)$*

Remark 5. *In other words, this theorem shows that if a line bundle L over a torus satisfies $L^* \cong L$, then L has to be trivial. This reflects the fact that $H^2(\mathbb{R}^n/\Gamma^*; \mathbb{Z}) = \bigwedge^2 \Gamma$ is torsion-free. We will give an elementary proof following the proof of* [HS89, Lemma 1.1].

Proof. We first note that is that if $\varphi(\theta) \in \mathcal{H}_\theta$ then $\overline{\varphi(\theta)} \in \mathcal{H}_{-\theta}$. Simplicity of $E_k(\theta)$ and the property $\overline{Pu} = P\bar{u}$ show that

$$E_k(\theta) = E_k(-\theta), \quad \overline{\varphi(\theta)} \in \ker(P|_{\mathcal{H}_{-\theta}} - E_k(\theta)).$$

Using this we will proceed by induction on the dimension n to show there is a continuous section. Then we will regularize it to get a real analytic section. Without loss of generality, we may assume $\Gamma = (2\pi\mathbb{Z})^n$ and $\Gamma^* = \mathbb{Z}^n$.

Step 1: Let $n = 1$. By Proposition 2.16, we can choose a continuous section $\tilde{\psi}(\theta)$ such that $P\tilde{\psi}(\theta) = E_k(\theta)\tilde{\psi}(\theta)$ and $\|\tilde{\psi}(\theta)\| = 1$ for $0 \leq \theta \leq 1/2$. We define $\tilde{\psi}(\theta) := \overline{\tilde{\psi}(-\theta)}$ for $-1/2 \leq \theta \leq 0$. One can check this defines a section except we want to glue at $\theta = 1/2$ and $\theta = -1/2$. Since $\|\tilde{\psi}(-1/2)\| = \|\tilde{\psi}(1/2)\| = 1$, there exists $\alpha \in \mathbb{R}$ such that $\tilde{\psi}(-1/2) = e^{-i\alpha}\tilde{\psi}(1/2)$. We then let

$$\psi(\theta) = e^{-i(\theta+1/2)\alpha}\tilde{\psi}(\theta),$$

so that $\psi(1/2) = \psi(-1/2)$. It glues to a global section on $\mathbb{R}/\mathbb{Z}$.

Step 2: By induction hypothesis, we may assume there exists a continuous section $\psi'(\theta')$ on $\mathbb{R}^{n-1}/\mathbb{Z}^{n-1} \times \{0\}$ such that $\overline{\psi'(\theta')} = \psi'(-\theta')$. Moreover, $P\psi'(\theta') = E_k(\theta', 0)\psi'(\theta')$ and $\|\psi'(\theta')\| = 1$. By Proposition 2.16, there exists a continuous extension to this section

$$\Psi(\theta) : (\mathbb{R}^{n-1}/\mathbb{Z}^{n-1})_{\theta'} \times [0, 1/2]_{\theta_n} \to \ker_{\mathcal{H}_\theta}(P - E_k(\theta)), \qquad \Psi(\theta', 0) = \psi'(\theta').$$

We now define Ψ on $\mathbb{R}^{n-1}/\mathbb{Z}^{n-1} \times [-\frac{1}{2}, 0]$ by $\Psi(-\theta) = \overline{\Psi(\theta)}$, and we want $\Psi(\theta', 1/2) = \Psi(\theta', -1/2)$ as before. In general one only has

$$\Psi(\theta', \tfrac{1}{2}) = e^{i\alpha(\theta')}\Psi(\theta', -\tfrac{1}{2})$$

where $\alpha(\theta') \in \mathbb{R}$ such that

$$\alpha(\theta' + \gamma) \equiv \alpha(\theta') \mod 2\pi\mathbb{Z}, \quad \gamma \in \mathbb{Z}^{n-1}.$$

Taking the conjugate we have

$$\Psi(-\theta', -\tfrac{1}{2}) = e^{-i\alpha(\theta')}\Psi(-\theta', \tfrac{1}{2})$$

or equivalently

$$\Psi(\theta', -\tfrac{1}{2}) = e^{-i\alpha(-\theta')}\Psi(\theta', \tfrac{1}{2}).$$

Thus $e^{i\alpha(\theta')} = e^{i\alpha(-\theta')}$, and

$$\alpha(\theta') \equiv \alpha(-\theta') \mod 2\pi\mathbb{Z}.$$

Since α is continuous at 0, we conclude $\alpha(\theta') = \alpha(-\theta')$. Since

$$\alpha\left(-\tfrac{1}{2}e_j + e_j\right) = \alpha\left(\tfrac{1}{2}e_j\right) = \alpha\left(-\tfrac{1}{2}e_j\right),$$

we conclude $\alpha(\theta' + \gamma) = \alpha(\theta')$ for $\gamma \in \mathbb{Z}^{n-1}$. Now define

$$\psi(\theta) := e^{-i(\theta_n+1/2)\alpha(\theta')}\Psi(\theta),$$

then

$$\psi(\theta', \tfrac{1}{2}) = e^{-i\alpha(\theta')}\Psi(\theta', \tfrac{1}{2}) = \Psi(\theta', -\tfrac{1}{2}) = \psi(\theta', -\tfrac{1}{2}).$$

Thus ψ gives a continuous global section over $\mathbb{R}^n/\mathbb{Z}^n$.

Step 3: Having obtained a continuous section $\psi : \mathbb{R}/\Gamma^* \to C^\infty(\mathbb{R}^n) \cap \mathcal{H}_\theta$, we want to regularlize it to get a real analytic section. Let $\chi(\theta) = (2\pi)^{-n/2}e^{-\theta^2/2}$ and $\chi_\varepsilon(\theta) = \varepsilon^{-n}\chi(\theta/\varepsilon)$, we define

$$\psi_\varepsilon(\theta, x) = \int_{\mathbb{R}^n} \chi_\varepsilon(\theta - \theta')e^{ix\cdot(\theta'-\theta)}\psi(\theta', x)d\theta'.$$

One checks

$$\psi_\varepsilon(\theta, x-\gamma) = \int_{\mathbb{R}^n} \chi_\varepsilon(\theta - \theta')e^{i(x-\gamma)\cdot(\theta'-\theta)}\psi(\theta', x-\gamma)d\theta' = e^{i\gamma\cdot\theta}\psi_\varepsilon(\theta, x),$$

so $\psi_\varepsilon(\theta, \cdot) \in \mathcal{H}_\theta$. Now $\psi_\varepsilon(\theta, \cdot)$ is a real analytic section and $\psi_\varepsilon(\theta, \cdot) \to \psi(\theta)$ in L^2 norm as $\varepsilon \to 0$. Taking $\varepsilon > 0$ small enough, we define

$$\varphi(\theta) = \frac{\varphi_0(\theta)}{\left(\int_{\mathbb{R}^n/\Gamma^*} \varphi_0(\theta)\varphi_0(-\theta)dx\right)^{1/2}}, \quad \varphi_0(\theta) = \Pi(\theta)\psi_\varepsilon(\theta).$$

By Lemma 5.4, $\varphi(\theta)$ gives a real analytic section satisfying all the required properties. $\square$

5.7. **Wannier functions and spectral localization to an isolated band.** Given the global section in Theorem 6, we see that

$$(\mathcal{B}\Pi_k\mathcal{C})L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta) = \{u(\theta, x) = f(\theta)\varphi(\theta, x) : f \in L^2(\mathbb{R}^n/\Gamma^*)\}.$$

Thus

$$\Pi_k L^2(\mathbb{R}^n) = \left\{ \int_{\mathbb{R}^n/\Gamma^*} f(\theta)\varphi(\theta, \cdot)d\theta : f \in L^2(\mathbb{R}^n/\Gamma^*) \right\}.$$

Expanding $f(\theta)$ into Fourier series, we obtain $f(\theta) = \sum_{\gamma\in\Gamma} a_\gamma e^{i\gamma\cdot\theta}$ and

$$\frac{1}{|\mathbb{R}^n/\Gamma^*|}\int_{\mathbb{R}^n/\Gamma^*} f(\theta)\varphi(\theta, \cdot)d\theta = \sum_{\gamma\in\Gamma} a_\gamma\varphi_\gamma(\theta)$$

where

$$\varphi_0(x) = \frac{1}{|\mathbb{R}^n/\Gamma^*|}\int_{\mathbb{R}^n/\Gamma^*} \varphi(\theta, x)d\theta \tag{5.19}$$

and $\varphi_\gamma(x) = \varphi_0(x - \gamma)$. We conclude

Proposition 5.5. *$\{\varphi_\gamma(x) : \gamma \in \Gamma\}$ gives an orthonormal basis of $\Pi_k L^2(\mathbb{R}^n)$. This basis gives an isomorphism $\Pi_k L^2(\mathbb{R}^n) \cong \ell^2(\Gamma)$.*

One can also check those properties directly. The basis φ_γ are called Wannier functions.

Theorem 6 has the following corollary about exponential decay of Wannier functions.

Proposition 5.6. *There exists a constant $C > 0$ such that for any $\alpha \in \mathbb{N}^n$ there is $C_\alpha > 0$ with*

$$|\partial^\alpha \varphi_0(x)| \leq C_\alpha e^{-|x|/C}. \tag{5.20}$$

Proof. Recall

$$\varphi_0(x-\gamma) = \frac{1}{|\mathbb{R}^n/\Gamma^*|}\int_{\mathbb{R}^n/\Gamma^*} e^{i\gamma\cdot\theta}\varphi(\theta,x)d\theta.$$

Using analyticity we can deform the contour from $\mathbb{R}^n/\Gamma^*$ to $\mathbb{R}^n/\Gamma^* + i\gamma/|\gamma|\varepsilon$, so we conclude that $\varphi_0(x-\gamma) = \mathcal{O}(e^{-\varepsilon|\gamma|})$. These estimates are uniform for x in the fundamental domain of Γ and (5.20) follows. $\square$

6. The tight binding model

6.1. Motivation and examples.

6.2. A warm up: a double well potential.

In this section we will consider the problem of a double well potential on the line

$$\begin{gathered} V(x) = V(-x), \quad V(1) = V'(1) = 0, \quad V''(1) > 0, \\ V|_{\mathbb{R}\setminus\{\pm 1\}} > 0, \quad \liminf_{|x|\to\infty} V(x) > 0, \quad V \in C^\infty(\mathbb{R}). \end{gathered} \tag{6.1}$$

A standard example is given by $V(x) = \frac{1}{2}(x^2-1)^2$. The corresponding semiclassical Schrödinger operator is given by

$$P(h) := -h^2\partial_x^2 + V(x). \tag{6.2}$$

The main result of this section concerns the exponentially small splitting between the two smallest eigenvalues of $P(h)$:

Theorem 7. *Suppose that $P(h)$ given by (6.2) with $V(x)$ satisfying (6.1). Then for $0 < h < h_0$,*

$$\operatorname{Spec}(P(h)) \cap [0, \alpha h] = \{\lambda_1(h), \lambda_2(h)\}, \quad \alpha < 3(\tfrac{1}{2}V''(1))^{\frac{1}{2}}, \tag{6.3}$$

and

$$\begin{gathered} \lambda_2(h) - \lambda_1(h) = 4h^{\frac{1}{2}}\sqrt{(\tfrac{1}{2}V''(1))^{\frac{1}{2}}/\pi}\, e^A e^{-S_0/h}(1+\mathcal{O}(h)), \\ S_0 := \int_{-1}^{1}\sqrt{V(x)}dx, \quad A := \lim_{\varepsilon\to 0+}\left(\int_{-1+\varepsilon}^{1+\varepsilon}\frac{1}{2}\sqrt{\frac{\frac{1}{2}V''(1)}{V(x)}} + \log\varepsilon + \log\sqrt{V''(1)/2}\right). \end{gathered} \tag{6.4}$$

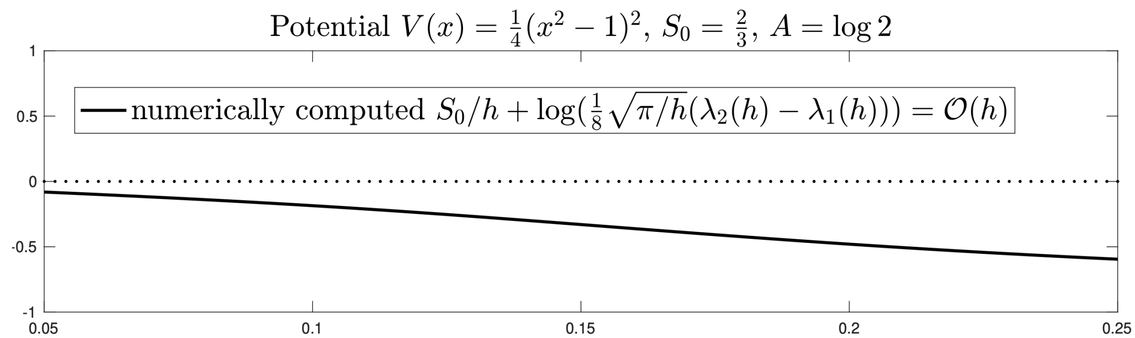
In the example $V(x) = \frac{1}{4}(x^2-1)^2$, we have

$$S_0 = \int_{-1}^{1} \sqrt{V(x)}dx = \tfrac{1}{2}\int_{-1}^{1}(1-x^2)dx = \tfrac{2}{3},$$

and, using (6.54),

$$A = \frac{1}{2}\lim_{\varepsilon\to 0+}\left(\int_{-1+\varepsilon}^{1-\varepsilon}\frac{1}{\frac{1}{2}(1-x^2)}dx + \log\varepsilon\right) = \lim_{\varepsilon\to 0+}\log(2+\varepsilon) = \log 2.$$

If we use the first 151 eigenfunctions of $(hD_x)^2 + x^2$ as an approximate basis of L^2 and compute the first two eigenvalues of $(hD_x)^2 + V(x)$ we obtain the following (admittedly, roughly computed) agreement with the theory:



We adapt, in a self-contained way, Helffer's presentation from [He88, §4.5] – see also earlier works by Landau–Lifshitz, Reed–Simon, and Harrell mentioned there. An interesting physics perspective on the double well problem is presented by Coleman in [Co77, §II.2] (with a *doubly well* done version in [Co77, Appendix B]).

There are many steps in the proof of Theorem 7 and they will be relevant to the solutions of the periodic problem. We retain some higher dimensional aspects of the argument (notably in the discussion of the Agmon–Lithner estimates) and this section can be considered as an introduction to the Helffer–Sjöstrand theory of semiclassical spectra for multi-well potentials – see [He88, §§3,4], [DS99, §§3,6] and references given there. Major simplifications due to working in 1D come in Proposition 6.3 (the WKB construction is particularly simple in 1D), the simple form of the Agmon metric (see Remark 6), and an easy calculation of the off diagonal terms in the interaction matrix (6.51) using a Wronskian (see (6.53)).

6.2.1. *Agmon–Lithner estimates.* We present these now classical estimates in all dimensions following [DS99, §6]. To formulate them we need some comments about Lipschitz functions. Suppose that $\Phi \in \mathrm{Lip}\,(\mathbb{R}^n)$, that is, there exists $M > 0$ such that

$$|\Phi(x) - \Phi(y)| \le M|x-y|. \tag{6.5}$$

We then use $\chi \in C^\infty_{\rm c}(B(0,1);[0,1])$, with $\int \chi = 1$ to define $\Phi_\varepsilon := \Phi * \chi_\varepsilon$, $\chi_\varepsilon(x) := \varepsilon^{-n}\chi(x/\varepsilon)$. The Lipshitz property shows that $\|\nabla \Phi_\varepsilon\|_{L^\infty}$ is uniformly bounded. In fact, since $\int \nabla \chi = 0$,

$$\begin{aligned}|\nabla \Phi_\varepsilon(x)| &\leq \varepsilon^{-n-1}\left|\int (\nabla\chi)(y/\varepsilon)(\Phi(x-y)-\Phi(x))dy\right| \\ &\leq M\varepsilon^{-n}\int |\nabla\chi(y/\varepsilon)||y/\varepsilon|dy = M\int |\nabla \chi(z)||z|dz.\end{aligned}$$

If we define $\nabla\Phi \in \mathscr{D}'(\mathbb{R}^n)$ using distribution theory, then $\Phi_\varepsilon \to \Phi$ in $\mathscr{D}'(\mathbb{R}^n)$ and, for $\varphi \in C^\infty_{\rm c}(\mathbb{R}^n;\mathbb{R}^n)$,

$$\nabla\Phi(\varphi) = \lim_{\varepsilon\to 0}\int \nabla\Phi_\varepsilon(x)\cdot\varphi(x)dx = \mathcal{O}(\|\varphi\|_{L^1}).$$

Hence, as L^∞ is the dual of L^1, $\nabla\Phi \in L^\infty(\mathbb{R}^n)$. That is the meaning of $\nabla\Phi$ in the estimates below. (We remark that Φ is in fact differentiable almost everywhere – see [Ev10, §5.8.3].) For $\Omega \subset \mathbb{R}^n$ with C^1 boundary we also recall the space

$$H^2 \cap H^1_0(\Omega) = \text{closure of } \{u \in C^2(\overline{\Omega}) : u|_{\partial\Omega} = 0\} \tag{6.6}$$

where the closure is in the norm given by $\sum_{|\alpha|\leq 2}\|\partial^\alpha u\|_{L^2(\Omega)}$.

Proposition 6.1. *Suppose $\Omega \subset \mathbb{R}^n$ is a bounded open set with a C^1 boundary, $\partial\Omega$, $V \in C(\overline{\Omega};\mathbb{R})$ and $\Phi \in \mathrm{Lip}(\overline{\Omega};\mathbb{R})$. Then for $P := -h^2\Delta + V$ and every $u \in H^2\cap H^1_0(\Omega;\mathbb{C})$ (see (6.6)), $h>0$,*

$$\|h\nabla(e^{\Phi/h}u)\|_{L^2(\Omega)} + \langle (V-|\nabla\Phi|^2)e^{\Phi/h}u, e^{\Phi/h}u\rangle_{L^2(\Omega)} = \mathrm{Re}\langle e^{\Phi/h}Pu, e^{\Phi/h}u\rangle_{L^2(\Omega)}. \tag{6.7}$$

Proof. We present a proof from [DS99] which has the advantage of generalising to the case of manifolds and forms (with modifications requiring an introduction of Riemannian metric; a sceptical reader can proceed by direct integration by parts). For that, we define an inner product on differential forms,

$$\|\omega\|^2_{L^2(\Omega)} := \sum_j \|\omega_j\|^2_{L^2(\Omega)}, \quad \omega := \sum_j \omega_j dx_j \in C^\infty_{\rm c}(\Omega, T^*\Omega).$$

The formal adjoint of $d : C^\infty_{\rm c}(\Omega)$, $du = \sum_j \partial_{x_j}u dx_j$, is then given by $d^*\omega = -\sum_j \partial_{x_j}\omega_j$. We start with $\Phi \in C^\infty(\overline{\Omega})$ and introduce

$$\begin{gathered} d\Phi\wedge : C^\infty_{\rm c}(\Omega) \to C^\infty_{\rm c}(\Omega, T^*\Omega), \quad d\Phi\wedge u := ud\Phi, \\ \nabla\Phi \lrcorner := (d\Phi\wedge)^* : C^\infty_{\rm c}(\Omega,T^*\Omega) \to C^\infty_{\rm c}(\Omega), \quad \nabla\Phi \lrcorner\, \omega = \sum_j \omega_j\partial_{x_j}\Phi.\end{gathered}$$

Since $-\Delta = d^*d$, we have a point-wise statement,

$$\begin{aligned} &e^{\Phi/h}(-h^2\Delta)e^{-\Phi/h} = e^{\Phi/h}(hd^*)e^{-\Phi/h}e^{\Phi/h}(hd)e^{-\Phi/h} \\ &= (hd^* + \nabla\Phi\lrcorner)(hd - d\Phi\wedge) = h^2d^*d - |\nabla\Phi|^2 - hd^*(d\Phi\wedge) + \nabla\Phi\lrcorner\, hd.\end{aligned} \tag{6.8}$$

We now assume that $u \in C_c^\infty(\Omega)$ and put $v = e^{\Phi/h}u$, so that

$$\operatorname{Re}\langle e^{\Phi/h}(-h^2\Delta)u, e^{\Phi/h}u\rangle_{L^2(\Omega)} = \operatorname{Re}\langle e^{\Phi/h}(-h^2\Delta)e^{-\Phi/h}v, v\rangle_{L^2(\Omega)}.$$

When we apply (6.8) we notice that $(\nabla\Phi \lrcorner d)^* = d^*(d\Phi\wedge)$, the last two terms disappear after taking of real parts. This gives (6.7) for $u \in C_c^\infty(\Omega)$. For the integration by parts, we only need $u \in C^2(\overline{\Omega})$ and $u|_{\partial\Omega} = 0$. By approximation we obtain the statement for $u \in H^2 \cap H_0^1(\Omega)$.

To prove (6.7) for $\Phi \in \operatorname{Lip}(\overline{\Omega})$, we first extend Φ to a Lipschitz function on $\mathbb{R}^n$ (and keep the same notation). We then define Φ_ε as in the discussion after (6.5) and note that (using the definition of convolution of distributions and compactly supported functions)

$$\nabla\Phi_\varepsilon(x) = \int \nabla\Phi(x)\chi_\varepsilon(x)dx.$$

Then $\nabla\Phi_\varepsilon \to \nabla\Phi$ in $L^1_{\rm loc}$ (see [Ho03, Theorem 1.3.2]) and hence there exists a sequence $\varepsilon_j \to 0$ such that $\nabla\Phi_{\varepsilon_j} \to \nabla\Phi$ almost everywhere (see [Ru87, Theorem 3.12]). We can then use that subsequence to pass to the limit from Φ_{ε_j} in Φ in (6.7) using the dominated convergence theorem. (In fact, $\nabla\Phi_\varepsilon \to \nabla\Phi$ almost everywhere if we use the more involved Lebesgue differentiation theorem [Ru87, Theorem 7.17].) $\square$

When considering operators on all of $\mathbb{R}^n$ we assume

$$V \in C(\overline{\Omega}; \mathbb{R}), \quad \exists\, E_0 \in \mathbb{R}\,\forall\, x \in \mathbb{R}^n \;\; V(x) > E_0. \tag{6.9}$$

We can then consider the Friedrichs extension (see Example 4 in §2.3) of $P := -h^2\Delta + V$, with the domain $D(P) \subset H^1(\mathbb{R}^n)$. In that case we have the following version of the Agmon–Lithner estimates:

Proposition 6.2. *Suppose that V satisfies (6.9) and $D(P)$ is the domain of the Friedrichs extension of $-h^2\Delta + V$. If $\Phi \in \operatorname{Lip}(\mathbb{R}^n; \mathbb{R})$ is constant outside of a compact set then for every $u \in D(P)$ (6.7) holds for $\Omega = \mathbb{R}^n$.*

Proof. Let $\chi \in C_c^\infty(B(0,2); [0,1])$ satisfy $\chi|_{B(0,1)} \equiv 1$. For $R > 1$ we define $\chi_R(x) = \chi(x/R)$. For u in the domain of the Friedrichs extension of P, we have $\chi_R u \in H^2 \cap H_0^1(B(0,2R))$ and hence we can apply Proposition 6.1 to u_R. Since $\operatorname{supp} u_R \Subset B(0,2R)$, the integration is now over $\mathbb{R}^n$.

$$\|h\nabla(e^{\Phi/h}u_R)\|_{L^2(\mathbb{R}^n)} + \langle (V - |\nabla\Phi|^2)e^{\Phi/h}u_R, e^{\Phi/h}u_R\rangle_{L^2(\mathbb{R}^n)} = \operatorname{Re}\langle e^{\Phi/h}Pu_R, e^{\Phi/h}u_R\rangle_{L^2\mathbb{R}^n}.$$

We now see that for $u \in D(P)$ and Φ constant outside of a compact set, we have, as $R \to \infty$,

$$u_R = \chi_R u \xrightarrow{L^2(\mathbb{R}^n)} u, \quad \nabla(e^{\Phi/h}u_R) = \chi_R\nabla(e^{\Phi/h}u) + R^{-1}(\chi')_R e^{\Phi/h}u \xrightarrow{L^2(\mathbb{R}^n)} \nabla(e^{\Phi/h}u),$$

and

$$Pu_R = \chi_R Pu - 2hR^{-1}(\nabla\chi)_R \cdot h\nabla\chi u - h^2R^{-2}(\Delta\chi)_R u \xrightarrow{L^2(\mathbb{R}^n)} Pu.$$

Passing to the limit gives (6.7) with $\Omega = \mathbb{R}^n$. □

Following [DS99, Proposition 6.2] it is useful to apply Proposition 6.1 and 6.2 as follows. In the setting those proposition, if $F_\pm \in L^\infty(\Omega; [0,\infty))$ ($\Omega = \mathbb{R}^n$ in the case of Proposition 6.2), satisfy

$$V(x) - |\nabla\Phi(x)|^2 = F_+(x)^2 - F_-(x)^2, \quad \text{almost everywhere,} \tag{6.10}$$

then, with norms in $L^2(\Omega)$,

$$\|h\nabla(e^{\Phi/h}u)\|^2 + \tfrac{1}{2}\|F_+e^{\Phi/h}u\|^2 \leq \|(F_+ + F_-)^{-1}e^{\Phi/h}Pu\|^2 + \tfrac{3}{2}\|F_-e^{\Phi/h}u\|^2. \tag{6.11}$$

Proof of (6.11). The definition of $F_\pm$ and (6.7) give

$$\begin{aligned} h^2\|\nabla(e^{-\Phi/h}u)\|^2 + \|F_+e^{\Phi/h}u\|^2 &= \operatorname{Re}(e^{\Phi/h}Pu, e^{\Phi/h}u) + \|F_-e^{\Phi/h}u\|^2 \\ &\leq \operatorname{Re}\left\langle e^{\Phi/h}(F_+ + F_-)^{-1}Pu, (F_+ + F_-)e^{\Phi/h}u\right\rangle + \|F_-e^{\Phi/h}u\|^2 \\ &\leq \left\|e^{\Phi/h}(F_+ + F_-)^{-1}Pu\right\|^2 + \tfrac{1}{4}\|(F_+ + F_-)e^{\Phi/h}u\|^2 + \|F_-e^{\Phi/h}u\|^2 \\ &\leq \left\|e^{\Phi/h}(F_+ + F_-)^{-1}Pu\right\|^2 + \tfrac{3}{2}\|F_-e^{\Phi/h}u\|^2 + \tfrac{1}{2}\|F_+e^{\Phi/h}u\|^2. \end{aligned}$$

Moving the last term to the left hand side gives (6.11). □

Example 14. Following [DS99, §6.a] we can apply (6.11) to positive Schrödinger operators as follows. Suppose that $V \geq 2\alpha > 0$. That means that $\inf \operatorname{Spec}(P) \geq 2\alpha$ and in particular $Pu = v$, $P = -\Delta + V$, (note that $h = 1$ here) has a solution $u \in D(P)$ for any $v \in L^2(\mathbb{R}^n)$. We obtain an exponential decay estimate on u if we restrict the support of v:

$$\left.\begin{array}{l} v \in L^2(\mathbb{R}^n), \quad \operatorname{supp} v \subset B(0, R_0), \\ \Phi(x) := \sqrt{\alpha}(|x| - R_0)\mathbb{1}_{\mathbb{R}^n \setminus B(0,R_0)}(x) \end{array}\right\} \Longrightarrow \sqrt{\alpha}\|e^\Phi\nabla u\| + \alpha\|e^\Phi u\| \leq 4\|v\|. \tag{6.12}$$

For that we first take

$$\Phi_R(x) := \sqrt{\alpha}(|x| - R_0)\mathbb{1}_{B(0,R)\setminus B(0,R_0)}(x) + \sqrt{\alpha}(R - R_0)\mathbb{1}_{\mathbb{R}^n\setminus B(0,R)}(x),$$

and $F_+ := \sqrt{V(x) - |\nabla\Phi_R(x)|^2} \geq \sqrt{\alpha}$ and $F_- = 0$ and apply (6.11) with $\Omega = \mathbb{R}^n$. (The details are left as an exercise with an answer in [DS99, §6.a].)

Since (6.12) gives exponential decay, we conclude from Rellich–Kodratchev's theorem (see [Ev10, §5.7]) that for $\chi \in C^\infty_c$, $P^{-1}\chi : L^2 \to L^2$ is a compact operator (both regularity and decay are improved). By adding a constant to V we conclude that

$$\begin{gathered} V > E_0 > \lambda \implies \\ \forall \chi \in C^\infty_c(\mathbb{R}^n) \ (P - \lambda)^{-1}\chi : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n) \text{ is a compact operator.} \end{gathered} \tag{6.13}$$

This gives a PDE proof (as opposed to the more general operator theoretical proof – see [DS99, Theorem 4.19]) of the following fact which we use in our analysis here:

$$\liminf_{|x|\to\infty} V(x) \geq E_0 \implies \inf \operatorname{Spec}_{\mathrm{ess}}(-\Delta + V) \geq E_0, \tag{6.14}$$

that is the spectrum of $-\Delta + V$ in $(-\infty, E_0)$ is discrete. To see this we proceed as follows. For any $E_1 < E_0$, there exists R_0 such that for $|x| > R_0$, $V(x) > E_1$. In the notation of the proof of Proposition 6.2, $V_0 := V + E_0\chi_{R_0} > E_1$ and (6.13) gives

$$(-\Delta + V_0 - \lambda_0)^{-1}\chi_{R_0} : L^2 \to L^2 \quad \text{is compact for } \lambda_0 < E_1.$$

Since

$$\begin{aligned}(-\Delta + V_0 - \lambda)^{-1}\chi_{R_0} &= (-\Delta + V_0 - \lambda_0)^{-1}\chi_{R_0} \\ &\quad + (-\Delta + V_0 - \lambda)^{-1}(\lambda_0 - \lambda)(-\Delta + V_0 - \lambda_0)^{-1}\chi_{R_0},\end{aligned}$$

it follows that for $\lambda \notin \operatorname{Spec}(-\Delta + V_0)$, $(-\Delta + V_0 - \lambda)^{-1}\chi_{R_0}$ is a compact operator on L^2. We now write

$$-\Delta + V - \lambda = (-\Delta + V_0 - \lambda)^{-1}(I + T(\lambda)), \quad T(\lambda) := (-\Delta + V_0 - \lambda)^{-1}E_0\chi_R.$$

Hence for $\lambda \notin \operatorname{Spec}(-\Delta + V_0)$ (and in particular for $\lambda < E_1$, since $V_0 > E_1$), $\lambda \notin \operatorname{Spec}(-\Delta + V)$ if and only of $I + T(\lambda)$ is invertible. But $\lambda \mapsto I + T(\lambda)$, $\lambda \in \mathbb{C}\setminus[E_1, \infty)$ is a holomorphic family of Fredholm operators invertible when $\lambda \notin \mathbb{C}$. Analytic Fredholm theory [DyZw2, Theorem C.8] shows that the poles of $(I + T(\lambda))^{-1}$ are discrete in $\mathbb{C} \setminus [E_1, \infty)$, Since $E_1 < E_0$ was arbitrary, (6.14) follows. □

6.2.2. *A single well.* We now present results concerning a single well potential in dimension one. For higher dimensional versions see [DS99, §3] and [He88, §2]. We consider a bounded interval $[a, b]$, $a < 0 < b$, and W satisfying,

$$W \in C^\infty([a, b]; \mathbb{R}), \quad W(0) = W'(0) = 0, \quad W''(0) > 0, \quad W|_{[a,b]\setminus\{0\}} > 0. \tag{6.15}$$

We start by a construction of an approximate ground state. We use the notation

$$a \sim a_0 + ha_1 + \cdots = \sum_{j=0}^{\infty} h^j a_j,$$

to mean that for every $N \geq 1$ there exists a constant such that

$$\left| a - \sum_{j=0}^{N-1} a_j h^j \right| \leq C_N h^N. \tag{6.16}$$

We recall that Borel's Lemma [Zw12, Theorem 4.15] shows that for any a_j's we can find an a (satisfying suitable bounds) so that (6.16) holds.

Proposition 6.3. *There exist $\varphi = \varphi(x, h)$ and $\lambda = \lambda(h)$ with asymptotic expansions*

$$\begin{gathered}\varphi(x, h) \sim \varphi(x) + h\varphi_1(x) + \cdots, \\ \varphi'(x) = (\operatorname{sgn} x)\sqrt{W(x)}, \quad \varphi(0) = 0, \quad \varphi \geq 0, \quad \varphi_j \in C^\infty([a, b]), \\ \varphi_1'(x) = \tfrac{1}{2}(\tfrac{1}{2}|W'(x)|/W(x)^{\frac{1}{2}} - (\tfrac{1}{2}W''(0))^{\frac{1}{2}})/((\operatorname{sgn} x)W(x)^{\frac{1}{2}}), \quad \varphi_1(0) = 0, \\ \lambda(h) \sim \lambda_1 h + \lambda_2 h^2 + \cdots, \quad \lambda_1 = \sqrt{\tfrac{1}{2}W''(0)},\end{gathered} \tag{6.17}$$

so that

$$((hD_x)^2 + W(x) - \lambda(h))(e^{-\varphi(x,h)/h}) = \mathcal{O}(h^\infty)e^{-\varphi(x)/h}, \tag{6.18}$$

uniformly for $x \in [a, b]$.

Proof. We want to find

$$\varphi(x, h) \sim \varphi(x) + h\varphi_1(x) + \cdots, \quad \lambda(h) \sim h\lambda_1 + h^2\lambda_2 + \cdots, \tag{6.19}$$

solving

$$e^{\varphi(x,h)/h}(-h^2\partial_x^2 + W(x) - \lambda(h))e^{-\varphi(x,h)/h} \sim 0 \tag{6.20}$$

in a suitable asymptotic sense. This will be achieved if we show that

$$-(\varphi'(x, h))^2 + W(x) + h\varphi''(x, h) - \lambda(h) \sim 0.$$

in the sense of (6.16). Inserting (6.19) into this equation gives $\varphi'(x) = (\operatorname{sgn} x)\sqrt{W(x)}$ and

$$-2\varphi_0'(x)\varphi_j'(x) - \sum_{\ell=1}^{j-1} \varphi_\ell'(x)\varphi_{j-\ell}'(x) + \varphi_{j-1}''(x) - \lambda_j = 0, \quad \varphi_0(x) := \varphi(x).$$

Since $\varphi_0'(x) = \sqrt{\frac{1}{2}W''(0)}x + \mathcal{O}(x^2)$, solving this requires a choice of λ_j for which we can divide by $\varphi_0'(x)$:

$$\lambda_j = \varphi_{j-1}''(0) - \sum_{\ell=1}^{j-1} \varphi_\ell'(0)\varphi_{j-\ell}'(0), \quad \lambda_1 = \sqrt{\tfrac{1}{2}W''(0)}.$$

We then get a recursive formula

$$\varphi_j'(x) = \frac{1}{2\varphi_0'(x)}\left(\varphi_{j-1}''(x) - \sum_{\ell=1}^{j-1} \varphi_\ell'(x)\varphi_{j-\ell}'(x) - \lambda_j\right).$$

In particular,

$$\varphi_1'(x) = \frac{1}{2(\operatorname{sgn} x)\sqrt{W(x)}}\left(\frac{|W'(x)|}{2\sqrt{W(x)}} - \sqrt{\tfrac{1}{2}W''(0)}\right),$$

where the function in brackets vanishes at 0 and hence can be divided $(\operatorname{sgn} x)\sqrt{W(x)} = (\frac{1}{2}W''(0))^{\frac{1}{2}}x + \mathcal{O}(x^2)$.

We conclude that for $\varphi(x, h)$ and $\lambda(h)$ given by (6.19) with φ_j and λ_j chosen above we obtain from (6.20)

$$(-h^2\partial_x^2 + W(x) - \lambda(h))e^{-\varphi(x,h)/h} = \mathcal{O}(h^\infty)e^{-\varphi(x,h)/h},$$

and it is clear that we can replace $\varphi(x, h)$ by $\varphi(x)$ on the right hand side. $\square$

We can normalise the WKB state so that

$$w(x) = c(h)h^{-1/4}\exp(-\varphi(x,h)/h), \quad \|w\|_{L^2(a,b)} = 1. \tag{6.21}$$

The normalising constant is computed by the method of steepest descent based on $\varphi(x) = \frac{1}{2}\sqrt{\frac{1}{2}W''(0)}x^2 + \mathcal{O}(x^3)$ – see [Zw12, Theorem 3.11] (the real version in which the phase $2i\varphi(x)/h$ is replaced by $2\varphi(x)/h$ is obtained in the same way). This gives,

$$c(h) = ((\tfrac{1}{2}W''(0))^{\frac{1}{2}}/\pi)^{1/4}(1+\mathcal{O}(h)). \tag{6.22}$$

In our applications of Proposition 6.1 we will use the following notation: for $\varphi \in \mathrm{Lip}$ of $S \in \mathbb{R}$,

$$\begin{gathered} u(x) = \widetilde{\mathcal{O}}(e^{-\varphi(x)/h}), \quad w(x) = \widetilde{\mathcal{O}}(e^{-S/h}) \\ \Longleftrightarrow \\ \forall\, \varepsilon > 0, k \in \mathbb{N}\ \exists\, C > 0 \ \ |\partial_x^k u(x)| \leq Ce^{-\varphi(x)/h+\varepsilon/h}, \quad |\partial_x^k w(x)| \leq Ce^{-S/h+\varepsilon/h}, \end{gathered} \tag{6.23}$$

where the estimates are valid in the region of definitions of the functions.

Proposition 6.4. *Suppose that W satisfies (6.15) and $P_0(h)$ is the Dirichlet realisation of $(hD_x)^2 + W(x)$ on $[a,b]$. Then for any $\alpha < 3(\frac{1}{2}W''(0))^{\frac{1}{2}}$ there exists h_0 such that for $0 < h < h_0$,*

$$\mathrm{Spec}(P_0(h)) \cap [0, \alpha h] = \{\lambda(h)\}, \tag{6.24}$$

where $\lambda(h)$ has an asymptotic expansion given in (6.17). Moreover, if u is the normalised eigenfunction corresponding to $\lambda(h)$ then, in the notation of (6.17) and (6.23),

$$u(x) = \widetilde{\mathcal{O}}(e^{-\varphi(x)/h}), \quad x \in [a,b]. \tag{6.25}$$

In fact, more precisely,

$$\exists\, N\, \forall\, k\, \exists\, C \ \ |(h\partial_x)^k u(x)| \leq Ch^{-N}e^{-\varphi(x)/h}, \quad x \in [a,b]. \tag{6.26}$$

In the proof and in the next section we will need the following lemma (which can be refined in many different ways but is sufficient for us here):

Lemma 6.5. *Suppose A is a self-adjoint operator, $A \geq 0$ and that $\Pi := \mathbb{1}_{[0,2\delta]}(A)$ has finite rank. Suppose that $\{u_j\}_{j=1}^J$ and $0 \leq \lambda \leq \delta$ satisfy*

$$u_j \in D(A), \quad \|u_j\| = 1, \quad \|(A-\lambda)u_j\| \leq \varepsilon, \quad |\langle u_i, u_j\rangle| \leq \varepsilon, \ i \neq j, \quad \varepsilon < \delta. \tag{6.27}$$

Then

$$\|(I-\Pi)u_j\| \leq \varepsilon/\delta. \tag{6.28}$$

If in addition $J(\varepsilon + (\varepsilon/\delta)^2) < 1$ then

$$\mathrm{tr}\,\Pi \geq J, \quad d(\lambda, \mathrm{Spec}(A)) \leq \varepsilon, \tag{6.29}$$

that is, there are at least J eigenvalues of A (counted with multiplicities) in $[0, 2\delta]$.

Proof. To see (6.28) we note that

$$\langle A(I-\Pi)u_j, u_j\rangle \geq 2\delta\|(I-\Pi)u_j\|^2.$$

On the other hand

$$\langle A(I-\Pi)u_j, u_j\rangle = \langle (I-\Pi)Au_j, u_j\rangle = \lambda\|(I-\Pi)u_j\|^2 + \langle r_j, (I-\Pi)u_j\rangle, \quad \|r_j\| \leq \varepsilon.$$

and hence

$$(2\delta-\lambda)\|(I-\Pi)u_j\|^2 \leq \langle r_i, (I-\Pi)u_j\rangle \leq \varepsilon\|(I-\Pi)u_j\|,$$

(6.28) follows.

For (6.29) it suffices to show that $w_j := \Pi u_j$, $j = 1, \cdots, J$, are linearly independent and for that we consider the Gramian matrix, G, with entries given by

$$\begin{aligned}\langle w_i, w_j\rangle &= \langle u_i, u_j\rangle + \langle (\Pi - I)u_i, u_j\rangle = \langle u_i, u_j\rangle + \langle (\Pi-I)u_i, (\Pi-I)u_j\rangle \\ &= \delta_{ij} + a_{ij}, \qquad |a_{ij}| \leq (\varepsilon/\delta)^2 + \varepsilon,\end{aligned} \tag{6.30}$$

where we used the estimate on $\langle u_i, u_j\rangle$ in (6.27) and (6.28). This means that $G = I + R$ where we can estimate the norm of R by $J(\varepsilon + (\varepsilon/\delta)^2)$ (using, for instance, the discrete version of the Schur estimate – see (2.9) and (2.10)). Hence, the assumption gives $\|R\| < 1$ and the Gramian is inverible, showing the independence of w_j's. $\square$

Proof of Proposition 6.4. We proceed in three steps:

Step 1. We start by proving that if $(P_0(h)-\lambda(h))u = 0$, $\|u\|_{L^2([a,b])} = 1$, $\lambda(h) \in [0, Mh]$ then (6.26) holds with N depending on M and the potential W (and on k). For that we will use (6.7) with $V(x) = W(x) - \lambda(h)$ and

$$\Phi(x) = \begin{cases} \varphi(x) - Ch\log C, & \varphi(x) \leq Ch, \\ \varphi(x) - Ch\log(\varphi(x)/h), & \varphi(x) \geq Ch. \end{cases} \tag{6.31}$$

Then for $\varphi(x) \geq Ch$, we use $\varphi'(x)^2 = W(x)$ (see (6.17)) and the assumption $\lambda(h) \leq Mh$ to see that

$$\begin{aligned} V(x) - \Phi'(x)^2 &= W(x) - \lambda(h) - \varphi'(x)^2 + 2Ch\frac{\varphi'(x)^2}{\varphi(x)} - C^2h^2\frac{\varphi'(x)^2}{\varphi(x)^2} \\ &= -\lambda(h) + Ch\frac{W(x)}{\varphi(x)}\left(2 - \frac{Ch}{\varphi(x)}\right) \geq -Mh + Ch\frac{W(x)}{\varphi(x)}. \end{aligned}$$

Since $W(x) \geq C_1\varphi(x)$, $x \in [a,b]$ (both functions are positive away from 0 and $W(x) = \frac{1}{2}W''(0)x^2 + \mathcal{O}(x^3)$, $\varphi(x) = \frac{1}{2}(\frac{1}{2}W''(0))^{\frac{1}{2}}x + \mathcal{O}(x^3)$ near 0), we see that we can choose C large enough so that for $\varphi(x) \geq Ch$,

$$V(x) - \Phi'(x)^2 \geq c_0 h, \quad c_0 > 0.$$

We now apply (6.11) with

$$F_-^2 = -(V - \Phi'(x)^2)\mathbb{1}_{\varphi(x)\leq Ch} = \lambda(h)\mathbb{1}_{\varphi(x)\leq Ch} \leq \mathbb{1}_{\varphi(x)\leq Ch}Mh,$$

and $F_+^2 = (V(x) - \Phi'(x)^2)\mathbb{1}_{\varphi(x)\geq Ch} \geq c_0 h$, $c_0 > 0$. Since $\|u\|_{L^2([a,b])} = 1$, (6.11) gives

$$\|h\partial_x(e^{\varphi/h}u)\|_{L^2([a,b])} + \|e^{\varphi/h}u\|_{L^2([a,b])} \leq C_1 h^{-1},$$

and Sobolev embedding[1] gives (6.26) with $k = 0$ and $N = 1$. For higher derivatives we use the equation: if $k \geq 1$,

$$(h\partial_x)(e^{\varphi/h}(h\partial_x)^k u) = e^{\varphi/h}(h\partial_x)^{k-1}[(W(x) - \lambda(h))u] + \varphi' e^{\varphi/h}(h\partial_x)^k u,$$

and the bound follows by induction.

Step 2. We now use Lemma 6.5 to obtain (6.24). We first note that if $\chi \in C_c^\infty((a,b);[0,1])$ is equal to 1 near 0 then we can use the normalized WKB state w in (6.21) to obtain $u_1 := \chi w/\|\chi w\|$ which satisfies the assumptions of Lemma 6.5 with $A = P_0(h)$, $J = 1$, $\delta = \alpha h$ and $\varepsilon = \mathcal{O}(h^\infty)$. This implies that $P_0(h)$ has an eigenvalue which is asymptotically given by $\lambda(h)$ in (6.17) (and we use the same notation for it).

Step 3. To see that there is exactly one eigenvalue in $[0, \alpha h]$, suppose that for some $\mu \in [0, Mh]$, $(P_0(h) - \mu)v = 0$, $\|v\|_{L^2([a,b])} = 1$, $v(a) = v(b) = 0$. By the argument in Step 1 of the proof, (6.26) holds for v. For $0 < \delta \ll 1$ we define

$$v_1(x) = \chi_0(h^{\frac{1}{2}-\delta}x)v(x), \quad \chi_0 \in C_c^\infty((-2,2);[0,1]), \quad \chi_0(x) = 1, \quad |x| \leq 1.$$

On the support of $\chi_0'(h^{\frac{1}{2}-\delta}x)$ the estimate (6.26) (which holds for v) gives

$$|(h\partial_x)^k v_1(x)| = \mathcal{O}(h^{-N}e^{-\varphi(x)/h}) = \mathcal{O}(h^{-N}e^{-h^{-2\delta}/C}) = \mathcal{O}(h^\infty).$$

(We recall that $\varphi(x) = \frac{1}{2}(\frac{1}{2}W''(0))^{\frac{1}{2}}x^2 + \mathcal{O}(x^3)$ and $\varphi(x) > 0$ for $x \neq 0$.) Hence,

$$(P_0(h) - \mu)u_1 = \mathcal{O}(h^\infty)_{L^2(\mathbb{R})}, \quad u_1 := v_1/\|v_1\|. \tag{6.32}$$

On the other hand,

$$P_0(h) = (hD_x)^2 + \tfrac{1}{2}W''(0)x^2 + \mathcal{O}(x^3), \quad \mathcal{O}(x^3)\chi_0(h^{\frac{1}{2}-\delta}x) = \mathcal{O}(h^{\frac{3}{2}-3\delta}),$$

and (6.32) gives

$$((hD_x)^2 + \tfrac{1}{2}W''(0)x^2 - \mu)u_1 = \mathcal{O}(h^{\frac{3}{2}-3\delta})_{L^2(\mathbb{R})}.$$

We can now apply Lemma 6.5 with $A = (hD_x)^2 + \frac{1}{2}W''(0)x^2$ to see that

$$d(\mu, (\tfrac{1}{2}W''(0))^{\frac{1}{2}}h(2\mathbb{N}+1)) = d(\mu, \operatorname{Spec}((hD_x)^2 + \tfrac{1}{2}W''(0)x^2)) = \mathcal{O}(h^{\frac{3}{2}-3\delta}),$$

where the spectrum of the harmonic oscillator was computed in §3.2.

Hence any eigenvalue of $P_0(h)$ in $[0, \alpha h]$ has to satisfy (for h small enough), $\mu = (\frac{1}{2}W''(0))^{\frac{1}{2}}h + \mathcal{O}(h^{\frac{3}{2}-3\delta})$. If there were $J > 1$ of them, we could use the orthonormal eigenfunctions of $P_0(h)$ cut-off by $\chi_0(h^{\frac{1}{2}-\delta}x)$ in Lemma 6.5 with $\varepsilon = \mathcal{O}(h^{\frac{3}{2}-3\delta})$. That would contradict the simplicity of the spectrum of the harmonic oscillator. This completes the proof of (6.24). $\square$

[1] Particularly simple in one case as for $u \in C^2$ with $u(a) = 0$, $|u(x)|^2 \leq 2\int_a^x |u(y)u_x(y)|dy \leq 2\|u\|_{L^2([a,b])}\|u_x\|_{L^2([a,b])}$.

The key fact is a comparison between the exact eigenfunction and the WKB state constructed in Proposition 6.3:

Proposition 6.6. *Suppose that $\psi := c(h)h^{-\frac{1}{4}}\exp(-\varphi(x,h)/h)$ is constructed in Proposition 6.3 with $c(h)$ given in (6.22), and $u(x) \geq 0$ given in Proposition 6.4. Then for any $\chi \in C_c^\infty((a,b);[0,1])$,*

$$\chi(u-\psi) = \mathcal{O}(h^\infty)e^{-\varphi/h} \text{ in } C^\infty([a,b]). \tag{6.33}$$

Proof. We choose $\widetilde{\chi} \in C_c^\infty((a,b);[0,1])$ such that $\widetilde{\chi} \equiv 1$ on a neighbourhood $[a',b'] \supset \operatorname{supp}\chi$, $a < a' < 0 < b' < b$. We then put $w := \widetilde{\chi}(u-\psi)$. Then (6.28) in Lemma 6.5 applied with $J = 1$ and $u_1 = \widetilde{\chi}\psi$, and the equation (see the proof of (6.26)) show that

$$w = \mathcal{O}(h^\infty)_{C^\infty([a,b])}.$$

Since both u and ψ satisfy (6.26), we also have (with estimates on derivatives)

$$w = \mathcal{O}(h^{-N_0})e^{-\varphi(x)/h}, \quad x \in [a,b].$$

Now,

$$\begin{aligned}(P-\lambda)w &= \widetilde{\chi}(P(h)-\lambda(h))(u-\psi) + [P,\widetilde{\chi}](u-\psi) \\ &= \mathcal{O}(h^\infty)e^{-\varphi/h} + r(h), \quad r(h) = \mathcal{O}(h^{-N_0})e^{-\varphi/h}, \quad \operatorname{supp} r \subset \operatorname{supp}\widetilde{\chi}'.\end{aligned} \tag{6.34}$$

We want to use this in (6.7) with an appropriate weight. To do that we change between weight used in Step 1 of the proof of Proposition 6.4 (to obtain (6.26)),

$$\Phi_0(x) = \varphi(x) - C\log\max(C, \varphi(x)/h),$$

to a weight $\Phi_1 < (1-\varepsilon)\varphi$ on the support of $\widetilde{\chi}'$. In dimension one that is very simple (see [DS99, Appendix to §6] for the higher dimensional version): choose a_0 and b_0 so that

$$\max\operatorname{supp}\widetilde{\chi}' \cap (a,0) < a_0 < a', \quad b' < b_0 < \min\operatorname{supp}\widetilde{\chi}' \cap (0,b),$$

and then put

$$\Phi_1(x) := \mathbb{1}_{[a,a_0]}(x)\Phi_0(a_0) + \mathbb{1}_{[a_0,b_0]}(x)\Phi_0(x) + \mathbb{1}_{[b_0,b]}(x)\Phi_0(b_0).$$

We can use (6.11) as in the proof (6.26) with $\Phi = \Phi_1$: the contribution of $e^{\Phi_1/h}r(h)$ (see (6.34)) is now $\mathcal{O}(h^\infty)$. Applying (6.11) to w as in Step 1 of the proof of Proposition 6.4 gives (6.33). ☐

6.2.3. *A double well.* We now assume that V satisfies (6.1) and start with an application of Proposition 6.2 to this case:

Proposition 6.7. *Suppose that V satisfies (6.1), $P(h) = (hD_x)^2 + V(x)$, and for some $M > 0$,*

$$(P(h)-\mu(h))u(h) = 0, \quad \|u(h)\|_{L^2(\mathbb{R})} = 1, \quad \mu(h) \in [0, Mh]. \tag{6.35}$$

If

$$d(x) := \min_{\pm} \varphi_\pm(x), \quad \varphi_\pm'(x) = \sqrt{V(x)}, \quad \varphi_\pm \geq 0, \quad \varphi_\pm(\pm 1) = 0, \tag{6.36}$$

then, in the notation of (6.23),

$$u(x) = \widetilde{\mathcal{O}}(e^{-d(x)/h}). \tag{6.37}$$

Remark 6. *If we define a degenerate metric on $\mathbb{R}$ by $g = V(x)dx^2$ then $d(x)$ is the distance of x to the set $\{-1, 1\}$, with respect to this metric. In any dimension and energy level we can define $g = (V(x)-E)_+dx^2$ where $f_+(x) := f(x)\mathbb{1}_{f(x)\geq 0}(x)$ and dx^2 is the Euclidean metric. This is the celebrated Agmon metric which is the analogue of the classical Jacobi metric $(E - V(x))_+dx^2$ for the classically forbidden region – see* [DS99, §6.b] *and* [He88, §3.2].

Proof of Proposition 6.7. We will apply Proposition (6.2) with $W = V - \mu(h)$, and

$$\Phi_R(x) := (1-\delta)d(x)\mathbb{1}_{\delta\leq d(x)\leq(1-\delta)d(R)}(x)+\delta(1-\delta)\mathbb{1}_{d(x)\leq\delta}(x)+(1-\delta)d(R)\mathbb{1}_{d(x)\geq(1-\delta)d(R)}(x).$$

We can then take $0 < \delta \ll 1$ and choose $F_\pm$ in (6.11) so that (we note that near ± 1, $d(x) \sim (x \pm 1)^2 \sim V(x)$)

$$F_+(x)|_{\delta\leq d(x)\leq(1-\delta)d(R)} = \sqrt{\delta V(x) - \mu(h)} \geq \tfrac{1}{2}\delta,$$
$$F_+(x)|_{d(x)\geq(1-\delta)d(R)} = \sqrt{V(x) - \mu(h)}, \quad F_+(x)|_{d(x)\leq\delta} = ((V - \mu(h))_+ + h)^{\frac{1}{2}},$$
$$F_-(x)|_{d(x)\geq\delta} \equiv 0, \quad F_-(x) = ((V - \mu(h))_- + h)^{\frac{1}{2}} = \mathcal{O}(h^{\frac{1}{2}}).$$

We then obtain (6.37) as in the proof of Proposition 6.4 and by taking $R \to \infty$. □

We can finally give

Proof of Theorem 7. We proceed in a number steps.

Step 1. We start by proving (6.3) using (6.24) and (6.37). For that we introduce

$$P_\pm(h) = (hD_x)^2 + V(x) \ \text{ with 0 boundary conditions on } \pm[-1+\eta, R_0]. \tag{6.38}$$

The parameters $0 < \eta \ll 1$ and $R_0 \gg 1$ will be chosen later. We introduce eigenfunctions of $P_\pm(h)$:

$$\begin{gathered}(P_+(h) - \lambda(h))u_+(h) = 0, \quad u_+(-1+\eta) = u_+(R_0) = 0, \\ \|u_+(h)\|_{L^2([-1+\eta,R_0])} = 1, \quad u_-(x,h) := u_+(-x,h),\end{gathered} \tag{6.39}$$

and recall from (6.25) that $u_\pm = \widetilde{\mathcal{O}}(e^{-\varphi_\pm/h})$, where $\varphi_\pm$ were introduced in (6.36).

We then take $\chi_+ \in C^\infty(\mathbb{R}, [0, 1])$ with $\operatorname{supp}\chi_+ \subset (-1 + 2\eta, R_0 - \eta)$, $\chi_+ = 1$ on $(-1 + 3\eta, R_0 - 2\eta)$, and put $\chi_-(x) = \chi_+(-x)$. We also put

$$S_0 := \int_{-1}^{1} \sqrt{V(x)}dx = \varphi_+(-1),$$

and choose R_0 large enough so that $\varphi_+(R_0) > 2S_0$. To streamline the notation we will modify (6.23) to

$$u(x) = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h}) \iff \forall\, \varepsilon,\, k,\, \eta\, \exists\, C \quad |\partial_x^k u(x)| \le C e^{-(S_0+\varepsilon+\gamma(\eta))/h}, \tag{6.40}$$

where $\lim_{\eta\to 0}\gamma(\eta) \to 0$. In this notation we have

$$\psi_\pm := \chi_\pm u_\pm, \quad (P(h) - \lambda(h))\psi_\pm = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h}), \tag{6.41}$$

and

$$\begin{gathered} \langle \psi_\pm, \psi_\pm\rangle = \langle u_\pm, u_\pm\rangle + \int (1-\chi_\pm^2)\widetilde{\mathcal{O}}(e^{-2\varphi_\pm(x)/h})dx = 1 + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}), \\ \langle \psi_+, \psi_-\rangle = \int_{-1-2\eta}^{1+2\eta} \widetilde{\mathcal{O}}(e^{-(\varphi_+(x)+\varphi_-(x))/h})dx = \widetilde{\mathcal{O}}(e^{-S_0/h}), \end{gathered} \tag{6.42}$$

since for $|x| \le 1$, $\varphi_+(x) + \varphi_-(x) = S_0$. Lemma 6.5 applied with $A = P(h)$ then shows that $P(h)$ has at least two eigenvalues in $[0, \alpha h]$.

We now reverse this argument and construct approximate eigenfunctions for $P_\pm$. Hence suppose that there exist $w_j(h) \in D(P(h))$, $j = 1, 2, 3$, such that

$$(P(h) - \lambda_j(h))w_j(h) = 0, \quad 0 \le \lambda_j(h) \le \alpha h, \quad \langle w_i(h), w_j(h)\rangle = \delta_{ij}.$$

Since $P(h)$ commutes with $Uf(x) := f(-x)$, we can assume that w_j's are either odd or even. Two of them have to be of the same parity, say w_1 and w_2.

We now introduce $\widetilde{\chi}_\pm \in C^\infty(\mathbb{R}, [0,1])$ with $\operatorname{supp}\widetilde{\chi}_+ \subset (2\eta, R_0 - \eta)$, $\widetilde{\chi}_+ = 1$ on $(3\eta, R_0 - 2\eta)$, and put $\widetilde{\chi}_-(x) = \widetilde{\chi}_+(-x)$. Then

$$\begin{gathered} (P(h) - \lambda_j(h))(\widetilde{\chi}_+ w_j) = \widetilde{\mathcal{O}}_\eta(e^{-S_0/2h}), \quad j = 1, 2, \\ 2\langle \widetilde{\chi}_+ w_i, \widetilde{\chi}_+ w_j\rangle = \sum_\pm \langle \widetilde{\chi}_\pm w_i, \widetilde{\chi}_\pm w_j\rangle = \delta_{ij} + \widetilde{\mathcal{O}}_\eta(e^{-S_0/2h}), \end{gathered} \tag{6.43}$$

where we used the fact that w_j, $j = 1, 2$, have the same parity. Since $\widetilde{\chi}_+ w_j$ are approximate eigenfunctions of the Dirichlet problem on $[-1+\eta, R_0]$ we see that we can replace $\lambda_j(h)$ by $\lambda(h)$ in (6.43). We can now apply Lemma 6.5 with $A = P_+(h)$, $\lambda = \lambda(h)$ and $u_j = w_j/\|w_j\|$ to conclude that $P_+(h)$ has *two* eigenvalues in $[0, \alpha h]$ which contradicts (6.24). Hence, (6.3) holds.

Step 2. Let $\Pi := \mathbb{1}_{[0,\alpha h]}(P(h))$ and, in the notation of (6.41), define

$$w_\pm = \Pi\psi_\pm, \quad \|w_\pm - \psi_\pm\| = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h}), \tag{6.44}$$

where the norm estimate follows from (6.28). As in (6.30) we see from this and (6.42) that

$$\langle w_\pm, w_\pm\rangle = 1 + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}), \quad \langle w_+, w_-\rangle = \langle \psi_+, \psi_-\rangle + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}). \tag{6.45}$$

We can assume that $\psi_\pm$ are real and put $t := \langle \psi_+, \psi_- \rangle = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h})$. The Gramian of $w_\pm$ is given by

$$
\begin{gathered}
G := \begin{pmatrix} \langle w_+, w_+ \rangle & \langle w_+, w_- \rangle \\ \langle w_-, w_+ \rangle & \langle w_-, w_- \rangle \end{pmatrix} = \begin{pmatrix} 1 & t \\ t & 1 \end{pmatrix} + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}), \\
G^{-\frac{1}{2}} = \begin{pmatrix} 1 & -\frac{1}{2}t \\ -\frac{1}{2}t & 1 \end{pmatrix} + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}),
\end{gathered}
\tag{6.46}
$$

and hence

$$
[\widetilde{w}_+, \widetilde{w}_-] := [w_+, w_-] G^{-1/2} \tag{6.47}
$$

is an orthonormal basis of ΠL^2 and

$$
\widetilde{w}_+ = w_+ - \tfrac{1}{2} t w_- + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}), \quad \widetilde{w}_- = w_- - \tfrac{1}{2} t w_+ + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}). \tag{6.48}
$$

Step 3. We now calculate the matrix of $\Pi P \Pi$ in the basis (6.47). We first note that

$$
\begin{aligned}
P(w_\pm - \psi_\pm) &= P(\Pi - I)\psi_\pm = (\Pi - I) P \psi_\pm \\
&= \lambda(\Pi - I)\psi_\pm + (\Pi - I) r_\pm, \quad r_\pm := [P, \chi_\pm] u_\pm,
\end{aligned}
\tag{6.49}
$$

where $u_\pm$ were defined in (6.39). Hence, (6.25) and (6.44) give

$$
P(w_\pm - \psi_\pm) = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h})_{L^2}.
$$

Consequently,

$$
\langle P w_\pm, w_\pm \rangle = \langle P\psi_\pm, \psi_\pm \rangle - \langle P(w_\pm - \psi_\pm), w_\pm - \psi_\pm \rangle = \langle P\psi_\pm, \psi_\pm \rangle + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h})_{L^2},
$$

and

$$
\langle P w_+, w_- \rangle = \langle P\psi_+, \psi_- \rangle + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h})_{L^2}.
$$

Using (6.42) and the definition of $r_\pm$ in (6.49) we see that, modulo $\widetilde{\mathcal{O}}_\eta(e^{-2S_0/h})$,

$$
\begin{pmatrix} \langle P\psi_+, \psi_+ \rangle & \langle P\psi_+, \psi_- \rangle \\ \langle P\psi_-, \psi_+ \rangle & \langle P\psi_-, \psi_- \rangle \end{pmatrix} \equiv \begin{pmatrix} \lambda + \langle r_+, \psi_+ \rangle & \lambda\langle \psi_+, \psi_- \rangle + \langle r_+, \psi_- \rangle \\ \lambda\langle \psi_-, \psi_+ \rangle + \langle r_-, \psi_+ \rangle & \lambda + \langle r_-, \psi_- \rangle \end{pmatrix}.
$$

Since

$$
[P, \chi_+] = -h^2 \chi_+' - 2h\chi_+' h\partial_x, \tag{6.50}
$$

and $\operatorname{supp} \chi_+' \subset [-1 + 2\eta, -1 + 3\eta] \cup [R_0 - 3\eta, R_0 - 2\eta]$, (6.25) shows that

$$
\langle r_\pm, \psi_\pm \rangle = \mathcal{O}_\eta(e^{-2S_0/h}).
$$

The transformation (6.48) eliminates $\langle \psi_+, \psi_- \rangle$ in the off-diagonal terms: in the notation of (6.46) and (6.48) we have, modulo $\widetilde{\mathcal{O}}_\eta(e^{-2S_0/h})$, we have the following matrix representation of $\Pi P \Pi$:

$$
\begin{aligned}
\Pi P \Pi &\equiv \begin{pmatrix} \langle P\tilde{w}_+, \tilde{w}_+ \rangle & \langle P\tilde{w}_+, \tilde{w}_- \rangle \\ \langle P\tilde{w}_-, \tilde{w}_+ \rangle & \langle P\tilde{w}_-, \tilde{w}_- \rangle \end{pmatrix} = G^{-\frac{1}{2}} \begin{pmatrix} \langle P\psi_+, \psi_+ \rangle & \langle P\psi_+, \psi_- \rangle \\ \langle P\psi_-, \psi_+ \rangle & \langle P\psi_-, \psi_- \rangle \end{pmatrix} G^{-\frac{1}{2}} \\
&\equiv \begin{pmatrix} \lambda & \beta \\ \beta & \lambda \end{pmatrix}, \quad \beta := \langle r_+, \psi_- \rangle.
\end{aligned}
\tag{6.51}
$$

Step 4. We now use Proposition 6.6 to calculate β in (6.51). Using (6.50) we obtain

$$\begin{aligned}\langle r_+, \psi_-\rangle &= -h^2 \int (\chi_+'' u_+ + 2\chi_+' u_+')\chi_- u_- dx = -h^2 \int (\chi_+' u_+' + (\chi_+' u_+)')\chi_- u_- dx \\ &= h^2 \int \chi_+' \chi_- (u_+ u_-' - u_+' u_-) dx + h^2 \int \chi_+' u_+ \chi_-' u_- dx.\end{aligned} \tag{6.52}$$

We note that the support properties of $\chi_\pm'$ show that the last term is $\widetilde{\mathcal{O}}_\eta(e^{-2S_0/h})$. We now notice that $\int \chi_+' \chi_- dx = 1$ and that the Wronskian $u_+ u_-' - u_+' u_-$ is constant on the support of $\chi_+' \chi_-$. Hence, in (6.51),

$$\beta = h^2 (u_+(0) u_-'(0) - u_+'(0) u_-(0)). \tag{6.53}$$

We now use Propositions 6.3 and 6.6 (and recall that $\varphi_-(x,h) = \varphi_+(-x,h)$ and that $\varphi_+(0) + \varphi_-(0) = S_0$) to see that

$$\begin{aligned}\beta &= 2c(h)^2 h^{\frac12} \varphi_+'(0,h) e^{-2\varphi_+(0,h)/h}(1 + \mathcal{O}(h^\infty)) \\ &= 2h^{\frac12} ((\tfrac12 V''(1))^{\frac12}/\pi)^{\frac12} \varphi_+'(0) e^{-2\varphi_{+,1}(0) - S_0/h}(1 + \mathcal{O}(h)).\end{aligned}$$

We also recall from (6.17) that,

$$\begin{aligned}-2\varphi_{+,1}(0) &= \int_0^1 \left((V(x)^{\frac12})'/V(x)^{\frac12} + (\tfrac12 V''(1))^{\frac12}/V(x)^{\frac12} \right) dx \\ &= \lim_{\varepsilon \to 0} \int_0^{1-\varepsilon} (\tfrac12 \log V(x))' + (\tfrac12 V''(1))^{\frac12}/V(x)^{\frac12} dx \\ &= \lim_{\varepsilon \to 0} \left(\int_0^{1-\varepsilon} \frac{\sqrt{\tfrac12 V''(1)}}{\sqrt{V(x)}} dx + \tfrac12 (\log V(1-\varepsilon)) \right) - \tfrac12 \log V(0).\end{aligned} \tag{6.54}$$

Since $\varphi_+'(0) = -\sqrt{V(0)}$ and

$$\tfrac12 (\log V(1-\varepsilon)) = \log \varepsilon + \frac12 \log (V''(1)/2) + \mathcal{O}(\varepsilon),$$

we obtain

$$\begin{aligned}\beta &= -2h^{\frac12} ((\tfrac12 V''(1))^{\frac12}/\pi)^{\frac12} e^{A - S_0/h}(1 + \mathcal{O}(h)), \\ A &:= \lim_{\varepsilon \to 0+} \left(\int_{-1+\varepsilon}^{1+\varepsilon} \tfrac12 \sqrt{\frac{\tfrac12 V''(1)}{V(x)}} dx + \log \varepsilon + \log \sqrt{V''(1)/2} \right).\end{aligned} \tag{6.55}$$

In view of (6.51), $\lambda_2(h) - \lambda_1(h) = -2\beta + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h})$, so by taking ε and η small we obtain (6.4). $\square$

Remark 7. *From (6.51) we conclude that the Dirichlet eigenvalue $\lambda_\eta(h)$, of $P(h)$ on $[-1+\eta, R_0]$, $R_0 \gg 1$, $0 < \eta \ll 1$, provides a good approximation for the eigenvalue of the double well problem:*

$$\lambda_1(h) = \lambda_\eta(h) + \beta + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}), \quad \lambda_1(h) - \lambda_2(h) = 2\beta + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}),$$

where $\beta < 0$ was given in (6.55) and we used the notation (6.40).

6.3. **The periodic case.** We now assume that $V \in C^\infty(\mathbb{R};\mathbb{R})$,

$$V(x+1) = V(x), \quad V(0) = V'(0) = 0, \quad V''(0) > 0, \quad V|_{\mathbb{R}\setminus\mathbb{Z}} > 0 \tag{6.56}$$

and consider

$$P(h) := -h^2\partial_x^2 + V(x) : H^2(\mathbb{R}) \to L^2(\mathbb{R}). \tag{6.57}$$

We can apply the Bloch–Floquet theory of §5.3 to $P(h)$.

Our goal is to describe the first band of the spectrum of $P(h)$, $E_0(\theta, h)$, as $h \to 0$. We denote by $P_\theta(h)$ the operator $P(h)$ acting on $\mathcal{H}_\theta$ given in (5.7) (with $\Gamma = \mathbb{Z}$ and $n = 1$, and the domain given by $H^2_{\rm loc}(\mathbb{R}) \cap \mathcal{H}_\theta$). Then $E_0(\theta, h)$ is the first eigenvalue of $P_\theta(h)$.

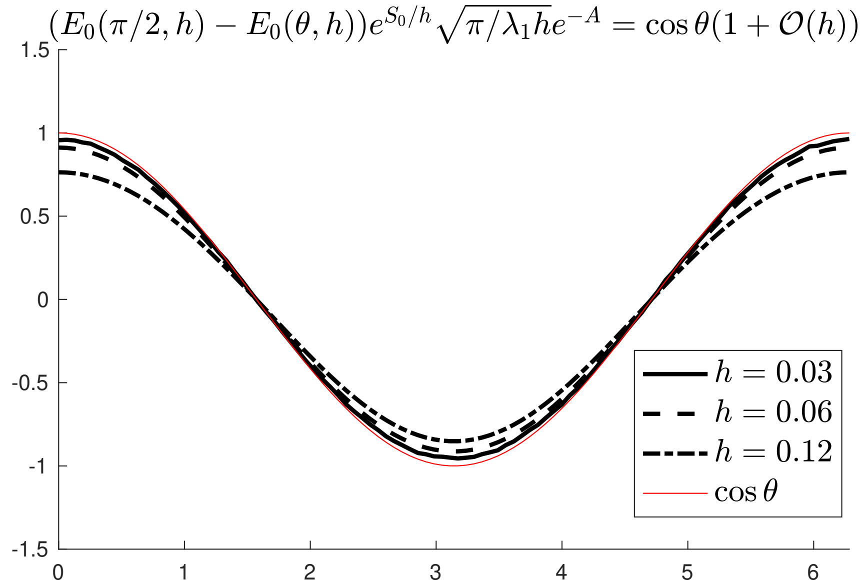
Theorem 8. *Under the assumptions (6.56) and in the notation above we have, for any $\varepsilon > 0$,*

$$\begin{gathered} E_0(\theta, h) = \lambda(h) - \beta(h)\cos\theta + \mathcal{O}_\varepsilon(e^{-(2S_0-\varepsilon)/h}), \\ \beta(h) = 4\sqrt{h\lambda_1/\pi}\, e^A e^{-S_0/h}(1 + \mathcal{O}(h)), \\ \lambda(h) \sim \lambda_1 h + \lambda_2 h^2 + \cdots, \quad \lambda_1 = \sqrt{\tfrac12 V''(0)}, \end{gathered} \tag{6.58}$$

where

$$S_0 = \int_0^1 V(x)^{\frac12} dx, \quad A = \lim_{\varepsilon\to 0} \tfrac12 \left(\int_\varepsilon^{1-\varepsilon} \lambda_1 V(x)^{-\frac12} dx + \log V(\varepsilon) \right). \tag{6.59}$$

We illustrate the theorem by computing the eigenvalues for to $V(x) = \sin^2 \pi x$ using $2^{10}+1$ Fourier modes ($S_0 = 2/\pi$, $\lambda_1 = \pi$ and $A = \log 2$ in this case):



For $0 < \eta \ll 1$ we define $P_0(h)$ as the Dirichlet realisation of $P(h) = (hD_x)^2 + V$ on $[-1+\eta, 1-\eta]$. This is an operator of the form described in §6.2.2.

Let $\lambda_\eta(h)$ be the first eigenvalue of the operator $P_0(h)$:

$$\begin{gathered}(P(h) - \lambda_\eta(h))u(h) = 0 \ \text{ on } I_\eta := [-1+\eta, 1-\eta], \\ \|u(h)\|_{L^2(I_\eta)} = 1, \quad u(h)|_{\partial I_\eta} = 0.\end{gathered} \tag{6.60}$$

Remark 8. *Just as in the case of the double well and in the notation of* (6.40) *we have that in* (6.58),

$$\lambda(h) = \lambda_\eta(h) + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}).$$

If $\chi \in C_c^\infty((-1+2\eta, 1-2\eta); [0,1])$ is equal to 1 in $(-1+3\eta, 1-3\eta)$ we put (dropping the dependence on h in the notation):

$$\psi := \chi u \implies P(h)\psi = \lambda(h)\psi + r, \quad r := [P(h), \chi]u. \tag{6.61}$$

We use ψ to construct a quasimode of $P_\theta(h)$:

$$\psi_\theta(x) := \sum_{k\in\mathbb{Z}} e^{-i\theta k}\psi(x-k). \tag{6.62}$$

Since

$$\begin{aligned}\psi_\theta(x-\ell) &= \sum_{k\in\mathbb{Z}} e^{-i\theta k}\psi(x-\ell-k) = e^{i\ell\theta}\sum_{k\in\mathbb{Z}} e^{-i\theta(k+\ell)}\psi(x-(k+\ell)) \\ &= e^{i\ell\theta}\psi_\theta(x),\end{aligned}$$

we see that $\psi_\theta \in \mathcal{H}_\theta \cap C^\infty(\mathbb{R})$. Also, in the notation of (6.61),

$$P_\theta(h)\psi_\theta = \lambda(h)\psi_\theta + r_\theta, \quad r_\theta := \sum_{k\in\mathbb{Z}} e^{-i\theta k} r(\bullet - k). \tag{6.63}$$

From (6.26) we see that (in the notation (6.40)) we have a pointwise estimate

$$\partial_x^k r_\theta(x) = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h}), \qquad S_0 := \int_0^1 \sqrt{V(x)}dx. \tag{6.64}$$

Proposition 6.8. *Let $P_\theta(h)$ be the Floquet operator defined after (6.57). Then for any $\alpha < 3(\frac{1}{2}V''(0))^{\frac{1}{2}}$ and h small enough,*

$$\operatorname{Spec}(P_\theta(h)) \cap [0, \alpha h] = \{\lambda_\theta(h)\}, \quad \lambda_\theta(h) = \lambda(h) + \widetilde{\mathcal{O}}_\eta(e^{-S_0/h}), \tag{6.65}$$

where $\lambda(h)$ was defined in (6.60) and we used the notation (6.40).

Proof. In view of (6.63) and (6.64) we already know that

$$d(\operatorname{Spec}(P_\theta(h)), \lambda(h)) = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h}),$$

and it remains to show that $\lambda(h) + \widetilde{\mathcal{O}}_\eta(e^{-S_0/h})$ is the only eigenvalue of $P_\theta(h)$ in $[0, \alpha h]$.

For that we recall Theorem 5 and consider

$$((hD_x - \theta)^2 + V(x))u_\theta(h) = E_\theta(h)u_\theta(h), \quad u_\theta(x+1) = u_\theta(x), \quad 0 \leq E_\theta(h) \leq \alpha h.$$

As explained in §5.4, $e^{ix\theta}u_\theta(h,x)$ is then an eigenfunction of $P_\theta(h)$ with eigenvalue $E(h)$. In particular estimates on $u_\theta(h)$ will translate to estimates on eigenfunctions of $P_\theta(h)$. An adaptation of the proof of Proposition 6.1 gives for any Lipschitz function on $\mathbb{R}/\mathbb{Z}$, Φ,

$$\begin{aligned}&\operatorname{Re}\langle e^{\Phi/h}(((hD_x - \theta)^2 + V(x) - E_\theta(h))u_\theta, e^{\Phi/h}u_\theta\rangle_{L^2(\mathbb{R}/\mathbb{Z})} = \\ &\quad \|(hD_x - \theta)(e^{\Phi/h}u_\theta)\|_{L^2(\mathbb{R}/\mathbb{Z})} + \langle (V - E_\theta(h) - |\nabla\Phi|^2)e^{\Phi/h}u_\theta, e^{\Phi/h}u_\theta\rangle_{L^2(\mathbb{R}/\mathbb{Z})}.\end{aligned}$$

Arguing as in Step 1 of the proof of Proposition 6.4 we see that (6.26) holds for $u_\theta(x)$ for $x \in K \Subset (-1,1)$. Consequently it remains true for the eigenfunctions of $P_\theta(h)$. Suppose $E_\theta^j(h)$, $1 \leq j \leq J$, are the eigenvalues of $P(\theta)$ in $[0, \alpha h]$ and $u^j(h)$ the corresponding eigenfunctions lying in $\mathcal{H}_\theta \cap C^\infty(\mathbb{R})$. The estimate (6.26) shows $\chi u^j(h)/\|\chi u^j\|_{L^2(I_\eta)}$ (with the same χ as in (6.61)) satisfy the assumptions of Lemma 6.5 with $A = P_0(h)$ and $\varepsilon = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h})$. But then the fact that $P_0(h)$ has only one eigenvalue in $[0, \alpha h]$ (see Proposition 6.4) shows that $J = 1$. □

Let $\Pi_\theta : \mathcal{H}_\theta \to \mathcal{H}_\theta$ be the orthogonal projection onto the eigenspace of $\lambda_\theta(h)$. Using (6.62) we define the following element of the eigenspace:

$$w_\theta = \Pi_\theta \psi_\theta, \quad \|w_\theta - \psi_\theta\| = \widetilde{\mathcal{O}}_\eta(e^{-S_0/h}),$$

where the bound follows from Lemma 6.5 using the argument described in the proof of Proposition 6.8, see (6.44). Then, as in (6.45)

$$\|w_\theta\|^2_{\mathcal{H}_\theta} = 1 + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}),$$

and

$$\langle P_\theta(h) w_\theta, w_\theta \rangle = \lambda(h) + \langle r_\theta, w_\theta \rangle = \lambda(h) + \langle r_\theta, \psi_\theta \rangle + \widetilde{\mathcal{O}}_\eta(e^{-2S_0/h}).$$

We now go back to (6.63) and compute (we can assume that ψ is real valued):

$$\langle r_\theta, \psi_\theta \rangle_{\mathcal{H}_\theta} = \sum_{k,\ell} e^{i\theta(k-\ell)} \int_0^1 r(x-\ell)\psi(x-k)dx.$$

Now,

$$\operatorname{supp} r(\bullet - \ell) \cap \operatorname{supp} \psi(\bullet - k) \cap [0,1] \neq \emptyset \implies \begin{cases} k=0, \ \ell=0, \\ k=0, \ \ell=1, \\ k=1, \ \ell=0. \end{cases}$$

Decay of ψ shows that $k=\ell=0$ contribute $\widetilde{\mathcal{O}}_\eta(e^{-2S_0/h})$ and hence, proceeding as in (6.52) and modulo that error term,

$$\begin{aligned}
\langle r_\theta, \psi_\theta \rangle_{\mathcal{H}_\theta} &\equiv 2\cos\theta \int_0^1 r(x)\psi(x-1)dx \\
&= -2h^2 \cos\theta \int_0^1 \int_0^1 (\chi'' u(x) + 2\chi' u'(x))\chi(x-1)u(x-1)dx \\
&= 2h^2 \cos\theta \int_0^1 \chi'(x)\chi(x-1)(u(x)u'(x-1) - u(x)' u(x-1))dx \\
&\quad + 2h^2 \cos\theta \int \chi'(x)u(x)\chi'(x-1)u(x-1)dx \\
&\equiv 2h^2 \cos\theta (u(\tfrac12)u'(-\tfrac12) - u(-\tfrac12)u'(\tfrac12)).
\end{aligned}$$

We now calculate the Wronskian using Propositions 6.3 and 6.6: for $|x| \leq 1-\eta$,

$$\begin{aligned}
u(x) &= c(h)h^{-\frac14} e^{-\varphi(x)/h} e^{-\varphi_1(x)}(1+\mathcal{O}(h)), \\
u'(x) &= -c(h)h^{-\frac54}(\varphi'(x) + \mathcal{O}(h))e^{-\varphi(x)/h}e^{-\varphi_1(x)}.
\end{aligned} \tag{6.66}$$

We have

$$\varphi(\tfrac12) = \int_0^{\frac12} \sqrt{V(x)}dx, \quad \varphi(-\tfrac12) = \int_{-\frac12}^0 \sqrt{V(x)}dx = \int_{\frac12}^1 \sqrt{V(x)}dx,$$

so that $\varphi(\frac{1}{2}) + \varphi(-\frac{1}{2}) = S_0$, where S_0 is given in (6.64). Finally,

$$
\begin{aligned}
\varphi_1(\tfrac{1}{2}) &= \tfrac{1}{2}\int_0^{\frac{1}{2}} \left((V(x)^{\frac{1}{2}})'/V(x)^{\frac{1}{2}} - (\tfrac{1}{2}V''(0))^{\frac{1}{2}}/V(x)^{\frac{1}{2}} \right) dx \\
&= \lim_{\varepsilon\to 0} \tfrac{1}{2}\int_\varepsilon^{\frac{1}{2}} (\tfrac{1}{2}\log V(x))' - (\tfrac{1}{2}V''(0))^{\frac{1}{2}}/V(x)^{\frac{1}{2}} dx \\
&= -\lim_{\varepsilon\to 0} \tfrac{1}{2}\left(\int_\varepsilon^{\frac{1}{2}} \frac{\sqrt{\frac{1}{2}V''(0)}}{\sqrt{V(x)}} dx + \tfrac{1}{2}(\log V(\varepsilon)) \right) + \tfrac{1}{4}\log V(\tfrac{1}{2}).
\end{aligned}
$$

From a similar formula for $\varphi_1(-\frac{1}{2})$ we obtain

$$
-\varphi_1(\tfrac{1}{2}) - \varphi_1(-\tfrac{1}{2}) = \lim_{\varepsilon\to 0} \tfrac{1}{2}\left(\int_\varepsilon^{1-\varepsilon} \frac{\sqrt{\frac{1}{2}V''(0)}}{\sqrt{V(x)}} dx + \log V(\varepsilon) \right) - \tfrac{1}{2}\log V(\tfrac{1}{2}).
$$

Hence

$$
u(\tfrac{1}{2})u'(-\tfrac{1}{2}) - u(-\tfrac{1}{2})u'(\tfrac{1}{2}) = 2h^{-\frac{3}{2}}((\tfrac{1}{2}V''(0))^{\frac{1}{2}}/\pi)^{\frac{1}{2}} e^{A} e^{-S_0/h}(1 + \mathcal{O}(h)),
$$

where A and S_0 are given by (6.59).

6.4. **Higher dimensional examples.**

7. Topology for band structures

7.1. **Line bundles through an example: the Bloch sphere.** In this section we introduce the concept of a line bundle over a surface, working with the specific example over 2-dimensional sphere $\mathbb{S}^2 = \{x \in \mathbb{R}^3 : |x| = 1\}$.

7.1.1. *Definition of a line bundle.* First we recall the definition in Section 2.7 specialized to line bundles.

Definition 7.1. *Let L, X be two topological spaces, and $\pi : L \to X$ be a continuous map. Then $\pi : L \to X$ is called a (continuous) complex line bundle if*

- *For any $x \in X$, $\pi^{-1}(x)$ is a 1-dimensional vector space over $\mathbb{C}$;*
- *There is an open covering $\{U_j\}$ of X such that there is a continuous map $h_j : \pi^{-1}(U_j) \to U_j \times \mathbb{C}$ which is a linear isomorphism on each fiber.*

$$
\begin{tikzcd}
\pi^{-1}(U_j) \arrow[r, "h_j"] \arrow[d, "\pi"'] & U_j \times \mathbb{C} \arrow[dl, "\mathrm{pr}_1"] \\
U_j &
\end{tikzcd}
$$

If L, X are smooth manifolds, π and h_j are all smooth maps, then $\pi : L \to X$ is called a smooth complex line bundle.

If L, X are complex manifolds, π and h_j are holomorphic maps, then $\pi : L \to X$ is called a holomorphic line bundle.

If $U_i \cap U_j \neq \varnothing$, then $h_i \circ h_j^{-1} : U_i \cap U_j \times \mathbb{C} \to U_i \cap U_j \times \mathbb{C}$ is given by $(x, \lambda) \mapsto (x, g_{ij}(x)\lambda)$. The maps $g_{ij} : U_i \cap U_j \to \mathbb{C}^*$ are called transition functions. Transitions function satisfy the following compatibility properties.

- $g_{ii}(x) = 1$;
- $g_{ij}(x)g_{ji}(x) = 1$;
- $g_{ij}(x)g_{jk}(x)g_{ki}(x) = 1$.

Conversely, if we are given a family of transition functions satisfying those compatibility properties, then we can recover the line bundle. The line bundle being smooth/holomorphic is equivalent to the transition functions being smooth/holomorphic.

We also define sections of a line bundle, as a generalization of functions.

Definition 7.2. *Let $\pi : L \to X$ be a line bundle, a section is a map $s : X \to L$ such that $\pi \circ s = \mathrm{id}_X$. It is called a continuous (smooth, holomorphic) section if $s : X \to L$ is continuous (smooth, holomorphic). The family of continuous (smooth, holomorphic) sections is denoted $C(X; L)$ ($C^\infty(X; L)$, $\mathcal{O}(X; L)$).*

Using local charts $X = \bigcup U_j$, a section can also be described by functions $s_j : U_j \to \mathbb{C}$ such that $g_{ij}s_j = s_i$.

7.1.2. *The Bloch sphere.* A concrete example of a line bundle, will be a bundle over $\mathbb{S}^2$ given by an eigenspace of a self-adjoint family of operators parametrized by $\mathbb{S}^2$. As we will see it is equivalent to the tautological line bundle over the projective space and, after taking unit vectors, to the Hopf fibration of $\mathbb{S}^3$.

The operator is defined using the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

From them we build a family of operators parameterized by $x \in \mathbb{S}^2$:

$$H(x) = \sum_j x_j \sigma_j = \begin{pmatrix} x_3 & x_1 - ix_2 \\ x_1 + ix_2 & -x_3 \end{pmatrix}. \tag{7.1}$$

It is clear that $H(x) = H(x)^* : \mathbb{C}^2 \to \mathbb{C}^2$ (as Hilbert space equipped with the standard inner product) and it is easy to check that $\mathrm{Spec}(H(x)) = \{\pm 1\}$.

On $\mathbb{S}^2$ we use two coordinate charts given by stereographic projections: let NP be the "north pole" given by $x_3 = 1$ and SP the "south pole" , $x_3 = -1$. We then have

$$U_0 := \mathbb{S}^2 \setminus \mathrm{NP} \ni x \mapsto z(x) = \frac{x_1 + ix_2}{1 - x_3} \in \mathbb{C}$$

and

$$U_1 := \mathbb{S}^2 \setminus \mathrm{SP} \ni y \mapsto w(y) = w = \frac{y_1 - iy_2}{1 + y_3} \in \mathbb{C}.$$

The transition map between them is $w = z^{-1}$.

We are interested in the line bundle given by $V_x = \ker(H(x) - 1) \subset \mathbb{C}^2$, considered as a subbundle of the rank 2 trivial bundle $\mathbb{S}^2 \times \mathbb{C}^2$. We have

$$V_x = \mathbb{C}\begin{pmatrix} z \\ 1 \end{pmatrix}, \quad x \neq \mathrm{NP}, \quad V_{\mathrm{NP}} = \mathbb{C}\begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

The sphere $\mathbb{S}^2$ can be identified with $\mathbb{CP}^1$ defined as the set of complex lines inside $\mathbb{C}^2$. In projective coordinates,

$$\mathbb{CP}^1 = \{[z_0 : z_1] : z_0 \neq 0 \text{ or } z_1 \neq 0, z_j \in \mathbb{C}\}.$$

Here the projective coordinate $[z_0 : z_1]$ means $[z_0 : z_1] = [z_0' : z_1']$ if and only if there exists $\lambda \in \mathbb{C}^*$ such that $(z_0, z_1) = \lambda(z_0', z_1')$. In local coordinates, we can use

$$[z_0 : z_1] \mapsto \begin{cases} z = z_1/z_0, & z_0 \neq 0; \\ z = z_0/z_1, & z_1 \neq 0. \end{cases}$$

The line bundle V is called the *tautological line bundle* because its fiber is nothing but the line that $[z_0 : z_1]$ represents in $\mathbb{CP}^1$. The trivialization map is given by projection to the second/first coordinate:

$$h_0([z_0 : z_1]) : \lambda\begin{pmatrix} z_1 \\ z_0 \end{pmatrix} \mapsto \lambda z_0, \quad z_0 \neq 0;$$

$$h_1([z_0 : z_1]) : \lambda\begin{pmatrix} z_1 \\ z_0 \end{pmatrix} \mapsto \lambda z_1, \quad z_1 \neq 0;$$

Thus $g_1 \circ g_0^{-1} : \lambda z_0 \mapsto \lambda z_1$ and the transition function $g_{10}([z_0 : z_1]) = z_1/z_0 = z$ on $U_0 \cap U_1$. This indeed gives V a holomorphic line bundle structure.

Sections of V is then given by $s_0, s_1 : \mathbb{C} \to \mathbb{C}$ such that $s_1(1/z) = g_{10}(z)s_0(z) = zs_0(z)$ for $z \in \mathbb{C}^*$.

Example 15. While V has a lot of smooth sections, the only holomorphic section of it is 0. This is because if we expand

$$s_0(z) = \sum_{k=0}^{\infty} a_k z^k, \quad s_1(w) = \sum_{l=0}^{\infty} b_l w^l,$$

FIGURE 10. Part of the foliation (7.2) with $\mathbb{R}^3 \simeq \mathbb{S}^3 \setminus \mathrm{NP}$ folliated by circles made out of *linked* key rings. See also an animated version.

then $s_1(1/z) = zs_0(z)$ implies that

$$a_0 z + a_1 z^2 + \cdots = b_0 + b_1 z^{-1} + \cdots$$

that is $a_k = b_l = 0$ for any k, l. There are other holomorphic line bundles with transition function $g_{10}(z) = z^{-k}$, that is $s_1(1/z) = z^{-k} s_0(z)$ (they are called $\mathcal{O}(k)$-bundles). Only when $k \geq 0$, there exists nonzero holomorphic sections.

Remark 9. *The bundle V is intimately related to the Hopf fibration of $\mathbb{S}^3$. For that we consider $\mathbb{S}^3 = \{(z_0, z_1) \in \mathbb{C}^2 : |z_0|^2 + |z_1|^2 = 1\} \subset \mathbb{C}^2$, $\iota : V_x \hookrightarrow \mathbb{C}^2$ the inclusion and*

$$\mathbb{S}^1 \simeq V_x \cap \mathbb{S}^3 \xrightarrow{\iota} \mathbb{S}^3 \xrightarrow{f} \mathbb{C}P^1 \simeq \mathbb{S}^2, \quad f(z_0, z_1) = [z_0 : z_1], \quad f \circ \iota = \mathrm{id}. \tag{7.2}$$

The circles $V_x \cap \mathbb{S}^3$ foliate the sphere $\mathbb{S}^3$ in a nontrivial way illustrated in Figure 10.

7.1.3. *Connections and curvature.* Now we define connections, which are generalizations of the exterior derivative.

Definition 7.3. *Let $L \to X$ be a smooth line bundle, a connection D on L is a linear map*

$$D : C^\infty(X; L) \to C^\infty(X; L \otimes T^*X)$$

such that $D(fs) = fDs + s \otimes df$ for any $f \in C^\infty(X)$ and $s \in C^\infty(X; L)$.

In local coordinates, a section s is represented by a family of functions $s_j : U_j \to \mathbb{C}$ such that $s_i(x) = g_{ij}(x)s_j(x)$. Suppose the section Ds is represented by $D_j s_j$, then by Leibniz rule we may assume

$$D_j s_j(x) = ds_j(x) + \theta_j(x)s_j(x), \quad \theta_j \in C^\infty(U_j; T^*X).$$

The compatibility condition is

$$g_{ij}(ds_j + \theta_j s_j) = ds_i + \theta_i s_i = d(g_{ij}s_j) + \theta_i g_{ij} s_j = g_{ij}(ds_j + \theta_i s_j) + s_j dg_{ij},$$

that is $\theta_j = \theta_i + g_{ij}^{-1} dg_{ij}$. A family of $\{\theta_j\}$ satisfying the compatibility condition will give a connection on L.

Given a connection D, we can define its curvature:

Proposition 7.4. *In local coordinates, we define $\Theta|_{U_j} := d\theta_j$, then Θ gives a globally defined closed 2-form on X.*

Proof. It is clear that it is closed. We only need to check it is the compatible on $U_i \cap U_j$:

$$d\theta_j = d\theta_i + d(g_{ij}^{-1} dg_{ij}) = d\theta_i + d(d(\log g_{ij})) = d\theta_i.$$

□

Θ is called the curvature form of the connection. It will depend on the choice of connection, but its cohomology class does not.

Proposition 7.5. *Suppose D_1, D_2 are two connections on L, Θ_1, Θ_2 are two corresponding curvature forms. Then there exists $\eta \in C^\infty(X; T^*X)$ such that $\Theta_1 = \Theta_2 + d\eta$.*

Proof. On $U_i \cap U_j$, $\Theta_1 - \Theta_2 = d(\theta_1 - \theta_2)$. We claim $\theta_1 - \theta_2$ defines a global 1-form η on X. It suffices to check that on $U_i \cap U_j$ we have $\theta_{1i} - \theta_{2i} = \theta_{1j} - \theta_{2j}$. But this follows from $\theta_{1j} - \theta_{1i} = \theta_{2j} - \theta_{2i} = g_{ij}^{-1} dg_{ij}$ □

As a corollary, when X is a 2-dimensional compact smooth manifold with a smooth line bundle L, one can define a number

$$c_1(L) = \frac{i}{2\pi} \int_X \Theta. \tag{7.3}$$

This is called the Chern number of the line bundle and is independent of the choice of the connection, thus a topological invariant. We will prove it is an integer.

Example 16. Let us come back to our example of the Bloch sphere. Recall we have the tautological line bundle V given by $\ker(H(x)-1)$ on the sphere $\mathbb{S}^2$. Denote $i : V \to \mathbb{S}^2 \times \mathbb{C}^2$ the inclusion to trivial bundle. For a section $s \in C^\infty(\mathbb{S}^2; V)$, $i \circ s$ gives a smooth function $\mathbb{S}^2 \to \mathbb{C}^2$ such that $i \circ s(x) \in \ker(H(x)-1)$. We can define a connection on V via

$$Ds(x) = \Pi_x(d(i \circ s)) \tag{7.4}$$

where Π_x is the orthogonal projection from $\mathbb{C}^2$ to $V_x = \ker(H(x)-1)$ under the standard Hermitian inner product on $\mathbb{C}^2$. It is easy to check it is a connection:

$$D(fs)(x) = \Pi_x(d(fi \circ s)) = \Pi_x(i \circ s \otimes df + fd(i \circ s)) = s \otimes df + fDs.$$

We compute the curvature of this connection using a different basis (that is a different trivialization). Let

$$u_0(x) = \frac{1}{(1+|z|^2)^{1/2}} \begin{pmatrix} z \\ 1 \end{pmatrix}, \quad u_1(x) = \frac{1}{(1+|w|^2)^{1/2}} \begin{pmatrix} 1 \\ w \end{pmatrix},$$

then $H(x)u_j(x) = u_j(x)$ and $|u_j(x)| = 1$. We have

$$d(s_j u_j) = u_j ds_j + s_j du_j$$

and

$$\Pi(d(s_j u_j)) = \langle u_j ds_j + s_j du_j, u_j \rangle u_j = u_j ds_j + s_j \langle du_j, u_j \rangle u_j.$$

So $D_j s_j = ds_j + s_j \langle du_j, u_j \rangle$.

We should note that the definition (7.4) does not rely on the special structure of V but only on the fact that we have an inclusion of V in the trivial bundle $\mathbb{S}^2 \times \mathbb{C}^2$. If we have an inclusion in a more general trivial bundle $\mathbb{S}^2 \times H$ where H is a Hilbert space, we can still use the definition (7.4).

This is a special case of a Hermitian connection the definition of which we now recall:

Definition 7.6. *A Hermitian metric on a line bundle $\pi : L \to X$ is a smooth family of Hermitian metrics $|\cdot|_x$ on each fiber $\pi^{-1}(x)$.*

In local coordinates, this can be written as $|v|_x^2 = h_j(x)|v|^2$. The compatibility condition gives

$$h_j(x)|s_j(x)|^2 = h_i(x)|s_i(x)|^2 = h_i(x)|g_{ij}(x)|^2|s_j(x)|^2,$$

that is

$$h_j(x) = h_i(x)|g_{ij}(x)|^2, \quad x \in U_i \cap U_j.$$

There are always many Hermitian structures on a line bundle by a partition of unity argument.

Definition 7.7. *Let D be a connection on the line bundle $L \to X$. D is called a Hermitian connection if*

$$d(\langle s(x), s'(x)\rangle_x) = \langle Ds(x), s'(x)\rangle_x + \langle s(x), Ds'(x)\rangle_x, \quad \forall s, s' \in C^\infty(X; L).$$

Equivalently, $|s(x)|_x$ is preserved under the parallel transport induced by D (parallel transport is defined via the equation $Ds(t)(\dot\gamma(t)) = 0$).

Let us choose a local frame u_j such that $|u_j| = 1$, then

$$d\langle s_j, s_j'\rangle = \langle ds_j, s_j'\rangle + \langle s_j, ds_j'\rangle$$

and

$$\langle Ds_j, s_j'\rangle + \langle s_j, Ds_j'\rangle = \langle ds_j + \theta_j s_j, s_j'\rangle + \langle s_j, ds_j' + \theta_j s_j'\rangle.$$

Thus D being Hermitian means $\langle \theta_j s_j, s_j'\rangle + \langle s_j, \theta_j s_j'\rangle = 0$, that is

$$\theta_j = -\overline{\theta}_j.$$

(Remember that this is when sections over U_j are written as $s(x) = s_j(x)u_j(x)$, $|u_j(x)|_x = 1$.)

If L is a holomorphic hermitian line bundle, we say D is *compatible with the holomorphic structure* if $D^{0,1} = \overline{\partial}$. There is a unique Hermitian connection on L compatible with the holomorphic structure, called the Chern connection.

Given a connection D on L and a curve $\gamma(t)$ on X, one can define the parallel transport of s via the equation $Ds(t)(\dot\gamma(t)) = 0$. Suppose D is Hermitian and γ is closed, that is $\gamma(0) = \gamma(1) = x \in X$, then $|s(0)|_x = |s(1)|_x$, and there exists $\theta \in \mathbb{R}$ such that $s(1) = e^{i\theta}s(0)$. The factor $e^{i\theta}$ is called the holonomy of the connection D on the curve γ, denoted by $\mathrm{hol}_D(\gamma)$. If γ is a simple closed curve inside a single chart U_j, then the equation

$$\frac{d}{dt}s_j(\gamma(t)) + \theta_j(\gamma(t))s_j(\gamma(t)) = 0$$

can be solved explicitly for $t \mapsto s_j(\gamma(t))$ and that gives

$$\mathrm{hol}_D(\gamma) = \exp\left(-\int_\gamma \theta_j\right) = \exp\left(-\int_\Omega \Theta\right) \tag{7.5}$$

where Ω is a region enclosed by γ and γ is positively oriented. (On surfaces that means that as we move along γ the region Ω is on the left.) The last term on the right is independent of the choice of charts and one can verify this formula works even if γ is not contained in a single chart U_j by a subdivision argument.

Exercise 7.8. Let us consider the Hermitian connection defined in (7.4). On can compute on U_0

$$\theta = \langle du_0, u_0 \rangle = \frac{1}{2(1+|z|^2)}(\bar{z}dz - zd\bar{z})$$

and

$$\Theta = d\theta = \frac{d\bar{z} \wedge dz}{(1+|z|^2)^2}.$$

For example, on the circle given by $z(t) = \dfrac{\sin\varphi e^{it}}{1-\cos\varphi}$ $(0 < \varphi < \pi)$, we can compute

$$\begin{aligned}
\mathrm{hol}_D(\gamma) &= \exp\left(\int_{|z|>\sin\varphi/(1-\cos\varphi)} \frac{d\bar{z} \wedge dz}{(1+|z|^2)^2} \right) \\
&= \exp\left(2\pi i \int_{\sin^2\varphi/(1-\cos\varphi)^2}^{\infty} \frac{ds}{(1+s)^2} \right) = \exp(\pi i(1-\cos\varphi)).
\end{aligned}$$

Now we prove the Chern number is an integer.

Theorem 9. *$c_1(L)$ defined in (7.3) is an integer.*

Proof. Let $x \in X$. Choose small neighbourhoods Ω_x converging to x and $\gamma = \partial\Omega_x$, then

$$\mathrm{hol}_D(\gamma) = \exp\left(-\int_{\Omega_x} \Theta \right) = \exp\left(\int_{X \setminus \Omega_x} \Theta \right).$$

Thus $\exp\left(\int_X \Theta\right) = 1$ and $\int_X \Theta \in 2\pi i\mathbb{Z}$. $\square$

If we are on the sphere $\mathbb{S}^2$, there is another simple proof: notice for the equator γ,

$$\int_X \Theta = \int_\gamma \theta_0 - \theta_1 = \int_\gamma g_{10}^{-1} dg_{10} = \int_\gamma d\log g_{10} \in 2\pi i\mathbb{Z}.$$

For the tautological line bundle V with connection Θ defined in (7.4), we have

$$\int_{\mathbb{S}^2} \Theta = \int_{\mathbb{C}} \frac{1}{(1+|z|^2)^2} d\bar{z} \wedge dz = 2\pi i.$$

Thus $c_1(V) = -1$.

7.2. **Line bundles over tori.** Let $\Gamma \subset \mathbb{R}^n$ be a lattice and $X = \mathbb{R}^n/\Gamma$ be an n-dimensional torus. We are interested in line bundles over the torus.

First we recall the notion of pullback. Let $f : Y \to X$ be a continuous map, then one can define the pullback bundle f^*L to be

$$f^*L = Y \times_X L = \{(y, v) \in Y \times L : f(y) = \pi(v)\}.$$

Suppose $\{U_i\}$ is a covering of X such that $\pi^{-1}(U_i)$ is trivial, then $\{f^{-1}(U_i)\}$ is a covering of Y such that $f^*L|_{f^{-1}(U_i)}$ is trivial. So f^*L is a line bundle over Y. When f is smooth/holomorphic, one can check f^*L is smooth/holomorphic.

When we look at a line bundle $L \to X$ over the torus $X = \mathbb{R}^n/\Gamma$, there is a natural quotient map $p : \mathbb{R}^n \to \mathbb{R}^n/\Gamma$. By Corollary 2.18, $p^*L \to \mathbb{R}^n$ must be a trivial line bundle, so we identify p^*L with $\mathbb{R}^n \times \mathbb{C}$. Now Γ has a natural action on p^*L by

$$\gamma \cdot (y, v) = (y + \gamma, v),$$

lifting the action on the base, that is

$$\begin{array}{ccc} \Gamma \times p^*L & \longrightarrow & p^*L \\ \downarrow & & \downarrow \\ \Gamma \times \mathbb{R}^n & \longrightarrow & \mathbb{R}^n \end{array}$$

and L is exactly the quotient bundle under the Γ-action

$$L = \{(y, v) \in Y \times L : p(y) = \pi(v)\}/(y + \gamma, v) \sim (y, v)) = p^*L/\Gamma.$$

Since we identify p^*L with the trivial bundle $\mathbb{R}^n \times \mathbb{C}$, the action of Γ can be written as

$$\gamma \cdot (x, \lambda) = (x + \gamma, e_\gamma(x)\lambda). \tag{7.6}$$

Those $e_\gamma(x)$'s are called *multipliers*. Because $(\gamma_1 + \gamma_2) \cdot (x, \lambda) = \gamma_1 \cdot (\gamma_2 \cdot (x, \lambda))$, they must satisfy

$$e_{\gamma_1+\gamma_2}(x) = e_{\gamma_1}(x + \gamma_2)e_{\gamma_2}(x), \quad e_0(x) = 1. \tag{7.7}$$

We can then describe sections of L as follows.

$$C^\infty(X; L) = \{u \in C^\infty(\mathbb{R}^n) : u(x + \gamma) = e_\gamma(x)u(x), \ \forall \gamma \in \Gamma\}. \tag{7.8}$$

Since the choice of trivialization $p^*L \to \mathbb{R}^n \times \mathbb{C}$ is not unique, if we change $e_\gamma(x)$ to

$$\tilde{e}_\gamma(x) = e^{g(x+\gamma)}e_\gamma(x)e^{-g(x)},$$

we will get an isomorphic line bundle L. Indeed, the family of line bundles over X up to isomorphism is given by

$$\{e_\gamma(x) : e_{\gamma_1+\gamma_2}(x) = e_{\gamma_1}(x + \gamma_2)e_{\gamma_2}(x)\}/e_\gamma(x) \sim \tilde{e}_\gamma(x) = e^{g(x+\gamma)}e_\gamma(x)e^{-g(x)}.$$

Let $L \to X = \mathbb{R}^n/\Gamma$ be a smooth line bundle, and h be a Hermitian metric on L. h then induces a metric on $p^*L \cong \mathbb{R}^n \times \mathbb{C}$ such that

$$h(x) = h(x + \gamma)|e_\gamma(x)|^2. \tag{7.9}$$

Conversely, any smooth function $h(x) : \mathbb{R}^n \to \mathbb{R}_+$ satisfying the above condition defines a Hermitian metric on L.

Similarly, connection D on L induces a connection on the pullback bundle $p^*L \cong \mathbb{R}^n \times \mathbb{C}$ such that

$$(p^*D)p^*s = p^*(Ds).$$

Suppose $(p^*D)s = ds + \theta s$ for some $\theta \in C^\infty(\mathbb{R}^n; T^*\mathbb{R}^n)$. Then θ has to satisfy for $s \in C^\infty(X; L)$

$$\begin{aligned} d(e_\gamma(x)s(x)) + \theta(x+\gamma)e_\gamma(x)s(x) &= ds(x+\gamma) + \theta(x+\gamma)s(x+\gamma) \\ &= e_\gamma(x)(ds(x) + \theta(x)s(x)), \end{aligned}$$

that is,

$$\theta(x+\gamma) = \theta(x) - e_\gamma(x)^{-1}de_\gamma(x).$$

The curvature is given by $\Theta = d\theta$. When $n = 2$, let $\Omega = \{s\gamma_1 + t\gamma_2 : 0 \le s, t \le 1\}$ be the fundamental domain, one can check that the Chern number is an integer directly in this case. We use (7.7) to see that

$$\begin{aligned} \int_X \Theta = \int_{\partial\Omega} \theta &= \int_{[0,1]\gamma_1} (\theta(x) - \theta(x+\gamma_2)) - \int_{[0,1]\gamma_2} (\theta(x) - \theta(x+\gamma_1)) \\ &= \int_0^1 (e_{\gamma_2}(t\gamma_1)^{-1}de_{\gamma_2}(t\gamma_1) - (e_{\gamma_1}(t\gamma_2)^{-1}de_{\gamma_1}(t\gamma_2)) \\ &= \log e_{\gamma_2}(\gamma_1) - \log e_{\gamma_2}(0) - \log e_{\gamma_1}(\gamma_2) + \log e_{\gamma_1}(0) \\ &\equiv \log e_{\gamma_1+\gamma_2}(0) - \log e_{\gamma_1+\gamma_2}(0) = 0 \mod 2\pi i\mathbb{Z}. \end{aligned} \tag{7.10}$$

We can simplify the multipliers a bit when $n = 2$.

Proposition 7.9. *If $\Gamma = \mathbb{Z}\gamma_1 \oplus \mathbb{Z}\gamma_2$, we can always choose $e_{\gamma_1}(x) = 1$.*

Proof. Recall a (complex) line bundle over the circle S^1 is always trivial, thus by an easy adaptation Proposition 2.16, any (complex) line bundle over $S^1 \times \mathbb{R}$ is also trivial. Consider the projection $p : \mathbb{R}^2/\gamma_1\mathbb{Z} \to X = \mathbb{R}^2/\Gamma$. The pullback p^*L must be a trivial line bundle. As before, there is a natural action of $\gamma_2\mathbb{Z}$ on p^*L such that $L = p^*L/\gamma_2\mathbb{Z}$. Suppose in a trivialization $p^*L \cong \mathbb{R}^2/\gamma_1\mathbb{Z} \times \mathbb{C}$, the action is given by

$$n\gamma_2 \cdot (x, \lambda) = (x + n\gamma_2, e_{n\gamma_2}(x)\lambda).$$

Then we can describe L by multipliers $e_{n\gamma_2}(x)$ and $e_{\gamma_1}(x) = 1$. ☐

Remark 10. *In higher dimensions, it is not true that any line bundle over $(\mathbb{R}/\mathbb{Z})^k \times \mathbb{R}^l$ is trivial. However, one can still play a similar game by choosing the generators carefully. There is also an analogous version in holomorphic case. For more details, see Griffiths–Harris* [GH14, Section 2.6].

As an application, we prove that if $c_1(L) = 0$ then L is trivial (Note this is not true in the holomorphic setting).

Proposition 7.10. *Let $n = 2$, $\Gamma = \gamma_1\mathbb{Z} \oplus \gamma_2\mathbb{Z}$. If $c_1(L) = 0$, then L is trivial.*

Proof. By Proposition 7.9, we may assume $e_{\gamma_1}(x) = 1$. Then $c_1(L) = 0$ implies that

$$\int_0^1 e_{\gamma_2}(t\gamma_1)^{-1} de_{\gamma_2}(t\gamma_1) = 0. \tag{7.11}$$

Since $d(e_{\gamma_2}(x)^{-1}de_{\gamma_2}(x)) = 0$, we can find $f \in C^\infty(\mathbb{R}^2)$ such that $df = e_{\gamma_2}(x)^{-1}de_{\gamma_2}(x)$. Modifying f by a constant gives $e_{\gamma_2}(x) = \exp(f(x))$. Since

$$e_{\gamma_2}(x+\gamma_1) = e_{\gamma_2}(x+\gamma_1)e_{\gamma_1}(x) = e_{\gamma_1+\gamma_2}(x) = e_{\gamma_1}(x+\gamma_2)e_{\gamma_2}(x) = e_{\gamma_2}(x),$$

$e_{\gamma_2}(x)$ is periodic in γ_1 and $f(x+\gamma_1) = f(x) + 2\pi ik$ for some $k \in \mathbb{Z}$. But (7.11) implies $k = 0$ and $f(x)$ is γ_1 periodic. Now we claim we can find $g \in C^\infty(\mathbb{R}^2/\gamma_1\mathbb{Z})$ such that

$$g(x+\gamma_2) - g(x) = f(x)$$

Let $\chi(x) \in C^\infty(\mathbb{R}^2/\gamma_1\mathbb{Z})$ be a cutoff function such that $\operatorname{supp}\chi \subset \{x = a_1\gamma_1 + a_2\gamma_2 : a_2 > -1\}$ and $\chi(x) = 1$ on $\{x = a_1\gamma_1 + a_2\gamma_2 : a_2 > 0\}$. Let

$$g(x) = \sum_{n=1}^{\infty} \chi(x - n\gamma_2)f(x - n\gamma_2) - (1 - \chi(x + (n-1)\gamma_2))f(x + (n-1)\gamma_2),$$

then $g \in C^\infty(\mathbb{R}^2/\gamma_1\mathbb{Z})$ since this is a finite sum. Moreover,

$$g(x+\gamma_2) - g(x) = \chi(x)f(x) + (1 - \chi(x))f(x) = f(x).$$

Now we let

$$\tilde{e}_\gamma(x) = e^{-g(x+\gamma)}e_\gamma(x)e^{g(x)},$$

Then $\tilde{e}_{\gamma_1}(x) = e^{g(x)-g(x+\gamma_1)} = 1$ and $\tilde{e}_{\gamma_2}(x) = e^{-f(x)}e_{\gamma_2}(x) = 1$. Thus L is isomorphic to the trivial line bundle. □

When $n = 2$, we identify $\mathbb{R}^2$ with $\mathbb{C}$, so that $\mathbb{C}/\Gamma$ is a complex manifold. It is called an elliptic curve (for reasons related to elliptic functions and elliptic integrals). It is a fact that every holomorphic line bundle over $\mathbb{C}$ is trivial. So we can do the same thing as above and get a family of holomorphic multipliers $e_\gamma(z) : \mathbb{C} \to \mathbb{C}^*$. Note that there are many different holomorphic structures on a smooth line bundle over an elliptic curve (in fact, they all differ by a translation).

Given a Hermitian connection $h(z)$, we can write down the Chern connection directly:

$$\theta(z) = \partial_z(\log h(z))dz = h(z)^{-1}\partial_z h(z)dz \tag{7.12}$$

It is direct to check it is Hermitian and $D^{0,1} = \overline{\partial}$. We check it is compatible:

$$\theta(z+\gamma) = \partial_z \log(h(z+\gamma))dz = \partial_z \log(h(x)|e_\gamma(x)|^{-2})dz = \theta(z) - e_\gamma(z)^{-1}\partial_z e_\gamma(z)dz.$$

A classical subject from 19th century is elliptic functions and theta functions. By Liouville's theorem, the only holomorphic function on $\mathbb{C}/\Gamma$ is constant. However there exist meromorphic functions on $\mathbb{C}/\Gamma$, which are called elliptic functions, and holomorphic sections of line bundles, which are called theta functions.

Definition 7.11. *Let $z, \tau \in \mathbb{C}, \operatorname{Im} \tau > 0$. The Jacobi theta function is*

$$\theta(z;\tau) = \sum_{n\in\mathbb{Z}} \exp(\pi i n^2 \tau + 2\pi i n z).$$

Let $l \in \mathbb{N}$, $a, b \in (1/l)\mathbb{Z}$, the theta function with rational characteristics a, b is defined as

$$\theta_{a,b}(z;\tau) = \sum_{n\in\mathbb{Z}} \exp(\pi i (n+a)^2 \tau + 2\pi i (n+a)(z+b)).$$

Since $\operatorname{Im}\tau > 0$, the series converges absolutely and defines a holomorphic function on $\mathbb{C}$. Here z is the variable on the universal cover $\mathbb{C}$ of $\mathbb{C}/\Gamma_\tau$, and τ should be thought of as the variable that parameterize the family of elliptic curves $\mathbb{C}/\Gamma_\tau$ with $\Gamma_\tau = \mathbb{Z} + \mathbb{Z}\tau$. The Jacobi theta function is quasi-periodic

$$\theta(z+1;\tau) = \theta(z;\tau), \quad \theta(z+\tau;\tau) = e^{-\pi i \tau - 2\pi i z}\theta(z;\tau).$$

In general,

$$\theta(z+m+n\tau;\tau) = e^{-\pi i n^2 \tau - 2\pi i n z}\theta(z;\tau).$$

If $e_{m+n\tau}(z) := \exp(-\pi i n^2 \tau - 2\pi i n z)$, then

$$\begin{aligned}
&e_{m_2+n_2\tau}(z+m_1+n_1\tau)e_{m_1+n_1\tau}(z) \\
&= \exp(-\pi i n_2^2\tau - 2\pi i n_2(z+m_1+n_1\tau) - \pi i n_1^2 \tau - 2\pi i n_1 z) \\
&= \exp(-\pi i (n_1+n_2)^2\tau - 2\pi i (n_1+n_2) z) \\
&= e_{m_1+m_2+(n_1+n_2)\tau}(z).
\end{aligned}$$

So $\{e_{m+n\tau}(z)\}$ defines a holomorphic line bundle over $\mathbb{C}/\Gamma_\tau$ and $\theta(z;\tau)$ is a nonzero holomorphic section of it.

One can check the metric given by $h(x) = \exp(-2\pi|\operatorname{Im} z|^2/|\operatorname{Im}\tau|)$ satisfies the compatibility condition (7.9). The corresponding Chern connection and curvature are given by

$$\theta(z) = \frac{\pi(z-\bar{z})}{\operatorname{Im}\tau}dz, \quad \Theta = \frac{\pi}{\operatorname{Im}\tau} dz \wedge d\bar{z}.$$

Hence,

$$c_1(L) = \frac{i}{2\pi}\int_X \Theta = 1.$$

It follows that the Jacobi theta function is a nontrivial holomorphic section of a line bundle of degree 1. In fact, Riemann–Roch theorem tells us this is the unique nontrivial holomorphic section of this line bundle (up to a scalar).

In general, there are more complicated line bundles of higher degrees. The theta functions with rational characteristics $\theta_{a,b}(lz;\tau)$ satisfies

$$\theta_{a,b}(l(z+1);\tau) = \theta_{a,b}(lz;\tau), \quad \theta_{a,b}(l(z+\tau);\tau) = e^{-\pi i l^2\tau - 2\pi i l^2 z}\theta_{a,b}(lz;\tau).$$

Thus they describe a holomorphic line bundle with $e_1(z) = 1$ and $e_\tau(z) = e^{-\pi i l^2\tau-2\pi i l^2 z}$. A simple calculation shows this line bundle has Chern number l^2, and again Riemann–Roch theorem implies that it has l^2 linearly independent holomorphic sections. Indeed, one can check directly that a basis is given by $\{\theta_{a,b}(z) : a, b \in \frac{1}{l}\mathbb{Z}/\mathbb{Z}\}$. We provide an elementary proof below.

Proposition 7.12. *Suppose* $\operatorname{Im}\tau > 0$*,* $\Gamma = \mathbb{Z} \oplus \mathbb{Z}\tau$*, and* $X = \mathbb{C}/\Gamma$*. Let* L *be a line bundle over* X *defined by multipliers*

$$e_1(z) = e^{i\alpha}, e_\tau(z) = e^{i\beta-2\pi i m z}, \quad \alpha, \beta \in \mathbb{C}, m \in \mathbb{Z}.$$

Then the dimension of holomorphic sections of L *(denoted by* $\mathcal{O}(X;L)$*) is equal to*

$$\dim_{\mathbb{C}} \mathcal{O}(X;L) = \begin{cases} m, & \text{if } m > 0; \\ 0, & \text{if } m < 0; \\ 0 \text{ or } 1, & \text{if } m = 0, \text{ depending on whether } L \text{ is trivial.} \end{cases}$$

Remark 11. *Note by* (7.10)*,* $m = c_1(L)$ *is the Chern number of the line bundle.*

Proof. Let w be a holomorphic section of L, we write

$$w(z) = e^{i\alpha z}u(z),$$

then $u(z+1) = u(z), u(z+\tau) = e^{i(\beta-\alpha\tau)-2\pi i m z}u(z)$. We can then expand u into Fourier series

$$u(z) = \sum_{n\in\mathbb{Z}} a_n(y)e^{2\pi i n z}.$$

Since $u(z)$ is holomorphic, $a_n(y)$ is also holomorphic, and $a_n(y) = a_n$ are constants. The condition $u(z+\tau) = e^{i(\beta-\alpha\tau)-2\pi i m z}u(z)$ gives

$$a_n e^{2\pi i n\tau} = e^{i(\beta-\alpha\tau)}a_{n+m}.$$

If $m = 0$ and $\beta - \alpha\tau \in 2\pi\tau\mathbb{Z}$ (i.e. when L is trivial), then one has a nonzero solution $a_n = \delta_{n,r}$ for $\beta - \alpha\tau = 2\pi i r\tau$. Otherwise we get $a_n = 0$ for all n.

For $m \neq 0$, the solution is determined by a choice of $a_0, a_1, \cdots, a_{|m|-1}$. If $m < 0$, the solution a_n would grow exponentially ($|a_n| \geq \frac{1}{C}e^{n^2/C}$) and the series would diverge. Thus there is no nonzero holomorphic sections when $m < 0$. If $m > 0$, then the solution a_n decays exponentially ($|a_n| \leq Ce^{-n^2/C}$) and gives holomorphic sections. So $\dim \mathcal{O}(X;L) = m$ for $m > 0$. $\square$

8. Topology in physics: the adiabatic theorem and decay of Wannier functions

Here we present two examples of consequences of non-trivial topology in physics. The first concerns adiabatic evolution. We first revisit the Bloch sphere (see §5.3) and see the emergence of holonomy in adiabatic evolution in that case. We then consider general line bundles over $\mathbb{R}^2/\Gamma^*$ (the *Brillouin zone*) given by Bloch eigenfunctions and show how their nontriviality affects decay of Wannier functions (see §5.6 for the first instance they appeared here, albeit in trivial topology).

8.1. **Adiabatic theorems and parallel transport.** In this section we introduce the adiabatic theorem. To gain respect for the general case proved in §8.2 below we first look at a special case of the Bloch operator (7.1).

Proposition 8.1. *Let $x(t) = (r\cos t, r\sin t, (1-r^2)^{1/2})$ be a curve on the sphere. Consider the initial value problem*

$$\begin{cases} i\varepsilon\partial_t w_\varepsilon = (H(x(t)) - 1)w_\varepsilon, \\ w_\varepsilon|_{t=0} \in V_{x(0)}. \end{cases}$$

Then there exists $w(t) \in V_{x(t)}$ independent of ε, such that

$$w_\varepsilon(t) = w(t) + \mathcal{O}(\varepsilon). \tag{8.1}$$

Remark 12. *If we write the equation as*

$$\begin{cases} i\partial_t w_\varepsilon = H(x(\varepsilon t))w_\varepsilon, \\ w_\varepsilon|_{t=0} \in V_{x(0)}, \end{cases}$$

then we will conclude $w_\varepsilon(t) = e^{-it}w(\varepsilon t) + \mathcal{O}(\varepsilon)$. The -1 term will just affect the phase. The adiabatic theorem describes behavior of a system under a slowly varying Hamiltonian.

Proof. Let

$$u_1 = \frac{1}{(1+\rho^2)^{1/2}}\begin{pmatrix}\rho e^{it} \\ 1\end{pmatrix}, \quad u_2 = \frac{1}{(1+\rho^2)^{1/2}}\begin{pmatrix}1 \\ -\rho e^{-it}\end{pmatrix}$$

be the normalized eigenvectors. Let $w_\varepsilon(t) = c_1(t)u_1(t) + c_2(t)u_2(t)$. Then

$$\begin{aligned} \dot c_1(t) &= -c_1\langle \dot u_1, u_1\rangle - c_2\langle \dot u_2, u_1\rangle, \\ \dot c_2(t) &= -c_1\langle \dot u_1, u_2\rangle - c_2\langle \dot u_2, u_2\rangle + \frac{2i}{\varepsilon}c_2. \end{aligned}$$

In other words,

$$\begin{aligned}\dot c_1(t) &= -ic_1\frac{\rho^2}{1+\rho^2} + ic_2\frac{\rho}{1+\rho^2}e^{-it},\\ \dot c_2(t) &= -ic_1\frac{\rho}{1+\rho^2}e^{it} + c_2\left(\frac{2i}{\varepsilon} + \frac{i\rho^2}{1+\rho^2}\right).\end{aligned}$$

Let $a_1(t) = c_1(t)$ and $a_2(t) = e^{-it}c_2(t)$, then

$$\begin{aligned}\dot a_1(t) &= -ia_1\frac{\rho^2}{1+\rho^2} + ia_2\frac{\rho}{1+\rho^2},\\ \dot a_2(t) &= -ia_1\frac{\rho}{1+\rho^2} + a_2\left(\frac{2i}{\varepsilon} + \frac{i\rho^2}{1+\rho^2} - i\right).\end{aligned}$$

This is an ordinary differential equation with constant coefficients. The matrix

$$\begin{pmatrix} -i\frac{\rho^2}{1+\rho^2} & i\frac{\rho}{1+\rho^2}\\ -i\frac{\rho}{1+\rho^2} & \frac{2i}{\varepsilon}+\frac{i\rho^2}{1+\rho^2}-i\end{pmatrix}$$

has eigenvalue $\lambda_1 = 2i/\varepsilon + i\rho^2/(1+\rho^2) - i + \mathcal{O}(\varepsilon)$ and $\lambda_2 = -i\rho^2/(1+\rho^2) + \mathcal{O}(\varepsilon)$ and eigenvectors $v_1 = \begin{pmatrix}0\\1\end{pmatrix} + \mathcal{O}(\varepsilon)$, $v_2 = \begin{pmatrix}1\\0\end{pmatrix} + \mathcal{O}(\varepsilon)$. Thus

$$\begin{aligned}\begin{pmatrix}a_1(t)\\a_2(t)\end{pmatrix} &= \exp\left(t\begin{pmatrix} -i\frac{\rho^2}{1+\rho^2} & i\frac{\rho}{1+\rho^2}\\ -i\frac{\rho}{1+\rho^2} & \frac{2i}{\varepsilon}+\frac{i\rho^2}{1+\rho^2}-i\end{pmatrix}\right)\begin{pmatrix}1\\0\end{pmatrix}\\ &= \exp((-i\rho^2/(1+\rho^2))t)\begin{pmatrix}1\\0\end{pmatrix} + \mathcal{O}(\varepsilon).\end{aligned}$$

In conclusion

$$w_\varepsilon(t) = \exp((-i\rho^2/(1+\rho^2))t)u_1(t) + \mathcal{O}(\varepsilon), \tag{8.2}$$

which gives (8.1). □

The general adiabatic theorem describes a system with slowly varying Hamiltonian. It was first proposed by Born and Fock, and later proved mathematically by Kato [Ka58]

Theorem 10. *Let $P(s), s \in [0,1]$ be a smooth family of bounded self-adjoint operators on a Hilbert space H, and $\lambda(s)$ be a smooth family of simple eigenvalues of $P(s)$ such that* $\mathrm{dist}(\lambda(s), \mathrm{Spec}(P(s)) \setminus \{\lambda(s)\}) > \delta > 0$ *is bounded from below. Consider the following initial data problem*

$$\begin{cases} i\varepsilon\partial_t u_\varepsilon = P(t)u_\varepsilon,\\ u_\varepsilon(0) = u_0 \in \ker(P(0) - \lambda(0)).\end{cases}$$

Then there exists $u(t) \in \ker(P(t) - \lambda(t))$ independent of ε such that

$$u_\varepsilon(t) = \exp\left(-\frac{i}{\varepsilon}\int_0^t \lambda(s)ds\right) u(t) + \mathcal{O}_H(\varepsilon).$$

We postpone the proof until §8.2.

Remark 13. *The boundedness assumption of $P(t)$ is not essential, and the proof adapts to unbounded cases under reasonable assumptions. We only prove the bounded case for simplicity.*

In order to understand the next theorem, we need to introduce parallel transport.

Definition 8.2. *Let $\pi : L \to X$ be a line bundle over a smooth manifold X, and $\gamma(t)$ be a smooth curve on X. The parallel transport of $s_0 \in \pi^{-1}(\gamma(0))$ is a section $s(t)$ of L along $\gamma(t)$ such that*

$$Ds(t)(\dot\gamma(t)) = 0. \tag{8.3}$$

Suppose $L \subset X \times H$ and the connection D is inherited from H as in (7.4). Then if we choose a local orthonormal frame u_1, D is given by $ds_1 + \langle du_1, u_1\rangle s_1$. The parallel transport equation can be rewritten as

$$\left\langle \frac{d}{dt}(s_1(t)u_1(\gamma(t))), u_1(\gamma(t))\right\rangle = 0.$$

Let $s(t) = s_1(t)u_1(\gamma(t))$, it is equivalent to $\langle \frac{d}{dt}s(t), s(t)\rangle = 0$ or $\langle s(t+\delta), s(t)\rangle = \langle s(t), s(t)\rangle + \mathcal{O}(\delta^2)$.

The following theorem of Barry Simon [Si83] gives an interpretation of the adiabatic theorem in terms of parallel transport.

Theorem 11. *Suppose X is a smooth manifold, $\gamma(s)$ is a smooth curve on X and suppose that $X \ni x \mapsto Q(x)$ is a smooth family of self-adjoint operators parametrised by X and such that there exists $x \mapsto \lambda(x)$ satisfying*

$$\mu(x) \in \operatorname{Spec}(Q(x)), \quad d(\mu(x), \operatorname{Spec}(Q(x)) \setminus \{\mu(x)\}) > \delta > 0, \quad x \in X.$$

Let $V_x = \ker(Q(x) - \lambda(x))$ be the line bundle defined by the eigenspace of $Q(x)$ and D be the inherited connection from H. Suppose that $[0,1] \ni t \mapsto \gamma(t)$ is a smooth curve in X and $P(t) := Q(\gamma(t))$. Then $u(t)$ given in Theorem 10 is the parallel transport of u_0 along $\gamma(t)$.

Proof. We may assume $\lambda(x) = 0$ and ignore the phase. Then $u(s) = \lim_{\varepsilon\to 0} u_\varepsilon(s)$. To prove $u(s)$ is the parallel transport, it suffices to show $\langle \frac{d}{ds}u(s), u(s)\rangle = 0$. For that in turn, it suffices to show for any $\varphi \in C_0^\infty((0,1))$ we have

$$\int \varphi(s)\left\langle \frac{d}{ds}u(s), u(s)\right\rangle ds = 0.$$

We calculate

$$\begin{aligned}
\int \varphi(s)\left\langle \frac{d}{ds}u(s), u(s)\right\rangle ds &= \lim_{\varepsilon\to 0}\int \varphi(s)\left\langle \frac{d}{ds}u(s), u_\varepsilon(s)\right\rangle ds \\
&= \lim_{\varepsilon\to 0} -\int \varphi'(s)\left\langle u(s), u_\varepsilon(s)\right\rangle ds - \int \varphi(s)\left\langle u(s), \frac{d}{ds}u_\varepsilon(s)\right\rangle ds \\
&= -\int \varphi'(s)ds + \lim_{\varepsilon\to 0}\frac{i}{\varepsilon}\int \varphi(s)\left\langle u(s), P(s)u_\varepsilon(s)\right\rangle ds \\
&= \lim_{\varepsilon\to 0}\frac{i}{\varepsilon}\int \varphi(s)\left\langle P(s)u(s), u_\varepsilon(s)\right\rangle ds \\
&= 0.
\end{aligned}$$

We conclude $\langle \frac{d}{ds}u(s), u(s)\rangle = 0$ and this finishes the proof. ☐

Remark 14. *A quick formal argument indicating validity of Theorem 11 goes as follows:*

$$\begin{aligned}
\left\langle \frac{d}{ds}u(s), u(s)\right\rangle &= \lim_{\varepsilon\to 0}\left\langle \frac{d}{ds}u_\varepsilon(s), u(s)\right\rangle = -\lim_{\varepsilon\to 0}\frac{i}{\varepsilon}\left\langle P(s)u_\varepsilon(s), u(s)\right\rangle \\
&= -\lim_{\varepsilon\to 0}\frac{i}{\varepsilon}\left\langle u_\varepsilon(s), P(s)u(s)\right\rangle = 0.
\end{aligned}$$

But we need to justify the change of order for limit and derivative. Thus we need the help of a test function $\varphi \in C_0^\infty$ in the actual proof.

As a corollary, we conclude

Corollary 8.3. *In Theorem 11, if $\gamma(0) = \gamma(1)$ and $\lambda = 0$, then $u(1) = \mathrm{hol}_D(\gamma)u(0)$.*

Remark 15. *One can check that the answer in (8.2) agrees with the computation in Example 7.8. In (8.2), $\rho = \sin\varphi/(1-\cos\varphi)$ and*

$$\begin{aligned}
\mathrm{hol}_D(\gamma) &= \exp\left(-\frac{2\pi i\rho^2}{1+\rho^2}\right) = \exp\left(\frac{2\pi i}{1+\rho^2}\right) = \exp\left(\frac{2\pi i(1-\cos\varphi)^2}{(1-\cos\varphi)^2+\sin^2\varphi}\right) \\
&= \exp(\pi i(1-\cos\varphi)).
\end{aligned}$$

8.2. **Proof of the Adiabatic Theorem.** In this section we give the proof of Theorem 10. The main idea is a new unitary evolution called the adiabatic evolution.

Proof of Theorem 10. **Step 1:** We may assume $\lambda(t) = 0$ without loss of generality. Let $U(t)$ be the unitary evolution defined by P:

$$i\varepsilon\partial_t U(t) = P(t)U(t), \quad U(0) = \mathrm{id}, \tag{8.4}$$

then $u_\varepsilon(t) = U(t)u_0$. Following Kato [Ka58] we define the adiabatic evolution to be

$$i\varepsilon\partial_t U_A(t) = (P(t) + i\varepsilon[\dot{\Pi}(t), \Pi(t)])U_A(t), \quad U_A(0) = \mathrm{id}$$

where

$$\Pi(t) := \frac{1}{2\pi i}\oint_\gamma (z-P(t))^{-1}dz$$

is the projection to the eigenspace with eigenvalue $\lambda(t)=0$ (γ is a simple closed curve such that $\lambda(t)$ lies inside and $\mathrm{Spec}(P(t))\setminus\{\lambda(t)\}$ lies outside). Note this defines a unitary evolution because $[\dot\Pi(t),\Pi(t)]$ is anti-self-adjoint. We claim

$$\Pi(t)U_A(t) = U_A(t)\Pi(0).$$

This is because

$$\begin{aligned}
&i\varepsilon\frac{d}{dt}(U_A(t)^*\Pi(t)U_A(t))\\
&= U_A(t)^*(-P(t)\Pi(t) - i\varepsilon[\dot\Pi(t),\Pi(t)]\Pi(t) + i\varepsilon\dot\Pi(t) + \Pi(t)P(t) + i\varepsilon\Pi(t)[\dot\Pi(t),\Pi(t)])U_A(t)\\
&= i\varepsilon U_A(t)^*(\dot\Pi(t) + 2\Pi(t)\dot\Pi(t)\Pi(t) - \dot\Pi(t)\Pi(t) - \Pi(t)\dot\Pi(t))U_A(t) = 0.
\end{aligned}$$

In the last step we use

$$\dot\Pi(t) = \frac{d}{dt}(\Pi(t)^2) = \dot\Pi(t)\Pi(t) + \Pi(t)\dot\Pi(t)$$

and consequently $\Pi(t)\dot\Pi(t)\Pi(t) = 2\Pi(t)\dot\Pi(t)\Pi(t) = 0$. As a consequence,

$$u(t) := U_A(t)u_0 = \Pi(t)U_A(t)u_0 \in \ker(P(t)-\lambda(t)).$$

Moreover, since $P(t)U_A(t)\Pi(0) = P(t)\Pi(t)U_A(t) = 0$, we have

$$i\varepsilon\partial_t u(t) = (P(t) + i\varepsilon[\dot\Pi(t),\Pi(t)])U_A(t)u_0 = i\varepsilon[\dot\Pi(t),\Pi(t)]u(t),$$

that is, $\partial_t u(t) = [\dot\Pi(t),\Pi(t)]u(t)$ which shows that $u(t)$ is independent of ε.

Step 2: It remains to prove $u_\varepsilon(t) - u(t) = \mathcal{O}_H(\varepsilon)$. We need to estimate

$$\begin{aligned}
U_A(t) - U(t) &= U(t)\int_0^t \frac{d}{ds}(U(s)^*U_A(s))ds\\
&= \frac{U(t)}{i\varepsilon}\int_0^t U(s)^*(-P(s) + P(s) + i\varepsilon[\dot\Pi(s),\Pi(s)])U_A(s)ds \qquad (8.5)\\
&= U(t)\int_0^t U(s)^*[\dot\Pi(s),\Pi(s)]U_A(s)ds.
\end{aligned}$$

The key now is to find a smooth family operator $s\mapsto X(s)$ such that

$$[\dot\Pi(s),\Pi(s)] = [X(s),P(s)]. \tag{8.6}$$

That is because we then have a chance of gaining an epsilon in (8.5) as (8.4) and (8.6) give

$$U(s)^*[X(s),P(s)]U(s) = \varepsilon\left(i\partial_s[U(s)^*XU(s)] - iU(s)^*[\partial_s X(s)]U(s)\right). \tag{8.7}$$

We claim that

$$X(s) := \frac{1}{2\pi i}\oint_\gamma (z-P(s))^{-1}\dot\Pi(s)(z-P(s))^{-1}dz$$

gives (8.6). Indeed,

$$
\begin{aligned}
[X(s), P(s)] &= \frac{1}{2\pi i}\oint_\gamma (z-P(s))^{-1}[\dot\Pi(s), P(s)](z-P(s))^{-1}dz \\
&= -\frac{1}{2\pi i}\oint_\gamma (z-P(s))^{-1}[\dot\Pi(s), z-P(s)](z-P(s))^{-1}dz \\
&= \frac{1}{2\pi i}\oint_\gamma [\dot\Pi(s), (z-P(s))^{-1}]dz \\
&= [\dot\Pi(s), \Pi(s)].
\end{aligned}
$$

So we can write the integrand in (8.5) as

$$
\begin{aligned}
U(s)^*[X(s), P(s)]U_A(s) = i\varepsilon\partial_s(U(s)^*X(s)U_A(s)) - i\varepsilon U(s)^*\dot X(s)U_A(s) \\
- i\varepsilon U(s)^*X(s)[\dot\Pi(s), \Pi(s)]U_A(s),
\end{aligned}
$$

Inserting this into (8.5) gives

$$
\begin{aligned}
\|U_A(t) - U(t)\| &\le \varepsilon\|U(t)^*X(t)U_A(t) - X(0)\| \\
&\quad + \varepsilon\int_0^t (\|\dot X(s)\| + \|X(s)[\dot\Pi(s), \Pi(s)]\|)ds = \mathcal{O}(\varepsilon).
\end{aligned}
$$

Thus $u_\varepsilon(t) - u(t) = (U(t) - U_A(t))u_0 = \mathcal{O}_H(\varepsilon)$, as claimed. □

8.3. **The line bundle of eigenfunctions over $\mathbb{R}^2/\Gamma^*$.** Suppose that

$$
\begin{gathered}
P(x, D) = \sum_{j=1}(D_{x_j} + A_j(x))^2 + V(x), \\
A_j(x+\gamma) = A_j(x), \quad V(x+\gamma) = V(x), \quad \gamma\in\Gamma, \quad x\in\mathbb{R}^2.
\end{gathered} \tag{8.8}
$$

We also assume that for some k (5.17) holds. We then define

$$
\begin{gathered}
L := \left\{[\theta, v] \in (\mathbb{R}^2\times L^2(\mathbb{R}^2/\Gamma))/\sim :\ v\in \ker_{L^2(\mathbb{R}^2/\Gamma)}(P(x, D-\theta) - E_k(\theta))\right\}, \\
[\theta, v] = [\theta', v'] \iff (\theta, v)\sim(\theta', v') \iff \exists\, p\in\Gamma^*,\ \theta' = \theta + p, \quad v' = \tau(p)v,
\end{gathered} \tag{8.9}
$$

where $[\tau(p)v](x) = e^{i\langle x, p\rangle}v(x)$.

The reason for $\tau(p)$ is the fact that it provides unitary equivalence

$$
P(x, D-\theta-p) = \tau(p)P(x, D-\theta)\tau(p)^*, \quad \theta\in\mathbb{R}^2, \quad p\in\Gamma^*.
$$

In particular, for $u\in H^2(\mathbb{R}/\Gamma)$,

$$
P(x, D-\theta)u(x) = Eu(x) \iff P(x, D-\theta-p)[\tau(p)u](x) = E[\tau(p)u](x).
$$

We have

Lemma 8.4. *Definition* (8.9) *gives a complex line bundle over* $\mathbb{C}/\Gamma^*$,

$$
\pi : L\to\mathbb{C}/\Gamma^*, \quad \pi : [\theta, v]\to[\theta]\in\mathbb{C}/\Lambda. \tag{8.10}
$$

Proof. Let $\mathbb{R}^n \ni \theta \mapsto u(\theta, \bullet) \in C^\infty(\mathbb{R}^2/\Gamma)$ be a smooth family of solutions to $P(x, D - \theta)u(\theta, x) = E_k(\theta)u(\theta, x)$, $\|u(\theta, \bullet)\|_{L^2(\mathbb{R}^2/\Gamma)} = 1$.

The action of the discrete group Γ^*, $p : (\theta, v) \mapsto (\theta + p, \tau(p)v)$ on the (trivial) complex line bundle

$$\widetilde{L} := \{(\theta, \tau u(\theta)) : \theta \in \mathbb{C}, \quad \tau \in \mathbb{C}\} \simeq \mathbb{C}_\theta \times \mathbb{C}_\tau, \tag{8.11}$$

is free and proper, and the quotient map is given by $F(\theta, \tau u(\theta)) = [\theta, \tau u(\theta)]$. Hence its quotient by that action, L, is a smooth manifold of dimension two. With π given by (8.10), $\pi^{-1}([\theta]) \simeq \ker_{L^2(\mathbb{R}^2/\Gamma)}(P(x, D - \theta) - E_k(\theta))$ and has a vector space structure and local coordinates θ provide the needed trivializations. $\square$

From the presentation in §7.2 we see that we can use $u(\theta, x)$, $\theta \in F$, F a fundamental domain of Γ^*, as a frame and then for $\theta \in F$, the connection is given by $D(su) = (ds + \eta s)u$,

$$\eta := \langle d_\theta u(\theta, \bullet), u(\theta, \bullet)\rangle_{L^2(\mathbb{R}^n/\Gamma)} = \langle \partial_{\theta_1} u, u\rangle d\theta_1 + \langle \partial_{\theta_2} u, u\rangle d\theta_2, \quad \theta \in F. \tag{8.12}$$

This is the *Berry connection* in the setting of Floquet eigenfunctions over $\mathbb{R}^2/\Gamma^*$. This gives the following formula for the curvature, called the *Berry curvature* in this setting:

$$\Theta = d\eta = -2i \operatorname{Im}\langle \partial_{\theta_1} u(\theta, \bullet), \partial_{\theta_2} u(\theta, \bullet)\rangle_{L^2(\mathbb{R}^2/\Gamma)} d\theta_1 \wedge d\theta_2, \quad \theta \in F. \tag{8.13}$$

(The other terms give $\langle \partial^2_{\theta_1\theta_2} u, u\rangle d\theta_2 \wedge d\theta_1 + \langle \partial^2_{\theta_2\theta_1} u, u\rangle d\theta_1 \wedge d\theta_2 = 0$.) We then have

$$c_1(L) = \frac{1}{\pi} \int_F \operatorname{Im}\langle \partial_{\theta_1} u, \partial_{\theta_2} u\rangle d\theta_1 d\theta_2. \tag{8.14}$$

In particular if the integral on the right hand side does not vanish then the line bundle is non-trivial.

Theorem 6 shows that in case of time reversal symmetry, in particular when $A_j \equiv 0$ in (8.8), the line bundle L is trivial and $c_1(L) = 0$. A yet stronger statement follows from symmetries of V:

Proposition 8.5. *Suppose that $P = -\Delta + V(x)$ and that (5.17) holds for $E(\theta) = E_k(\theta)$. If for some x_0,*

$$V(x_0 + x) = V(x_0 - x), \tag{8.15}$$

then the Berry curvature given by (8.13) satisfies

$$\Theta \equiv 0. \tag{8.16}$$

Proof. We can assume that $x_0 = 0$. In view of (8.13),

$$\Omega = -\int_{\mathbb{R}^2/\Gamma} d_\theta u(\theta, x) \wedge \overline{d_\theta u(\theta, x)} dx.$$

Since we assumed that the eigenvalue $E(\theta)$ is simple, $V(x) = \overline{V(x)}$ and $V(x) = V(-x)$ imply that

$$\overline{u(\theta, x)} = \alpha_1(\theta)u(-\theta, x), \quad u(-\theta, x) = \alpha_2(\theta)u(\theta, -x), \quad |\alpha_j(\theta)| = 1.$$

Hence with $\alpha(\theta) := \alpha_1(\theta)\alpha_2(\theta)$,

$$\overline{u(\theta, x)} = \alpha(\theta)u(\theta, -x), \quad \alpha \in C^\infty(\mathbb{R}^n/\Gamma^*). \tag{8.17}$$

The periodicity and smoothness of α hold as for $p \in \Gamma^*$ we have

$$\alpha(\theta + p) = \int_{\mathbb{R}^2/\Gamma} \overline{u(\theta + p, x)u(\theta + p, -x)}dx = \int_{\mathbb{R}^2/\Gamma} \overline{e^{i\langle x,p\rangle}u(\theta, x)e^{i\langle -x,p\rangle}u(\theta, -x)} = \alpha(\theta).$$

This gives

$$\begin{aligned}\Omega &= -\int_{\mathbb{R}^2/\mathbb{Z}^2} d_\theta u(\theta, x) \wedge d_\theta(\alpha(\theta)u(\theta, -x))dx \\ &= -\alpha(\theta)\int_{\mathbb{R}^2/\mathbb{Z}^2} d_\theta u(\theta, x) \wedge d_\theta u(\theta, -x)dx + d\alpha(\theta) \wedge \int_{\mathbb{R}^2/\mathbb{Z}^2} u(\theta, -x)d_\theta u(\theta, x)dx.\end{aligned}$$

The first term vanishes since

$$\begin{aligned}\int_{\mathbb{R}^2/\mathbb{Z}^2} d_\theta u(\theta, x) \wedge d_\theta u(\theta, -x)dx &= \int_{\mathbb{R}^2/\mathbb{Z}^2} d_\theta u(\theta, -x) \wedge d_\theta u(\theta, x)dx \\ &= -\int_{\mathbb{R}^2/\mathbb{Z}^2} d_\theta u(\theta, x) \wedge d_\theta u(\theta, -x)dx.\end{aligned}$$

For the second term we notice that

$$\int_{\mathbb{R}^2/\mathbb{Z}^2} u(\theta, -x)d_\theta u(\theta, x)dx = \tfrac{1}{2}d_\theta \int_{\mathbb{R}^2/\mathbb{Z}^2} u(\theta, -x)u(\theta, x)dx = \tfrac{1}{2}d_\theta(\alpha(\theta)^{-1}),$$

so that

$$d\alpha(\theta) \wedge \int_{\mathbb{R}^2/\mathbb{Z}^2} u(\theta, -x)d_\theta u(\theta, x)dx = \tfrac{1}{2}d\alpha(\theta) \wedge d_\theta(\alpha(\theta)^{-1}) = 0,$$

and the conclusion (8.16) follows. □

8.4. **Berry connection and curvature via perturbation theory.** In the notation of §8.3 and assuming (5.17) again we can express the connection (8.12) and its curvature using formulas from second order perturbation theory. Since we will consider other energy levels we now write $u = u_k$ nad $E = E_k$ – see (5.17).

We first note that $(P(x, D - \theta) - E_k(\theta))u_k(\theta, x) = 0$ implies that

$$(P(x, D - \theta) - E_k(\theta))\partial_{\theta_\ell} u_k(\theta) = \partial_{\theta_\ell} E_k(\theta)u_k(\theta) - 2(D_{x_\ell} - \theta_\ell)u_k(\theta).$$

Since the inner product of the left hand side with u_k vanishes we see that the right is also orthogonal to u_k (and that $\partial_{\theta_\ell} E_k(\theta) = 2\langle (D_{x_\ell} - \theta_\ell) u_k(\theta), u_k(\theta)\rangle$). This means that, for $\alpha(\theta) \in \mathbb{R}$,

$$\partial_{\theta_\ell} u_k(\theta) = \langle \partial_{\theta_\ell} u_k(\theta), u_k(\theta)\rangle u_k(\theta) + 2\sum_{j\neq k} \frac{\langle D_{x_\ell} u_k(\theta), u_j(\theta)\rangle}{E_k - E_j} u_j(\theta).$$

Then, for the curvature (8.13) we get $\Theta = H(\theta) d\theta_1 \wedge d\theta_2$ where

$$\begin{aligned} H(\theta) &:= -2i \operatorname{Im}\langle \partial_{\theta_1} u_k(\theta), \partial_{\theta_2} u_k(\theta)\rangle \\ &= -8i \sum_{j\neq k} \frac{\operatorname{Im}\left(\langle D_{x_1} u_k(\theta), u_j(\theta)\rangle \overline{\langle D_{x_2} u_k(\theta), u_j(\theta)\rangle}\right)}{(E_k - E_j)^2}. \end{aligned} \tag{8.18}$$

8.5. **Decay of Wannier functions.** We again suppose that (5.17) holds and we denote by $\Pi_k = \mathbb{1}_{I_k}(P)$, the spectral projection associated to the isolated band I_k. In §5.7 we discussed the basis of $\Pi_k L^2(\mathbb{R}^2)$ for time reversible operators P, $\overline{Pu} = P\bar{u}$ (for instance, $P = -\Delta + V$, with V real valued). We now consider a more general case.

Definition 8.6. *Suppose that the condition* (5.17) *holds. Then φ_0 is a Wannier function associated to the band I_k if $\{\varphi_0(x-\gamma)\}_{\gamma\in\Gamma}$ form an orthonormal basis of of $\mathbb{1}_{I_k}(P) L^2(\mathbb{R}^2)$.*

We note that that

$$\varphi(\theta, \bullet) := |\mathbb{R}^n/\Gamma^*|^{1/2} \mathcal{B}\varphi_0(\theta, \bullet) \in \ker_{\mathcal{H}_\theta}(P - E_k(\theta)).$$

The condition that $\{\varphi_0(x-\gamma)\}_{\gamma\in\Gamma}$ forms an orthonormal basis implies $\|\varphi(\theta,\bullet)\|_{\mathcal{H}_\theta} = 1$: let F be a fundamental domain of $\mathbb{R}^n/\Gamma$,

$$\begin{aligned} \|\varphi(\theta,\bullet)\|^2_{\mathcal{H}_\theta} &= \sum_{\gamma,\gamma'\in\Gamma} \int_F e^{i(\gamma'-\gamma)\cdot\theta} \varphi_0(x-\gamma)\overline{\varphi_0(x-\gamma')} dx \\ &= \sum_{\gamma\in\Gamma} e^{i\gamma\cdot\theta} \int_{\mathbb{R}^n} \varphi_0(x)\overline{\varphi_0(x-\gamma)} dx = \int_{\mathbb{R}^n} |\varphi_0(x)|^2 dx = 1. \end{aligned}$$

Conversely, (see §5.6) any normalized family $\varphi(\theta, x) \in L^2(\mathbb{R}^2/\Gamma^*_\theta; \mathcal{H}_\theta)$ satisfying $P\varphi(\theta) = E_k(\theta)\varphi(\theta)$ and $\|\varphi(\theta)\|_{\mathcal{H}_\theta} = 1$ produces a Wannier function

$$\varphi_0(x) := \varphi_0(x) = \frac{1}{|\mathbb{R}^n/\Gamma^*|} \int_{\mathbb{R}^n/\Gamma^*} \varphi(\theta, x) d\theta. \tag{8.19}$$

Hence we always have a Wannier function once (5.17) is satisfied.

The simplicity assumption in (5.17) then shows that $\varphi(\theta,\bullet)$ is uniquely determined up to a multiplicative (measurable) factor $f(\theta)$, $|f(\theta)| = 1$, and that

$$\mathcal{B}\mathbb{1}_{I_k}(P) L^2(\mathbb{R}^2) = \{ g(\theta)\varphi(\theta, x) : g \in L^2(\mathbb{R}^2/\Gamma^*)\}.$$

We also note that for $\alpha, \beta \in \Gamma$,

$$\begin{aligned}\frac{1}{|\mathbb{R}^2/\Gamma^*|}\langle e^{-i\langle\alpha,\theta\rangle}\varphi, e^{-i\langle\beta,\theta\rangle}\varphi\rangle_{L^2(\mathbb{R}^2/\Gamma^*;\mathcal{H}_\theta)} &= \frac{1}{|\mathbb{R}^2/\Gamma^*|}\int_{\mathbb{R}^2/\Gamma^*}\int_{\mathbb{R}^2/\Gamma} e^{-i\langle\alpha-\beta,\theta\rangle}|\varphi(\theta,x)|^2 dx d\theta \\ &= \frac{1}{|\mathbb{R}^2/\Gamma^*|}\int_{\mathbb{R}^2/\Gamma^*} e^{-i\langle\alpha-\beta,\theta\rangle} d\theta = \delta_{\alpha\beta}.\end{aligned}$$

Writing $g(\theta) = \sum_{\alpha\in\Gamma} a_\alpha e^{-i\langle\alpha,\theta\rangle}$, $\{a_\alpha\} \in \ell^2(\Gamma)$, we see from this that

$$\{\varphi_0(x-\gamma)\}_{\gamma\in\Gamma} \text{ is an orthonormal basis of } \mathbb{1}_{I_k}(P)L^2(\mathbb{R}^2). \tag{8.20}$$

We now make a general statement about the relation between regularity of in θ and decay in x (which holds in any dimension):

Lemma 8.7. *Suppose $u \in \mathscr{S}(\mathbb{R}^2)$ and that $\widetilde{\mathcal{B}}$ is the modified Bloch transform (see §5.3). Then $D_{\theta_j}\widetilde{\mathcal{B}}u = \widetilde{B}(x_j u)$ and*

$$\int_{\mathbb{R}^2/\Gamma}\int_{\mathbb{R}^2/\Gamma^*} |D_{\theta_j}\widetilde{\mathcal{B}}u(\theta,x)|^2 d\theta dx = C_\Gamma \int_{\mathbb{R}^2} |x_j u(x)|^2 dx. \tag{8.21}$$

For $v \in \mathscr{S}'(\mathbb{R}^2 \times \mathbb{R}^2/\Gamma)$ satisfying $v(\theta+p, x+\gamma) = \tau(p)v(\theta,x)$, we then define

$$\|v\|^2_{H^k_\tau(\mathbb{R}^2/\Gamma^*\times\mathbb{R}^2/\Gamma)} := \sum_{|\alpha|\le k}\int_{\mathbb{R}^2/2\Gamma^*} |D^\alpha_\theta v(\theta,x)|^2 d\theta, \tag{8.22}$$

provided that the right hand side (with distributional derivatives on $\mathbb{R}^2\times\mathbb{R}^2/\Gamma$ and the integral over a fundamental domain of a larger lattice 2Γ) is finite. It follows that

$$\|\widetilde{\mathcal{B}}u\|_{H^k_\tau(\mathbb{R}^2/\Gamma^*\times\mathbb{R}^2/\Gamma)} \simeq \|\langle x\rangle^k u\|_{L^2(\mathbb{R}^2)}, \tag{8.23}$$

and that $\widetilde{\mathcal{B}}u \in H^k_\tau(\mathbb{R}^2/\Gamma^*\times\mathbb{R}^2/\Gamma)$ if and only if $\langle x\rangle^k u \in L^2(\mathbb{R}^2)$.

Proof. For $u \in \mathscr{S}(\mathbb{R}^2)$ we have

$$\widetilde{\mathcal{B}}u(\theta,x) = c_\Gamma \sum_{\gamma\in\Gamma} e^{i\langle x-\gamma,\theta\rangle}u(x-\gamma) \in C^\infty(\mathbb{R}^2_\theta, C^\infty(\mathbb{R}^2/\Gamma_x)).$$

Then

$$D_{\theta_j}\widetilde{\mathcal{B}}u(\theta,x) = c_\Gamma \sum_{\gamma\in\Gamma} e^{i\langle x-\gamma,\theta\rangle}(x_j-\gamma_j)u(x-\gamma) = \widetilde{\mathcal{B}}[\bullet_j u](\theta,x),$$

and (8.21) and (8.22) follow. A density argument then gives the last conclusion. □

Let us assume that $\Gamma = \mathbb{Z}^2$ and that $c_1(L) \neq 0$. Then, using the results of §7.2 we choose $\varphi(\theta,x)$ such that

$$\varphi(\theta+p,x) = e_p(\theta)[\tau(p)\varphi](\theta,x), \quad p\in\mathbb{Z}^2, \quad e_{\mathbf{e}_1}(\theta)\neq 1, \quad e_{\mathbf{e}_2}(\theta) = 1. \tag{8.24}$$

Using Definition 8.6 we now formulate

Theorem 12. *Suppose that P is given by (8.8) and that for some k, (5.17) holds. Let L be the line bundle over $\mathbb{R}^2/\Gamma^*$ given by (8.9). Then the following are equivalent:*

(1) there exists a Wannier function satisfying $|\partial^\alpha \varphi_0(x)| \leq C_\alpha e^{-c|x|}$, $c > 0$;
(2) there exists a Wannier function satisfying $\int_{\mathbb{R}^2} |x|^2 |\varphi_0(x)|^2 dx < \infty$;
(3) $c_1(L) = 0$.

Remark 16. *A more general version of this result valid for multiple bands and dimension three was provided in [Mo*18]. It is also optimal as far as the exponent 2 in (2) is concerned. Localization of Wannier functions and its link to topology is related to interesting physical phenomena such as superconductivity – see [Va18].*

Remark 17. *We have shown that for line bundles over tori $c_1(L) = 0$ is equivalent to L being trivial (in fact, in full generality, $c_1(L)$ is the only topological invariant of a line bundle, see [BoTu82]). Hence, the theorem states that having a decaying Wannier function is equivalent to triviality of the line bundle of L, that is for having a smooth family $\mathbb{R}^2 \ni \theta \mapsto \varphi(\theta) \in C^\infty(\mathbb{R}^2/\Gamma)$, satisfying $\tau(p)\varphi(\theta) = \varphi(\theta+p)$, $\|\varphi(\theta)\|_{L^2(\mathbb{R}^2/\Gamma)} = 1$, $P(x, D_x - \theta)\varphi(\theta) = E_k(\theta)\varphi(\theta)$.*

Proof of Theorem 12. The implication (1) $\Rightarrow$ (2) is obvious. To see that (2) $\Rightarrow$ (3) we use (8.23) to see that $\varphi(\theta, x) := |\mathbb{R}^n/\Gamma^*|^{1/2} \widetilde{\mathcal{B}} \varphi_0 \in H^1_\tau$. But this means that $\theta \mapsto e^{-i\langle x,\theta\rangle}\varphi(\theta, x)$ form $\mathbb{R}/\Gamma^* \to \ker_{\mathcal{H}_\theta}(P - E_k(\theta)) \subset \mathcal{H}_\theta$ is an H^1 section satisfying $\|\varphi(\theta)\|_{L^2(\mathbb{R}^2/\Gamma)} = 1$. We then use the following lemma:

Lemma 8.8. *Let L be a smooth complex line bundle over $\mathbb{R}^2/\Gamma^*$, and there exists a unitary H^1 section $s : \mathbb{R}^2/\Gamma^* \to L$, then L is trivial.*

Proof. Let $1 = \sum_j \chi_j$ be a partition of unity on $\mathbb{R}^2/\Gamma^*$ such that $\operatorname{supp} \chi_j \subset U_j$ and L is trivial over U_j (see Definition 7.1). We then choose $\varphi_j : \pi^{-1}(U_j) \to U_j \times \mathbb{C}$ be a trivialization. Let $\psi \in C^\infty_{\rm c}(B(0,1); \mathbb{R})$ with $\int \psi(x)dx = 1$ and put $\psi_\varepsilon(x) = \varepsilon^{-2}\psi(x/\varepsilon)$. Then

$$s_\varepsilon := \sum_j \varphi_j^* (\psi_\varepsilon * s_j) \in C^\infty(\mathbb{R}^2/\Gamma^*; L), \quad s_j := \varphi_{j*}(\chi_j s), \quad \|s_\varepsilon - s\|_{H^1} \to 0, \ \varepsilon \to 0.$$

We now denote by $|v|$ the Hermitian length of $v \in L$ defined using the L^2 norm (see §8.3) and introduce a distance function, $d : L \times L \to [0, \infty)$, on L (for instance by introducing a Riemannian metric). We can now estimate the distance between $s_\varepsilon(x) \in L$ and the compact subset $\{v \in L : |v| = 1\}$ of L:

$$\begin{aligned} d(s_\varepsilon(x), \{v \in L : |v| = 1\})^2 &\leq \min_{|x-y|<\varepsilon} d(s_\varepsilon(x), s(y))^2 \leq C\varepsilon^{-2} \int_{|x-y|<\varepsilon} d(s_\varepsilon(x), s(y))^2 dy \\ &\leq C \sum_j \varepsilon^{-2} \int_{|x-y|<\varepsilon} \left(|\psi_\varepsilon * s_j(x) - s_j(y)|^2 + |x-y|^2 \right) dy, \end{aligned} \tag{8.25}$$

where the $\mathcal{O}(|x-y|^2)$ term came from the change of the Hermitian metric on different fibers. Its overall contribution after integration is $\mathcal{O}(\varepsilon^2)$.

To estimate the first term, we recall the Poincaré inequality (see for instance [Ev10, §5.8.1])

$$\varepsilon^{-2}\int_{|x-y|<\varepsilon} |[s_j]_{x,\varepsilon} - s_j(y)|^2\, dy \le C \int_{|x-y|<\varepsilon} |\nabla s_j(y)|^2 dy,$$

where

$$[s_j]_{x,\varepsilon} := \frac{1}{\pi\varepsilon^2}\int_{|x-y'|<\varepsilon} s_j(y')dy'$$

is the average of s_j over the disc $B(x,\varepsilon)$. We also note that by the Cauchy–Schwarz inequality and properties by ψ_ε we have

$$\begin{aligned} |\psi_\varepsilon * (s_j - [s_j]_{x,\varepsilon})(x)|^2 &= \left|\int_{|x-y|<\varepsilon} \psi_\varepsilon(x-y)(s_j(y) - [s_j]_{x,\varepsilon})dy\right|^2 \\ &\le C\varepsilon^{-2}\int_{|x-y|<\varepsilon} |s_j(y) - [s_j]_{x,\varepsilon}|^2 dy. \end{aligned} \tag{8.26}$$

Thus,

$$\begin{aligned} &\varepsilon^{-2}\int_{|x-y|<\varepsilon} |\psi_\varepsilon * s_j(x) - s_j(y)|^2 dy \\ &\qquad = \varepsilon^{-2}\int_{|x-y|<\varepsilon} |\psi_\varepsilon * (s_j - [s_j]_{x,\varepsilon})(x) - (s_j(y) - [s_j]_{x,\varepsilon})|^2 dy \\ &\qquad \le C_1|\psi_\varepsilon * (s_j - [s_j]_{x,\varepsilon})(x)|^2 + 2\varepsilon^{-2}\int_{|x-y|<\varepsilon} |s_j(y)[s_j]_{x,\varepsilon}|^2 dy \\ &\qquad \le C_2\varepsilon^{-2}\int_{|x-y|<\varepsilon} |s_j(y) - [s_j]_{x,\varepsilon}|^2 dy \\ &\qquad \le C_3\int_{|x-y|<\varepsilon} |\nabla s_j(y)|^2 dy \to 0, \quad \varepsilon \to 0, \end{aligned}$$

where we used (8.26) to obtain the penultimate inequality.

Returning to (8.25), we have shown that $d(s_\varepsilon(x), \{v \in L : |v| = 1\}) \to 0$ as $\varepsilon \to 0$, and hence s_ε is a smooth, nonvanishing section of L. Thus L must be trivial. □

It remains to show that (3) ⇒ (1). From Proposition 7.10 we see that the line bundle L is trivial. That implies existence of a C^∞ non-vanishing section, that is of a smooth map $\theta \mapsto \varphi(\theta, x)$, $\|\varphi(\theta)\|_{L^2(\mathbb{R}^2/\Gamma)} = 1$ (see above). But then the regularization procedure in the proof of Theorem 6 gives us a real analytic section $\tilde\varphi(\theta)$. (The only modification needed is in the normalization where we need to divide by the square root of $\langle \varphi_0(\theta), \varphi_0(\bar\theta)\rangle_{L^2(\mathbb{R}^2/\Gamma)}$ to guarantee holomorphy.) Exponentially decaying Wannier function is then obtained as in Proposition 5.20. □

9. Two examples of topology in band theory

Here we present two cases of non-trivial line bundles arising in condensed matter physics. The first one is motivated by the work of Thouless [Th83] and has physical implications which we do not discuss but provide references for. The second comes from considering 2D Landau Hamiltonians of §3 with rational magnetic fluxes. It turns out that in that case one can use *magnetic translations* to develop an analogue of Bloch–Floquet theory and that leads to non-trivial topology.

9.1. **Thouless pumping.** Suppose that $P := D_x^2 + V(x)$ where $V(x+2\pi) = V(x)$, $V \in C^\infty(\mathbb{R};\mathbb{R})$ (regularity is irrelevant here and could for instance consider the Kronig–Penney model of Example 11). Following §5.4 we have

$$\operatorname{Spec}(P) = \bigcup_{j=1}^{\infty} I_j, \quad I_j := \{E_j(\theta) : \theta \in \mathbb{R}/\mathbb{Z}\}.$$

Suppose that $E(\theta) = E_k(\theta)$ and (5.17) holds, that is the band I_k is isolated. It follows from Theorem 6 that there exists $u(\theta, x) \in C^\infty(\mathbb{R} \times \mathbb{R})$ satisfying

$$((D_x - \theta)^2 + V(x))u(\theta, x) = E(\theta)u(\theta, x), \quad u(\theta + p, x + 2\pi\ell) = e^{ipx}u(\theta, x), \quad p, \ell \in \mathbb{Z}.$$

(We have $u(\theta, x) = e^{ix\theta}\varphi(\theta, x)$, where φ is the (normalized) Bloch eigenfunction of Theorem 6.) We then consider the periodic family of operators

$$P(\lambda) := D_x^2 + V(x - \lambda), \quad P(\theta, \lambda) := (D_x - \theta)^2 + V(x - \lambda).$$

The eigenfunction corresponding to $E(\theta)$ is given by $u(\theta, \lambda)(x) = u(\theta, x - \lambda)$ and

$$u(\theta + p, x + 2\pi\ell) = e^{-i\lambda p}\tau(p)u(\theta, \lambda), \quad [\tau(p)v](x) := e^{ixp}v(x). \tag{9.1}$$

As in §8.3, we consider the following natural line bundle defined in a way similar to (8.9):

$$\begin{gathered} L_{\mathrm{T}} := \left\{ (\lambda, [\theta, v]) \in \mathbb{R} \times (\mathbb{R} \times L^2(\mathbb{R}/\mathbb{Z}))/\sim : \ v \in \ker_{L^2(\mathbb{R}/\mathbb{Z})}(P(\theta, \lambda) - E_k(\theta)) \right\}, \\ [\theta, v] = [\theta', v'] \iff (\theta, v) \sim (\theta', v') \iff \exists\, p \in \mathbb{Z} \ \ \theta' = \theta + p, \ \ v' = \tau(p)v. \end{gathered} \tag{9.2}$$

We define the connection using the Hermitian structure inherited from $L^2(\mathbb{R}/2\pi\mathbb{Z})$ – see (7.4): for $(\theta, \lambda) \in (0,1) \times (0, 2\pi)$, using the frame $s(\theta, \lambda) = ((\theta, \lambda), f(\theta, \lambda)u(\theta, \lambda))$,

$$Ds(\theta, \lambda) = ((\theta, \lambda), (d_{\theta,\lambda} f + \langle d_{\theta,\lambda} u, u \rangle f)u(\theta, \lambda)).$$

The curvature is then given by

$$\begin{aligned} \Theta &= \partial_\lambda \langle u_\theta, u \rangle d\lambda \wedge d\theta + \partial_\theta \langle u_\lambda, u \rangle d\theta \wedge d\lambda \\ &= (\langle u_\lambda, u_\theta \rangle - \langle u_\theta, u_\lambda \rangle) d\theta \wedge d\lambda = 2i \operatorname{Im}\langle u_\lambda, u_\theta \rangle d\theta \wedge d\lambda \end{aligned} \tag{9.3}$$

The Chern number is given as in (8.14) but with $\theta_1 = \lambda$ and $\theta_2 = \theta$. Since

$$\partial_\lambda u(\theta, x - \lambda) = -\partial_x u(\theta, x - \lambda)$$

and u is periodic in x, we get

$$\begin{aligned} c_1(L_{\mathrm{T}}) &= \frac{i}{2\pi}\int_{[0,1]\times[0,2\pi]} \Theta \\ &= -\frac{1}{\pi}\int_0^1 \int_0^{2\pi} \left(\int_0^{2\pi} \operatorname{Im}\left(\partial_x u(\theta, x-\lambda)\overline{\partial_\theta u(\theta, x-\lambda)}\right) dx \right) d\lambda d\theta \\ &= -2\int_0^{2\pi}\int_0^1 \operatorname{Im}\left(\partial_x u(\theta,x)\overline{\partial_\theta u(\theta,x)}\right) dx d\theta. \end{aligned} \tag{9.4}$$

We now observe (see (9.3)) that

$$-2\operatorname{Im}(\partial_x u(\theta,x)\overline{\partial_\theta u(\theta,x)})d\theta\wedge dx = id(u_\theta \bar{u} d\theta + u_x \bar{u} dx),$$

so that the Stokes theorem gives

$$c_1(L_T) = i\int_0^1 ([u_\theta\bar{u}](\theta,0) - [u_\theta \bar{u}](\theta,2\pi))d\theta + i\int_0^{2\pi} ([u_x\bar{u}](1,x) - [u_x\bar{u}](0,x))dx.$$

We now use (9.1) to see that

$$u(\theta, 2\pi) = u(\theta, 0), \quad u(1,x) = e^{ix}u(0,x).$$

This gives

$$[u_\theta\bar{u}](\theta,0) - [u_\theta\bar{u}](\theta,2\pi) = 0, \quad [u_x\bar{u}](1,x) - [u_x\bar{u}](0,x)] = i|u(0,x)|^2.$$

Since $\int_0^{2\pi}|u(0,x)|^2dx = 1$ (u is normalied in L^2) we conclude that

$$c_1(L_T) = -1. \tag{9.5}$$

In particular the line bundle L_T is nontrivial.

Remark 18. *We could also evaluate $c_1(L_T)$ using multpliers* (7.7) *as in* (7.10)*. From* (9.1) *we get that $e_{(k,2\pi\ell)}(\theta,\lambda) = e^{ip\lambda}$ and that give* (9.5).

For physical aspects of this example, involving the concept of *polarization* and *Thouless pumping*, see [MoMo18, §4.1] and [Va18, §1.1.2]. For a youtube presentation see `https://topocondmat.org/w3_pump_QHE/pumps.html` (thanks to Zhen Huang for this suggestion).

Mathematical treatment of the more subtle case of $D_x^2+W(x)+V(x-\lambda)$, $W(x+2\pi) = W(x)$, was recently given in [Dr21]. An argument similar to the one presented here appeared in [Go20] (thanks to Alexis Drouot for these references). Those results were motivated by the study of spectral flows rather than by Thouless pumping.

9.2. **Landau levels revisited.** We now return to §3.4 and consider the two dimensional Landau Hamiltonian in the symmetric gauge and recall that with $w = x_1 + ix_2$,

$$P_B = A_B^* A_B + B, \qquad A_B := e^{-B|w|^2/4}(2D_{\bar{w}})e^{B|w|^2/4} = 2D_{\bar{w}} - \tfrac{1}{2}iBw. \tag{9.6}$$

The infinitely degenerate ground states are given by

$$u(w,\bar{w}) = f(w)e^{-\frac{B|w|^2}{4}}, \quad f \in \mathscr{O}(\mathbb{C}), \quad \int |f(w)|^2 e^{-\frac{B|w|^2}{2}} dm(w) < \infty. \tag{9.7}$$

To describe this space using Bloch–Floquet theory we need operators which commute with P_B and replace $\gamma \mapsto u(x-\gamma)$, $\gamma \in \Gamma$.

Definition 9.1. *Let* Γ *be a lattice in* $\mathbb{C}$*. For magnetic field* B *and* $\gamma \in \Gamma$ *a* magnetic translation *by* γ *is defined on* $L^2(\mathbb{C}, dm(w))$ *as*

$$T_\gamma^B u(w) = e^{\frac{1}{4}B(w\bar{\gamma} - \bar{w}\gamma)} u(w-\gamma). \tag{9.8}$$

We immediately check that

$$A_B T_\gamma^B = T_\gamma^B A_B, \quad (T_\gamma^B)^* = T_{-\gamma}^B, \quad T_\gamma^B T_{\gamma'}^B = e^{\frac{1}{2}B(\gamma'\bar{\gamma} - \bar{\gamma}'\gamma)} T_{\gamma'}^B T_\gamma^B, \tag{9.9}$$

and

$$P_B T_\gamma^B = T_\gamma^B P_B, \quad \gamma \in \Gamma. \tag{9.10}$$

Remark 19. *This definition, due to Zak (see* [HS89] *and references given there), can be generalized to all dimensions so that* (9.10) *holds. We restrict ourselves to* $\mathbb{R}^2 \simeq \mathbb{C}$ *to keep the presentation simple.*

The problem with a generalization of Bloch–Floquet theory is that the magnetic translations do *not* commute – see (9.9). However if

$$\tfrac{1}{2}B(\gamma'\bar{\gamma} - \bar{\gamma}'\gamma) \in 2\pi i\mathbb{Z}, \quad \gamma, \gamma' \in \Gamma, \tag{9.11}$$

then $T_\gamma^B T_{\gamma'}^B = T_{\gamma'}^B T_\gamma^B$ and we can define

$$\mathscr{H}_{\mathbf{k}}^B := \{u \in L^2_{\mathrm{loc}}(\mathbb{C}) : \ \forall\, \gamma \in \Gamma \ T_\gamma^B u = e^{\frac{i}{2}(\bar{\mathbf{k}}\gamma + \mathbf{k}\bar{\gamma})} u\}, \quad \mathbf{k} \in \mathbb{C}.$$

The point is that $\{T_\gamma^B\}_{\gamma\in\Gamma}$ is an abelian group on two generators and it irreducible representations are one dimensional and are given by

$$\gamma \mapsto \pi_{\mathbf{k}}(\gamma) : \mathbb{C} \to \mathbb{C}, \quad \pi_{\mathbf{k}}(\gamma) z = e^{\frac{i}{2}(\mathbf{k}\bar{\gamma} + \bar{\mathbf{k}}\gamma)} z, \quad \mathbf{k} \in \mathbb{C}/\Gamma^*.$$

For $u \in \mathscr{S}(\mathbb{C})$, the magnetic Bloch transform is given by,

$$\mathcal{B}^B u(\mathbf{k}, x) := \frac{1}{|\mathbb{C}/\Gamma^*|^{\frac{1}{2}}} \sum_\gamma e^{-\frac{i}{2}(\bar{\mathbf{k}}\gamma + \mathbf{k}\bar{\gamma})} T_\gamma^B u(x) \in L^2(\mathbb{C}/\Gamma^*; \mathscr{H}_{\mathbf{k}}^B). \tag{9.12}$$

It extends to a unitary operators as for $u \in \mathscr{S}(\mathbb{C})$ we have

$$\begin{aligned}
&\sum_{\gamma\in\Gamma}\sum_{\gamma'\in\Gamma}\int_{\mathbb{C}/\Gamma}\frac{1}{|\mathbb{C}/\Gamma^*|}\left(\int_{\mathbb{C}/\Gamma^*} e^{-\frac{i}{2}(\bar{\mathbf{k}}(\gamma-\gamma')+\mathbf{k}(\bar\gamma-\bar\gamma')}dm(\mathbf{k})\right)e^{\frac14(w(\bar\gamma-\bar\gamma')-\bar w(\gamma-\gamma'))}\times \\
&\qquad\qquad u(w-\gamma)\overline{u(w-\gamma')}dm(w) \\
&\quad = \sum_{\gamma\in\Gamma}\sum_{\gamma'\in\Gamma}\int_{\mathbb{C}/\Gamma}\delta_{\gamma\gamma'}e^{\frac14(w(\bar\gamma-\bar\gamma')-\bar w(\gamma-\gamma'))}u(w-\gamma)\overline{u(w-\gamma')}dm(w) \\
&\quad = \int_{\mathbb{C}}|u(w)|^2 dm(w).
\end{aligned}$$

As is easily seen from (9.12), the inverse of $\mathcal{B}^B$ is given by

$$\mathcal{C}^B v(x) := \frac{1}{|\mathbb{C}/\Gamma^*|^{1/2}}\int_{\mathbb{C}/\Gamma^*} v(\mathbf{k},x)dm(\mathbf{k}).$$

(See also the proof of Theorem 4.) Hence, as in §5.4,

$$\mathcal{B}^B P_B \mathcal{C}^B v(\mathbf{k},x) = [P_B v(\mathbf{k},\bullet)](x),$$

We are interested in the space corresponding to the ground state:

$$V_{\mathbf{k}}^B := \ker_{\mathscr{H}_{\mathbf{k}}^B}(P_B - B) = \ker_{\mathscr{H}_{\mathbf{k}}^B} A_B. \tag{9.13}$$

It is convenient now to specialize to specific lattices of the form

$$\Gamma = \mathbb{Z}\oplus\tau\mathbb{Z}, \quad \operatorname{Im}\tau > 0, \quad \Gamma^* = \frac{2\pi i}{\operatorname{Im}\tau}\Gamma.$$

(A general lattice is given by $\omega_1\mathbb{Z}\oplus\omega_2\mathbb{Z} = \omega_1(\mathbb{Z}\oplus(\pm\omega_2/\omega_1)\mathbb{Z})$ and we can arrange the sign of $\operatorname{Im}\tau$, $\tau = \omega_2/\omega_1$). The condition (9.11) becomes

$$N_B := \frac{B}{2\pi}\operatorname{Im}\tau \in \mathbb{Z}. \tag{9.14}$$

Theorem 13. *Suppose that (9.14) holds. Then the vector subspace of $\mathscr{H}_{\mathbf{k}}^B$ corresponding to the ground state of B (see (9.13)) is finite dimensional and*

$$\dim\ker_{\mathscr{H}_{\mathbf{k}}^B}(P_B - B) = N_B.$$

Proof. In (9.7) it is convenient to write $f(w) = g(w)\exp(Bw^2/4)$, so that for $u \in \mathscr{H}_{\mathbf{k}}^B$,

$$\begin{aligned}
T_1^B u(w) &= e^{\frac{i}{2}B\operatorname{Im}w}u(w-1) = e^{\frac{i}{2}B\operatorname{Im}w}e^{-\frac14 B(w-1)(\bar w-1)}e^{\frac14 B(w-1)^2}g(w-1) \\
&= e^{\frac{i}{2}B\operatorname{Im}w}e^{\frac14 B(-1+(w+\bar w))}e^{\frac14 B(1-2w)}e^{-\frac14 B|w|^2+\frac14 Bw^2}g(w-1) \\
&= e^{-\frac14 B|w|^2+\frac14 Bw^2}g(w-1).
\end{aligned}$$

Since $T_1^B u = e^{i\operatorname{Re}\mathbf{k}}u = e^{i\operatorname{Re}\mathbf{k}}e^{-\frac14 B|w|^2+\frac14 Bw^2}g(w)$, we conclude that

$$g(w-1) = e^{i\operatorname{Re}\mathbf{k}}g(w). \tag{9.15}$$

Similarly,

$$\begin{aligned} T^B_\tau u(w) &= e^{\frac{i}{2}B\operatorname{Im}(w\bar\tau)}u(w-\tau) = e^{\frac{i}{2}B\operatorname{Im}(\bar\tau w)}e^{-\frac14 B(w-\tau)(\bar w-\bar\tau)}e^{\frac14 B(w-\tau)^2}g(w-\tau) \\ &= e^{\frac{i}{2}B\operatorname{Im}(w\bar\tau)}e^{\frac14 B(-|\tau|^2+(\bar\tau w+\tau\bar w)}e^{\frac14 B(\tau^2-2\tau w)}e^{-\frac14 B|w|^2+\frac14 Bw^2}g(w-\tau) \\ &= e^{\frac{i}{2}B\operatorname{Im}\tau(\tau-2w)}e^{-\frac14 B|w|^2+\frac14 Bw^2}g(w-\tau). \end{aligned}$$

Again, $T^B_\tau u(w) = e^{\frac{i}{2}(\bar{\mathbf{k}}\tau+\mathbf{k}\bar\tau)}u(w)$, we obtain

$$g(w-\tau) = e^{\frac{i}{2}(\bar{\mathbf{k}}\tau+\mathbf{k}\bar\tau)-\frac{i}{2}B\operatorname{Im}\tau(\tau-2w)}g(w) = e^{\frac{i}{2}(\bar{\mathbf{k}}\tau+\mathbf{k}\bar\tau)-i\pi N_B(\tau-2w)}g(w) \tag{9.16}$$

This means that we can consider g as a section of a holomorphic line bundle over $\mathbb{C}/\Gamma$. Proposition 7.12 tells us holomorphic sections form a vector space of dimension N_B.

One can also see the dimension from Riemann–Roch theorem. Residue theorem shows that the number of zeros of g is given by N_B and the theorem follows from the Riemann–Roch theorem: suppose g_1 and g_2 satisfy (9.15) and (9.16). Then $g_1(w)/g_2(w)$ is a meromorphic function on $\mathbb{C}/\Gamma$ with at most N_B poles at locations (counted with multiplicities) of the zeros N_B. But that space has dimension N_B. $\square$

Suppose $N_B = 1$. In that case we obtain a vector bundle over $\mathbb{C}/\Gamma^*$. To set it up we take the map

$$\begin{gathered} \tau_{\mathbf{k}} : \mathscr{H}^B_{\mathbf{k}} \to \mathscr{H}^B_{\mathbf{0}}, \quad u(w) \longmapsto \tau_{\mathbf{k}}u(w) := e^{\frac{i}{2}(\bar w\mathbf{k}+w\bar{\mathbf{k}})}u(w), \\ \tau_{\mathbf{k}}P_B\tau^*_{\mathbf{k}} = P_B(\mathbf{k}) := (A_B-\mathbf{k})^*(A_B-\mathbf{k})+B. \end{gathered} \tag{9.17}$$

We also note that for $\mathbf{p}\in\Gamma^*$, we have a unitary map

$$\tau_{\mathbf{p}} : \mathscr{H}^B_{\mathbf{0}} \to \mathscr{H}^B_{\mathbf{0}}, \quad \tau^*_{\mathbf{p}}P_B(\mathbf{k})\tau_{\mathbf{p}} = P_B(\mathbf{k}+\mathbf{p}). \tag{9.18}$$

As in §8.3 this leads to a definition of a natural line bundle over $\mathbb{C}/\Gamma^*$:

$$\begin{gathered} L_B := \left\{[\mathbf{k},v]\in(\mathbb{C}\times\mathscr{H}^B_{\mathbf{0}})/\sim:\ v\in\ker_{\mathscr{H}^B_{\mathbf{0}}}(P_B(\mathbf{k})-B)\right\}, \\ [\mathbf{k},v]=[\mathbf{k}',v'] \iff (\mathbf{k},v)\sim(\mathbf{k}',v') \iff \exists\,\mathbf{p}\in\Gamma^*,\ \mathbf{k}'=\mathbf{k}+\mathbf{p},\quad v'=\tau_{\mathbf{p}}v, \end{gathered} \tag{9.19}$$

Remark 20. *Under an assumption stronger than (9.11) (or equivalently (9.14)),*

$$\tfrac12\operatorname{Im}B(\gamma_1\bar\gamma_2)\in 2\pi\mathbb{Z},\quad \gamma_j\in\Gamma, \tag{9.20}$$

we can identify $\mathscr{H}^B_{\mathbf{0}}$ with L^2-sections of a line bundle over $\mathbb{C}/\Gamma$:

$$\mathscr{H}^B_{\mathbf{0}} \simeq L^2(\mathbb{C}/\Gamma; E_B), \tag{9.21}$$

where $E_B\to\mathbb{C}/\Gamma$ is the line bundle defined using (7.6) with multipliers $e_\gamma(z) := e^{\frac{i}{2}B\operatorname{Im}(z\bar\gamma)}$. We first check that this function satisfies the cocycle condition (7.7):

$$e_{\gamma_1+\gamma_2}(z) = e^{\frac{i}{2}B\operatorname{Im}(z(\bar\gamma_1+\bar\gamma_2)} = e^{\frac{i}{2}B\operatorname{Im}((z+\gamma_2)\bar\gamma_1)}e^{\frac{i}{2}\operatorname{Im}(z\bar\gamma_2)}e^{-\frac{i}{2}B\operatorname{Im}(\gamma_2\bar\gamma_1)} = e_{\gamma_1}(z+\gamma_2)e_{\gamma_2}(z),$$

where the last equality comes from (9.20). Now, $u\in\mathscr{H}^B_{\mathbf{0}}$ means that (see (9.8)) $u(z+\gamma)=e_\gamma(z)u(z)$ which in view of (7.8) gives (9.21).

We have

Theorem 14. *Definition* (9.19) *gives a holomorphic line bundle with a hermitian metric defined by* $\|v\|^2_{\mathscr{H}^B_{\mathbf{0}}}$ *and the Chern number* $c_1(L_B) = -1$.

Proof. Let us consider the function g in the proof of Theorem 13 for $\mathbf{k} = 0$. It satisfies

$$g \in \mathscr{O}(\mathbb{C}), \quad g(z+1) = g(z), \quad g(z+\tau) = e^{-i\pi(2z+\tau)} g(z).$$

This means that up to a multiplicative constant

$$g(z) = \theta(z,\tau) := \sum_{n \in \mathbb{Z}} \exp(\pi i n^2 \tau + 2\pi i n z),$$

that is g is the theta function from Definition 7.11. (Uniqueness follows an argument similar to the proof of Proposition 7.12 – see [Mu83, §I.1]; we also comment that the zero of $g(z)$ in the fundamental domain spanned by 1 and τ is at $\frac{1}{2}(\tau+1)$ – see [Mu83, I, Lemma 4.1].)

We now define

$$F_{\mathbf{k}}(z) := e^{-\frac{i}{2}(z-\bar{z})\mathbf{k}} \frac{\theta(z - i\mathbf{k}/B, \tau)}{\theta(z,\tau)},$$

so that

$$F_{\mathbf{k}}(z+1) = F_{\mathbf{k}}(z), \quad F_{\mathbf{k}}(z+\tau) = e^{-\frac{i}{2}(\tau-\bar{\tau})\mathbf{k}} e^{-2\pi\mathbf{k}/B} F_{\mathbf{k}}(z) = e^{(\operatorname{Im}\tau - 2\pi/B)\mathbf{k}} F_{\mathbf{k}}(z) = F_{\mathbf{k}}(z).$$

where we used (9.14) with $N_B = 1$. Let $u \in \ker_{\mathscr{H}^B_{\mathbf{0}}}(A_B)$, $u(z) = e^{-\frac{1}{4}B|z|^2} e^{\frac{1}{4}Bz^2} g(z)$. Then

$$u(\mathbf{k},z) := F_{\mathbf{k}}(z)u(z) \in \ker_{\mathscr{H}^B_{\mathbf{0}}}(A_B - \mathbf{k}), \quad u(\mathbf{k}+\mathbf{p},z) = e_{\mathbf{p}}(\mathbf{k})^{-1} \tau_{\mathbf{p}} u(\mathbf{k},z), \tag{9.22}$$

where $\tau_{\mathbf{p}}$ was defined in (9.17) and for $\mathbf{p} = iB(n+m\tau)$,

$$e_{\mathbf{p}}(\mathbf{k}) := e^{\pi i m^2 \tau + 2\pi m \mathbf{k}/B} \tag{9.23}$$

and we check that this a multiplier, that is, it satisfies (7.7).

The action of Γ^*, $\mathbf{p} : (\mathbf{k}, v) \mapsto (\mathbf{k}+\mathbf{p}, \tau_{\mathbf{p}} v)$ on the (trivial) complex line bundle

$$\widetilde{L} := \{(\mathbf{k}, \tau u(\mathbf{k})) : \mathbf{k} \in \mathbb{C}, \quad \tau \in \mathbb{C}\} \simeq \mathbb{C}_{\mathbf{k}} \times \mathbb{C}_{\tau}, \tag{9.24}$$

is free and proper, and the quotient map is given by $\pi_\tau(k, \tau u(k)) = [k, \tau u(k)]$. Hence its quotient by that action, L, is a smooth complex manifold of dimension 2. We then define the action of Γ^* on $\widetilde{L}$ as in (7.6):

$$\mathbf{p} \cdot (\mathbf{k}, \kappa u(\mathbf{k})) = (\mathbf{k}+\mathbf{p}, e_{\mathbf{p}}(\mathbf{k}) \kappa u(\mathbf{k}+\mathbf{p})), \quad \mathbf{p} \in \Gamma^*,$$

so that

$$\pi_\tau(\mathbf{k}, \kappa u(\mathbf{k})) = \pi_\tau(\mathbf{k}+\mathbf{p}, e_{\mathbf{p}}(\mathbf{k}) \kappa u(\mathbf{k}+\mathbf{p})).$$

This gives L the structure of a complex line bundle over $\mathbb{C}/\Gamma^*$.

The hermitian structure is inherited from $L^2(\mathbb{C}/\Gamma)$ and the resulting hermitian structure on $\widetilde{L}$ of (9.24). In coordinates (k,τ) on $\widetilde{L}$, we get

$$h(\mathbf{k}) = \|u(\mathbf{k})\|^2_{\mathscr{H}_{\mathbf{0}}^B},$$

This gives us also a hermitian structure on L: from (9.22) we see that

$$h(\mathbf{k}) = |e_{\mathbf{p}}(\mathbf{k})|^2 h(\mathbf{k}+\mathbf{p}), \quad \mathbf{p} \in \Gamma^*. \tag{9.25}$$

To h we associate the Chern connection (7.12) and the curvature Θ – see Proposition 7.4. Then we use (7.10):

$$c_1(L_B) = \frac{i}{2\pi}\int_{\mathbb{C}/\Gamma^*} \Omega = -1, \tag{9.26}$$

completing the proof. $\square$

Remark 21. *Another way to compute the Chern number is to use* (7.10)*:*

$$c_1(L_B) = \frac{i}{2\pi}\left(\log e_{iB\tau}(iB) - \log e_{iB\tau}(0) - \log e_{iB}(iB\tau) + \log e_{iB}(0)\right) = \frac{i(iB)}{B} = -1.$$

Remark 22. *Since* $\ker_{L^2(\mathbb{C}/\Gamma)}(P_B(\mathbf{k}) - B)$ *is one dimensional we can always choose a holomorphic gauge:*

$$0 = D_{\bar{\mathbf{k}}}[(A_B - \mathbf{k})v(\mathbf{k})] = (A_B - \mathbf{k})[D_{\bar{\mathbf{k}}}v(\mathbf{k})] \implies D_{\bar{\mathbf{k}}}v(\mathbf{k}) = a(\mathbf{k})v(\mathbf{k}),$$

and a *can be replaced by* 0 *by choosing changing* v *to* $v_1 := e^{-ia(\mathbf{k})\bar{w}/2}v$.

10. 2D periodic structures in constant magnetic field: effective Hamiltonians

We now study the case with a smooth periodic potential $V(x) \in C^\infty(\mathbb{R}^2)$ and $V(x+\gamma) = V(x)$ for any $\gamma \in \Gamma$. Let

$$\begin{gathered} P_{B,0} := \sum_{j=1}^{2}(D_{x_j} + A_j(x))^2, \quad A(x) = (-Bx_2/2, Bx_1/2), \quad D_{x_j} = \frac{1}{i}\partial_{x_j}, \\ P_B = P_{B,V} = P_{B,0} + V. \end{gathered} \tag{10.1}$$

We will use our knowledge of the cases $B = 0$ and $V = 0$ and our goal is to consider the problem perturbatively as $B \to 0$. The perturbation is very singular but a careful study of the case $B = 0$ combined with the magnetic translations will provide a needed framework. We follow the proof given by Helffer–Sjöstrand [HS89]. For a presentation of more general perturbations of periodic structures and references, see [DS99, Chapter 12] and [Te03].

We consider the simplest case of an isolated band, that is we assume that (5.17) and we are interested in the spectrum of P_B for small B.

The basic result is a mathematical version is the construction of an effective Hamiltonian: there exists a family of function on $\mathbb{R}^2/\Gamma^*$, depending holomorphically on z and smoothly on B,

$$\mathbb{R}^2/\Gamma^* \ni (x,\xi) \mapsto b(z,x,\xi,B) = b_0(z,x,\xi) + Bb_1(z,x,\xi) + \mathcal{O}(B^2)$$

such that for λ near $I_k = \{E_k(\theta) : \theta \in \mathbb{R}^2/\Gamma^*\}$,

$$\lambda \in \mathrm{Spec}_{L^2(\mathbb{R}^2)}(P_B) \iff 0 \in \mathrm{Spec}_{L^2(\mathbb{R})}(b^{\mathrm{w}}(\lambda, x, BD_x, B)).$$

Here $b^{\mathrm{w}}(\lambda, x, BD_x, B)$ is the Weyl quantization of the periodic function $b \in S(\mathbb{R}^2)$, see (10.23). The linear eigenvalue problem for P_B is replaced by a lower dimensional nonlinear eigenvalue problem. Also, the operator $b^{\mathrm{w}}(z, x, BD_x, B)$ can be used to understand the density of states – see §11.

We have

$$b_0(z,x,\xi) = z - E_k(x,\xi), \tag{10.2}$$

and that is known as the *Peierls substitution*. This shows that the first approximation of the spectrum is given by the spectrum of $E_k(x, BD_x)$ on $L^2(\mathbb{R})$ (see the discussion of the Harper operator in §10.6). The first correction term is given in (10.28). On the "energy surface" $b_0(z,x,\xi,B) = z - E_k(x,\xi) = 0$ (which is most relevant to correction terms in Bohr–Sommerfeld rules for z) we have (see (10.30) for a derivation)

$$\begin{aligned} \tilde{b}_1(x,\xi) &:= b_1(x,\xi,z)|_{b_0(z,x,\xi)=0} \\ &= -\tfrac{i}{2}\int_{\mathbb{R}^2/\Gamma} (P(\tau) - E_k(\tau))\nabla_\tau u(\tau,y) \wedge \nabla_\tau \overline{u(\tau,y)} dy, \quad \tau = (x,\xi), \end{aligned} \tag{10.3}$$

which is a formula appearing in the physics literature – see for instance [Fu*10, equation (10)].

10.1. **Periodic potentials revisited.** In order to consider magnetic field as a perturbation we analyze a Grushin problem $P := -\Delta + V$ under the isolated band assumption (5.17). Theorem 12 then shows that the topology of the band is trivial. In particular, we have exponentially decaying Wannier functions $\varphi_\alpha(x) = \varphi_0(x-\alpha)$ such that $|\varphi_0(x)| \le Ce^{-|x|/C}$ for some $C > 0$.

Proposition 10.1. *With the notation introduced above, let*

$$\mathcal{P}(z) = \begin{pmatrix} P - z & R_- \\ R_+ & 0 \end{pmatrix} : H^2(\mathbb{R}^2) \times l^2(\Gamma) \to L^2(\mathbb{R}^2) \times l^2(\Gamma)$$

where $R_-u_- := \sum_{\alpha\in\Gamma} u_-(\alpha)\varphi_\alpha(x)$ *and* $R_+u(\alpha) = \langle u, \varphi_\alpha\rangle$. *Then for* $z \in \mathrm{nbhd}_{\mathbb{C}}(I_k)$, $\mathcal{P}(x)$ *is invertibile with*

$$\begin{aligned} \mathcal{P}(z)^{-1} = \mathcal{E}(z) &:= \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix}, \\ E_{-+}(z)f(\alpha) &= zf(\alpha) - \sum_\gamma \widehat{E}(\alpha-\gamma)f(\gamma). \end{aligned} \tag{10.4}$$

where $\widehat{E}(\gamma) = |\mathbb{R}^2/\Gamma^*|^{-1}\int_{\mathbb{R}^2/\Gamma^*} e^{-i\gamma\cdot\theta}E(\theta)d\theta$.

Proof. Let $\Pi = \Pi_k = \mathbb{1}_{I_k}(P)$ be the spectral projection to the band I_k. One can verify directly that

$$E(z) = (I-\Pi)(P-z)^{-1}(I-\Pi), \quad E_-(z) = R_+, \quad E_+(z) = R_-$$

and $E_{-+}(z)$ given above solve the equation. □

Since the magnetic field introduces a very strong perturbation near infinite, we will need *weighted* estimates for $\mathcal{E}(z)$:

Proposition 10.2. *Let* $f \in C^2(\mathbb{R}^2;\mathbb{R})$ *and* $e^f(v,v_+) = (e^{f(x)}v(x), e^{f(\alpha)}v_+(\alpha))$. *If* $\|f'\|_\infty + \|f''\|_\infty$ *is sufficiently small, then* $e^f\mathcal{P}(z)e^{-f}$ *is invertible with bounded inverse*

$$\|e^f\mathcal{P}(z)^{-1}e^{-f}\|_{L^2\times l^2\to H^2\times l^2} \le C.$$

Proof. We estimate each term in

$$e^f\mathcal{P}(z)e^{-f} = \begin{pmatrix} e^f(P-z)e^{-f} & e^fR_-e^{-f} \\ e^fR_+e^{-f} & 0 \end{pmatrix}.$$

Notice $e^f(P-z)e^{-f} = \sum(D_{x_j} + i\partial_{x_j}f)^2 + V(x) - z$, we have

$$e^f(P-z)e^{-f} - (P-z) = i(\nabla f\cdot D_x + D_x\cdot\nabla f) - |\nabla f|^2.$$

This is small in $H^2 \to L^2$ norm once $\|f'\|_\infty + \|f''\|_\infty$ is small. The term on R_+ gives

$$e^fR_+e^{-f}u = e^{f(\alpha)}\langle e^{-f(x)}u(x), \varphi_\alpha(x)\rangle = \langle u, e^{f(\alpha)-f(x)}\varphi_\alpha(x)\rangle$$

and $(e^fR_+e^{-f} - R_+)u = \langle u, (e^{f(\alpha)-f(x)} - 1)\varphi_\alpha(x)\rangle$. So we can estimate

$$\begin{aligned} |(e^{f(\alpha)-f(x)} - 1)\varphi_\alpha(x)| &= \left|\int_0^1 (f(\alpha)-f(x))e^{t(f(\alpha)-f(x))}dt\right| |\varphi_\alpha(x)| \\ &\le C\|f'\|_\infty|\alpha-x|e^{\|f'\|_\infty|\alpha-x|}e^{-|x-\alpha|/C}. \end{aligned} \tag{10.5}$$

Now,

$$(e^fR_+e^{-f} - 1)u(\alpha) = \int_{\mathbb{R}^2} K(\alpha,x)u(x)dx, \quad K(\alpha,x) := (e^{f(\alpha)-f(x)} - 1)\varphi_\alpha(x),$$

and we showed in (10.5) that if $\|f'\|_\infty < 1/C$ is sufficiently small,

$$|K(\alpha,x)| \le Ce^{-c|x-\alpha|}, \quad c > 0.$$

Hence $e^f R_+ e^{-f} - R_+ : L^2 \to l^2$ is bounded with a small norm by Schur's inequality (see (2.9), (2.10)).

Similarly we also obtain the smallness of $\|e^f R_- e^{-f} - R_-\|_{l^2 \to L^2}$. Since $\mathcal{P}(z)$ is invertible and $e^f \mathcal{P}(z) e^{-f} - \mathcal{P}(z)$ has small norm as an operator $H^2 \times l^2 \to L^2 \times l^2$, we conclude $e^f \mathcal{P}(z) e^{-f}$ is invertible with a bounded inverse. $\square$

10.2. **Functional spaces associated to P_B.** The operator $P_{B,0}$ is essentially self-adjoint as was discussed in Example 5. The domain was given by

$$\mathcal{D}(P_{B,0}) = \{u \in L^2(\mathbb{R}) : P_{B,0} u \in L^2(\mathbb{R}^2)\},$$

where $P_{B,0}u$ was considered as an element of $\mathscr{S}'$ after distributional differentiation (2.4). It is convenient to give a different characterization of the domain using *magnetic Sobolev spaces* which we define as follows. For $\alpha \in \mathbb{N}^2$, we put

$$(D_x + A)^\alpha = (D_{x_1} - Bx_2/2)^{\alpha_1} (D_{x_2} + Bx_1/2)^{\alpha_2}.$$

(We note that the order matters but the commutator of $D_{x_1} - Bx_2/2$ and $D_{x_2} + Bx_1/2$ is given by multiplication by B.) With that notation we define

$$H^k_B(\mathbb{R}^n) = \{u \in L^2(\mathbb{R}^2) : (D_x + A)^\alpha u \in L^2(\mathbb{R}^2), \quad |\alpha| \le k\}, \quad k \in \mathbb{N},$$

where again the derivatives are taken in the sense of distributions. We note that $C^\infty_{\rm c}(\mathbb{R}^2)$ is dense in $H^k_B(\mathbb{R}^2)$.

To relate H^2_B to the domain of $P_{B,0}$ we have

Lemma 10.3. *There exist C_1 such that for $u \in C^\infty_{\rm c}(\mathbb{R}^2)$*

$$\|(D_x + A)^\alpha u\|_{L^2} \le C_1 (\|P_{B,0} u\|_{L^2} + \|u\|_{L^2}), \quad |\alpha| \le 2. \tag{10.6}$$

Proof. This is based on the observation that for $\xi_0 := A(x_0) := (-Bx_{0,2}/2, Bx_{0,1}/2)$ we have

$$e^{i\langle \xi_0, x\rangle} (D_x + A(x))^\alpha e^{-i\langle \xi_0, x\rangle} = (D_x + A(x - x_0))^\alpha = (D_y + A(y))^\alpha, \quad x = x_0 + y,$$

and $e^{i\langle \xi_0, x\rangle} P_{B,0}(x, D_x) e^{-i\langle \xi_0, x\rangle} = P_{B,0}(y, D_y)$.

Local elliptic estimates (see the proof of Lemma 5.2 or [Zw12, Theorem 7.1] for a detailed elementary presentation) then show that

$$\|(D_y + A(y))^\alpha v\|_{L^2(B(0,1))} \le C_0 (\|P_{B,0}(y, D_y) v\|_{L^2(B(0,2))} + \|v\|_{L^2(B(0,2))}), \quad |\alpha| \le 2.$$

Applying this to $v(y) = e^{i\langle \xi_0, x_0 + y\rangle} u(x_0 + y)$, gives

$$\|(D_x + A(x))^\alpha u\|_{L^2(B(x_0,1))} \le C_0 (\|P_{B,0} u\|_{L^2(B(x_0,2))} + \|u\|_{L^2(B(x_0,2))}), \tag{10.7}$$

where the constant is independent of x_0. We can now use a cover, say, $\mathbb{R}^2 = \bigcup_{p \in \frac14 \mathbb{Z}^2} B(p, 1)$, so that (10.7) applied with $x_0 = p$ and summed over $\frac14 \mathbb{Z}^2$ gives (10.6) with $C_1 = 64 C_0$. $\square$

If $u, P_{B,0} \in L^2$ then approximation by elements of C_c^∞ shows that (10.6) remains valid and that $\mathcal{D}(P_{B,0}) = H_B^2(\mathbb{R}^2)$. The estimate remains true when $P_{B,0}$ is replaced by $P_{B,V}$ and it can also be used to show that $P_{B,V}$ is essentially self-adjoint (apply the definitions from §2.3) with the same domain.

10.3. **Grushin problem for small constant magnetic fields.** In the notation of §10.2 we consider the following Grushin problem:

$$\mathcal{P}_B(z) = \begin{pmatrix} P_B - z & R_-^B \\ R_+^B & 0 \end{pmatrix} : H_B^2(\mathbb{R}^2) \times l^2(\Gamma) \to L^2(\mathbb{R}^2) \times l^2(\Gamma) \tag{10.8}$$

where

$$R_-^B u_-(x) := \sum_{\alpha \in \Gamma} u_-(\alpha) T_\alpha^B \varphi_0(x), \quad R_+^B u(\alpha) := \langle u, T_\alpha^B \varphi_0 \rangle,$$

The boundedness of

$$R_-^B : \ell^2(\Gamma) \to L^2(\mathbb{R}^2), \quad R_+^B : L^2(\mathbb{R}^2) \to \ell^2(\Gamma),$$

follows from the Schur criterion (2.10) and the exponential decay of $\varphi_0(x)$:

$$R_-^B u_-(x) = \sum_{\alpha \in \Gamma} K(x, \alpha) u_-(\alpha), \quad K(x, \alpha) := T_\alpha^B \varphi_0(x), \quad |K(x, \alpha)| \leq C e^{-c_0 |x - \alpha|},$$

with the similar statement for R_+^B.

We define

$$\tau_\gamma^B v(\alpha) := e^{\frac{1}{4} B(\alpha \bar{\gamma} - \bar{\alpha} \gamma)} v(\alpha - \gamma)$$

as the discrete analogue of (9.8) and

$$\mathcal{T}_\gamma^B := \begin{pmatrix} T_\gamma^B & 0 \\ 0 & \tau_\gamma^B \end{pmatrix},$$

then

$$\mathcal{T}_\gamma^B \mathcal{P}_B(z) = \mathcal{P}_B(z) \mathcal{T}_\gamma^B. \tag{10.9}$$

This means that the operator obtained from the Grushin problem commutes with the magnetic translation. We only need to check $T_\gamma^B R_+^B = R_+^B T_\gamma^B$ as the other one is dual to this one.

$$\begin{aligned}
\tau_\gamma^B R_+^B u(\alpha) &= e^{\frac{1}{4} B(\alpha \bar{\gamma} - \bar{\alpha} \gamma)} \langle u, \varphi_{\alpha - \gamma}(x) \rangle = e^{\frac{1}{4} B(\alpha \bar{\gamma} - \bar{\alpha} \gamma)} \langle u, e^{\frac{1}{4} B(x \overline{(\alpha - \gamma)} - \bar{x}(\alpha - \gamma))} \varphi_0(x - \alpha + \gamma) \rangle \\
&= \langle e^{\frac{1}{4} B(x \bar{\gamma} - \bar{x} \gamma)} u(x - \gamma), e^{\frac{1}{4} B(x \bar{\alpha} - \bar{x} \alpha)} \varphi_0(x - \alpha) \rangle \\
&= \langle T_\gamma^B u, \varphi_\alpha \rangle = R_+^B [T_\gamma^B u](\alpha).
\end{aligned}$$

We now show that our Grushin problem is well posed:

Theorem 15. *For $z \in \operatorname{nbhd}_{\mathbb{C}}(I_k)$ and $|B| \ll 1$, the operator*

$$\mathcal{P}_B(z) : H_B^2(\mathbb{R}^2) \times l^2(\Gamma) \to L^2(\mathbb{R}^2) \times l^2(\Gamma)$$

is invertible with uniformly bounded inverse.

Proof. We choose a partition of unity θ_γ such that

$$\sum_{\gamma\in\Gamma}\theta_\gamma(x)=1,\quad \theta_\gamma(x)=\theta_0(x-\gamma),\quad \theta_0(x)\in C_0^\infty(\mathbb{R}^2;[0,1]).$$

Let

$$\Theta_\gamma(x)=\begin{pmatrix}\theta_\gamma(x) & 0\\ 0 & \delta_\gamma\end{pmatrix} \tag{10.10}$$

and $\mathcal{E}_0(z)=\mathcal{P}_0(z)^{-1}$, we construct the approximate inverse $\mathcal{F}_B$ as

$$\mathcal{F}_B=\sum_{\gamma\in\Gamma}\mathcal{T}_\gamma^B\mathcal{E}_0\mathcal{T}_{-\gamma}^B\Theta_\gamma=\sum_{\gamma\in\Gamma}\mathcal{T}_\gamma^B\mathcal{E}_0\Theta_0\mathcal{T}_{-\gamma}^B.$$

We claim $\|\mathcal{F}_B\|_{L^2\times l^2\to H_B^2\times l^2}\le C<\infty$. We need to estimate

$$\begin{pmatrix}(D+A)^\alpha & 0\\ 0 & 1\end{pmatrix}\mathcal{F}_B=\sum_{\gamma\in\Gamma}\mathcal{T}_\gamma^B\begin{pmatrix}(D+A)^\alpha & 0\\ 0 & 1\end{pmatrix}\mathcal{E}_0\Theta_0\mathcal{T}_{-\gamma}^B.$$

Let $\eta>0$; denote

$$K=\begin{pmatrix}e^{\eta\langle\cdot\rangle} & 0\\ 0 & e^{\eta\langle\cdot\rangle}\end{pmatrix}\begin{pmatrix}(D+A)^\alpha & 0\\ 0 & 1\end{pmatrix}\mathcal{E}_0\Theta_0.$$

By weighted estimate (Proposition 10.2), $K:L^2\times l^2\to L^2\times l^2$ is bounded for η sufficiently small and $|\alpha|\le 2$. We now choose $\tilde\theta_0\in C_0^\infty(\mathbb{R}^2)$ so that the corresponding $\widetilde\Theta_0$ defined as in (10.10) satisfies $\widetilde\Theta_0\Theta_0=\Theta_0$. We then have

$$\begin{pmatrix}(D+A)^\alpha & 0\\ 0 & 1\end{pmatrix}\mathcal{F}_B=\sum_{\gamma\in\Gamma}A_\gamma,\quad A_\gamma:=\mathcal{T}_\gamma^B\begin{pmatrix}e^{-\eta\langle\cdot\rangle} & 0\\ 0 & e^{-\eta\langle\cdot\rangle}\end{pmatrix}K\widetilde\Theta_0\mathcal{T}_{-\gamma}^B. \tag{10.11}$$

To prove the boundedness of the sum of A_γ's we need the classical Cotlar–Stein Lemma:

Proposition 10.4. *Suppose that $B_j:H_1\to H_2, j\in\mathbb{N}$ are bounded operators between Hilbert spaces H_1 and H_2, and that there exists $M>0$ such that for all j,*

$$\sum_{k\in\mathbb{N}}\|B_j^*B_k\|^{\frac12}\le M,\quad \sum_{k\in\mathbb{N}}\|B_jB_k^*\|^{\frac12}\le M,$$

then $Bu:=\sum_{j\in J}B_ju$ converges in H_2 and defines an operator satisfying

$$\|B\|_{H_1\to H_2}\le M.$$

Proof. Let us first assume that $B_j=0$ for $j>J$ so that B is well defined. Since B^*B is self-adjoint, the spectral theorem (Theorem 1) implies that $\|B\|^{2m}=\|(B^*B)^m\|$. In addition,

$$(B^*B)^m=\sum_{j_1,\dots,j_{2m}=1}^{J}B_{j_1}^*B_{j_2}\dots B_{j_{2m-1}}^*B_{j_{2m}}=:\sum_{j_1,\dots,j_{2m}=1}^{J}B_{j_1,\dots,j_{2m}},$$

where we note that we have $2m$ sums. The summands are estimated as follows:

$$\|B_{j_1,\dots,j_{2m}}\| \leq \|B_{j_1}^* B_{j_2}\| \|B_{j_3}^* B_{j_4}\| \dots \|B_{j_{2m-1}}^* B_{j_{2m}}\|,$$

and

$$\|B_{j_1,\dots,j_{2m}}\| \leq \|B_{j_1}\| \|B_{j_2} B_{j_3}^*\| \dots \|B_{j_{2m-2}} B_{j_{2m-1}}^*\| \|B_{j_{2m}}\|.$$

Since $\|B_j\| = \|B_j^* B_j\|^{\frac{1}{2}} \leq M$, multiplying these estimates and taking square roots we obtain

$$\|B_{j_1,\dots,j_{2m}}\| \leq M \|B_{j_1}^* B_{j_2}\|^{1/2} \|B_{j_2} B_{j_3}^*\|^{1/2} \dots \|B_{j_{2m-2}}^* B_{j_{2m-1}}^*\|^{1/2} \|B_{j_{2m-1}}^* B_{j_{2m}}\|^{1/2}.$$

The advantage lies in having products of $2m-1$ terms which we can sum separately:

$$\begin{aligned} \|B\|^{2m} &= \|(B^*B)^m\| \leq \sum_{j_1,\dots,j_{2m}=1}^{J} \|B_{j_1,\dots,j_{2m}}\| \\ &\leq M \sum_{j_1,\dots,j_{2m}=1}^{J} \|B_{j_1} B_{j_2}^*\|^{1/2} \dots \|B_{j_{2m-1}}^* B_{j_{2m}}\|^{1/2} \leq MJM^{2m-1}, \end{aligned}$$

where the J factor came from having $2m$ sums and only $2m-1$ factors in the summands. Hence

$$\|B\| \leq J^{\frac{1}{2m}} M \longrightarrow M \quad \text{as } m \to \infty. \tag{10.12}$$

For the general case we take $u \in H_1$ of the form $u = B_k^* v$ for some k and some $v \in H_2$. Then

$$\|\sum_{j=1}^{\infty} B_j u\| = \|\sum_{j=1}^{\infty} B_j B_k^* v\| \leq \sum_{j=1}^{\infty} \|B_j B_k^*\|^{1/2} \|B_j B_k^*\|^{1/2} \|v\| \leq M^2 \|v\|.$$

We conclude that $\sum_{j=1}^{\infty} B_j u$ converges for $u \in \Sigma := \operatorname{span}\{B_k^*(H_2) \mid k = 1, \dots\}$.

We have proved $\|\sum_{j=1}^{J} B_j\| \leq M$ for any J, and that $\sum_{j=1}^{\infty} B_j u$ converges for any $u \in \Sigma$. Hence, the series converges for any $u \in \overline{\Sigma}$ (the closure of Σ in H_1). In fact, if suffices to show that for $u \in \overline{\Sigma}$, we have the Cauchy sequence property: $\|\sum_{j=L}^{K} B_j u\| < \varepsilon$, if $L, K > N$. For that we choose $u_0 \in \Sigma$ such that $\|u - u_0\| < \varepsilon/(2M)$ and for which $\|\sum_{j=L}^{K} B_j u_0\| < \varepsilon/2$, if $L, K > N$. Then

$$\|\sum_{j=L}^{K} B_j u\| \leq \|\sum_{j=L}^{K} B_j u_0\| + \|\sum_{j=L}^{K} B_j (u - u_0)\| < \tfrac{1}{2}\varepsilon + M\|u - u_0\| < \varepsilon,$$

where we used the fact for any finite sum of B_j we have the bound (10.12). It also follows that

$$\|\sum_{j=1}^{\infty} B_j u\| \leq \limsup_{J \to \infty} \left(\|\sum_{j=1}^{J} B_j u\| + \|\sum_{j=J+1}^{\infty} B_j u\| \right) \leq M\|u\|.$$

If u is orthogonal to $\overline{\Sigma}$, then $u \in \ker(B_k)$ for all k; in which case $\sum_{j=1}^{\infty} B_j u = 0$. Hence the series $\sum_{j=1}^{\infty} B_j u$ converges in norm for all $u \in H_1$ and defines an operator of norm bounded by M. $\square$

We want to apply this proposition with the index set $\mathbb{N}$ replaced by Γ and B_j given by A_γ, $\gamma \in \Gamma$ defined in (10.11). First of all, since $K : L^2 \times l^2 \to L^2 \times l^2$ is bounded, each $A_\gamma : L^2 \times l^2 \to L^2 \times l^2$ is uniformly bound. Moreover,

$$A_\alpha A_\beta^* = \mathcal{T}_\alpha^B \begin{pmatrix} e^{-\eta\langle\cdot\rangle} & 0 \\ 0 & e^{-\eta\langle\cdot\rangle} \end{pmatrix} K \widetilde{\Theta}_0 \mathcal{T}_{-\alpha}^B \mathcal{T}_\beta^B \widetilde{\Theta}_0 K^* \begin{pmatrix} e^{-\eta\langle\cdot\rangle} & 0 \\ 0 & e^{-\eta\langle\cdot\rangle} \end{pmatrix} \mathcal{T}_{-\beta}^B.$$

For $|\alpha - \beta| \gg 1$, $\widetilde{\Theta}_0 \mathcal{T}_{-\alpha}^B \mathcal{T}_\beta^B \widetilde{\Theta}_0 = 0$ by the support property. So $\sum_{\beta\in\Gamma} \|A_\alpha A_\beta^*\|^{\frac{1}{2}} \le C$ for some $C > 0$. On the other hand,

$$A_\alpha^* A_\beta = \mathcal{T}_\alpha^B \widetilde{\Theta}_0 K^* \begin{pmatrix} e^{-\eta\langle\cdot\rangle} & 0 \\ 0 & e^{-\eta\langle\cdot\rangle} \end{pmatrix} \mathcal{T}_{-\alpha}^B \mathcal{T}_\beta^B \begin{pmatrix} e^{-\eta\langle\cdot\rangle} & 0 \\ 0 & e^{-\eta\langle\cdot\rangle} \end{pmatrix} K \widetilde{\Theta}_0 \mathcal{T}_{-\beta}^B.$$

Thus

$$\|A_\alpha^* A_\beta\| \le C \|e^{-\eta\langle\cdot\rangle} \mathcal{T}_{-\alpha}^B \mathcal{T}_\beta^B e^{-\eta\langle\cdot\rangle}\| \le C \sup_x e^{-\eta\langle x\rangle} e^{-\eta\langle x-(\beta-\alpha)\rangle} \le C e^{-\eta|\beta-\alpha|}.$$

So we conclude $\sum_{\beta\in\Gamma} \|A_\alpha^* A_\beta\|^{\frac{1}{2}} \le C$ for some $C > 0$. Using Proposition 10.4 and recalling (10.11), we proved that

$$\begin{pmatrix} (D+A)^\alpha & 0 \\ 0 & 1 \end{pmatrix} \mathcal{F}_B : L^2 \times l^2 \to L^2 \times l^2, \quad |\alpha| \le 2$$

is bounded and therefore $\mathcal{F}_B : L^2 \times l^2 \to H_B^2 \times l^2$ is bounded.

Now we compute

$$\mathcal{P}_B \mathcal{F}_B = \sum_{\gamma\in\Gamma} \mathcal{T}_\gamma^B \mathcal{P}_B \mathcal{E}_0 \Theta_0 \mathcal{T}_{-\gamma}^B = I + K, \quad K = \sum_{\gamma\in\Gamma} \mathcal{T}_\gamma^B (\mathcal{P}_B - \mathcal{P}_0) \mathcal{E}_0 \Theta_0 \mathcal{T}_{-\gamma}^B. \tag{10.13}$$

We claim $\|K\|_{L^2\times\ell^2\to L^2\times\ell^2} = \mathcal{O}(B)$ and thus $\mathcal{F}_B$ is an approximate right inverse. In order to estimate the norm K, we compute

$$P_B - P_0 = \sum \mathcal{O}(B) x_i D_{x_j} + \mathcal{O}(B)|x|^2 + \mathcal{O}(B)$$

and

$$\begin{aligned} |T_\gamma^B \varphi_0 - T_\gamma \varphi_0| &= |e^{\frac{B}{4}(x\bar\alpha - \bar x\alpha)} - 1||\varphi_0(x-\alpha)| \le C|B||x-\alpha||\alpha| e^{-|x-\alpha|/C} \\ &\le C|B\alpha| e^{-|x-\alpha|/C'}, \\ |\partial_x^\beta (T_\gamma^B \varphi_0 - T_\gamma \varphi_0)| &\le C_\beta (|B\alpha| + |B\alpha|^{|\beta|}) e^{-|x-\alpha|/C}. \end{aligned}$$

Thus as in the proof of Proposition 10.2, for $\|f'\|_\infty$ sufficiently small we have

$$e^{-f} \langle\bullet\rangle^{-1} (R_+^B - R_+^0) e^f = \mathcal{O}_{L^2\to l^2}(B); \quad e^{-f} (R_-^B - R_-^0) \langle\bullet\rangle^{-1} e^f = \mathcal{O}_{l^2\to L^2}(B).$$

Now we write

$$(\mathcal{P}_B - \mathcal{P}_0)\mathcal{E}_0\Theta_0 = \begin{pmatrix} e^{-\eta\langle\cdot\rangle} & 0 \\ 0 & e^{-\eta\langle\cdot\rangle} \end{pmatrix} K_B, \quad K_B := \begin{pmatrix} e^{\eta\langle\cdot\rangle} & 0 \\ 0 & e^{\eta\langle\cdot\rangle} \end{pmatrix} (\mathcal{P}_B - \mathcal{P}_0)\mathcal{E}_0\Theta_0.$$

By Proposition 10.1, we conclude $\|K_B\|_{L^2\times l^2 \to L^2\times l^2} = \mathcal{O}(B)$. We now write

$$K = \sum_{\gamma\in\Gamma} \mathcal{T}_\gamma^B \begin{pmatrix} e^{-\eta\langle\cdot\rangle} & 0 \\ 0 & e^{-\eta\langle\cdot\rangle} \end{pmatrix} K_B \mathcal{T}_{-\gamma}^B.$$

Using Cotlar–Stein Lemma as before, we conclude $\|K\|_{L^2\times l^2 \to L^2\times l^2} = \mathcal{O}(B)$. For B sufficiently small $\|K\| < 1$ and we can define

$$\mathcal{E}_B = \mathcal{F}_B \sum_{j=0}^{\infty} (-K)^j \text{ so that } \mathcal{P}_B\mathcal{E}_B = I.$$

A similar construction gives an approximate left inverse by defining

$$\mathcal{G}_B = \sum_{\gamma\in\Gamma} \Theta_\gamma \mathcal{T}_\gamma^B \mathcal{E}_0 \mathcal{T}_{-\gamma}^B = \sum_{\gamma\in\Gamma} \mathcal{T}_\gamma^B \Theta_0 \mathcal{E}_0 \mathcal{T}_{-\gamma}^B.$$

We will then get the left inverse $\mathcal{E}_B'$ such that $\mathcal{E}_B'\mathcal{P}_B = I$. Since the left inverse and right inverse must be equal, we conclude that $\mathcal{E}_B' = \mathcal{E}_B$ is the inverse of $\mathcal{P}_B$ and the proof is finished. ∎

We conclude this section with an analogue of Proposition 10.2:

Proposition 10.5. *For f with properties from Proposition 10.2 and $\mathcal{P}_B$ given by (10.8) then $e^f\mathcal{P}_B(z)e^{-f}$ is invertible with bounded inverse, and*

$$\|e^f\mathcal{P}_B(z)^{-1}e^{-f}\|_{L^2\times l^2 \to H_B^2\times l^2} \le C.$$

The proof follows the same lines as the proof in the case of $B = 0$.

10.4. **Stability of spectral gaps.** In §10.3 we considered z in a neighbourhood of an isolated band of $P_0 = -\Delta + V(x)$. It is also natural to ask what happens when $z_0 \notin \mathrm{Spec}(-\Delta + V(x))$. In that case we proceed as in the proof of Theorem 15 but *without* setting up a Grushin problem, that is using invertibility of $(P_0 - z_0)^{-1}$. In the notation of (10.10) we put

$$F_B = \sum_{\gamma\in\Gamma} T_\gamma^B (P_0 - z_0)^{-1} \Theta_0 T_{-\gamma}^B,$$

where T_γ^B are magnetic translations (9.8). A simpler version of the analysis of (10.13) then shows that

$$(P_B - z)F_B = I + K_B, \quad K_B = \mathcal{O}(B) : L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2).$$

which provides us with a right inverse. Similarly we obtain a left inverse. This proves the following theorem of Nenciu and of Simon. We note that no assumption on the spectrum are made here. All we need is that z_0 is outside the spectrum of P_0.

Theorem 16. *Suppose* $P_B = (D_{x_1} - Bx_2/2)^2 + (D_{x_2} + iBx_1/2)^2 + V(x)$, $V \in C^\infty(\mathbb{R}^2;\mathbb{R})$, $V(x+\gamma) = V(x)$, $\gamma \in \Gamma$. *Then for* B *sufficiently small*

$$z_0 \notin \operatorname{Spec}(P_0) \implies z_0 \notin \operatorname{Spec}(P_B). \tag{10.14}$$

A modification of the proof gives in fact a stronger statement than (10.14) (see [Sj89, Proposition 2.4]): if $z_0 \notin \operatorname{Spec}(P_{B_0})$ then there exists $\varepsilon > 0$ such that

$$|z_0 - z| + |B - B_0| < \varepsilon \implies z_0 \notin \operatorname{Spec}(P_B).$$

10.5. **Effective Hamiltonian for small magnetic fields.** In view of Theorem 15 we can define

$$\mathcal{P}_B(z)^{-1} =: \mathcal{E}_B(z) = \begin{pmatrix} E^B(z) & E^B_+(z) \\ E^B_-(z) & E^B_{-+}(z) \end{pmatrix} : L^2(\mathbb{R}^2) \times \ell^2(\Gamma) \to H^2_B(\mathbb{R}^2) \times \ell^2(\Gamma). \tag{10.15}$$

In view of (2.16) the operator $E^B_{-+}(z)$ is the *effective Hamiltonian* in the sense that the existence of its inverse controls invertibility of $P_B - z$:

$$(P_B - z)^{-1} = E^B(z) - E^B_+(z) E^B_{-+}(z)^{-1} E^B_-(z), \quad z \in \operatorname{nbhd}_{\mathbb{C}}(I_k). \tag{10.16}$$

We now have an analogue of (10.4):

Proposition 10.6. *There exists* $(z, B, \alpha) \mapsto f(z, B, \alpha)$, $z \in \operatorname{nbhd}_{\mathbb{C}}(I_k)$, $B \in \operatorname{nbhd}_{\mathbb{R}}(0)$, $\alpha \in \Gamma$, *satisfying, uniformly in* z *and* B,

$$|f(z, B, \alpha)| \le C e^{-c|\alpha|}, \quad c > 0, \tag{10.17}$$

such that, in the notation of (10.15),

$$[E^B_{-+}(z) v](\alpha) = \sum_{\beta \in \Gamma} e^{\frac{i}{2} B \alpha \wedge \beta} f(z, B, \alpha - \beta) v(\beta). \tag{10.18}$$

Proof. From (10.9) we conclude that for all $\gamma \in \Gamma$, $\tau^B_\gamma E^B_{-+}(z) = E^B_{-+}(z) \tau^B_\gamma$. On the level of the matrix elements of $E^B_{-+}(z)$ that means that

$$\begin{aligned} e^{\frac{i}{2} B \rho \wedge \gamma} \sum_\beta E^B_{-+}(z, \rho - \gamma, \beta) v(\beta) &= \sum_\beta E^B_{-+}(z, \rho, \beta) e^{\frac{i}{2} B \beta \wedge \gamma} v(\beta - \gamma) \\ &= \sum_\beta E^B_{-+}(z, \rho, \beta + \gamma) e^{\frac{i}{2} B \beta \wedge \gamma} v(\beta), \end{aligned}$$

that is,

$$e^{\frac{i}{2} B \rho \wedge \gamma} E^B_{-+}(z, \rho - \gamma, \beta) = e^{\frac{i}{2} B \beta \wedge \gamma} E^B_{-+}(z, \rho, \beta + \gamma),$$

or, by putting $\rho = \alpha - \beta$ and taking $\gamma = -\beta$,

$$E^B_{-+}(z, \alpha, \beta) = e^{-\frac{i}{2} B(\alpha - \beta) \wedge (-\beta) + \frac{i}{2} B \beta \wedge (-\beta)} E^B_{-+}(z, \alpha - \beta, 0) = e^{\frac{i}{2} B \alpha \wedge \beta} E^B_{-+}(z, \alpha - \beta, 0).$$

Hence we can put

$$f(z,B,\gamma) := E_{-+}^B(z,\gamma,0).$$

To obtain exponential decay we note that Proposition 10.5 applied with $f(x) = c_0\langle x\rangle$, $0 < c_0 \ll 1$, shows that

$$e^{c_0\langle\gamma\rangle} f(z,B,\gamma) = e^{c_0\langle\gamma\rangle} E_{-+}^B(z)(e^{-c_0\langle\bullet\rangle}\delta_0(\bullet))(\gamma) \in \ell^2(\Gamma).$$

In particular, the left hand side is bounded and that gives (10.17). □

10.6. **Harper's operator.** We will show that f is a smooth function of B and hence the first approximation of $E_{-+}^B(z)$ is given by

$$v(\alpha) \mapsto zv(\alpha) - M_B v(\alpha), \quad M_B v(\alpha) := \sum_{\beta\in\Gamma} e^{\frac{i}{2}B\alpha\wedge\beta}\widehat{E}(\alpha-\beta).$$

In the simplest *tight binding model*, $\Gamma = \mathbb{Z}^2$, $\Gamma^* = 2\pi\mathbb{Z}^2$, and

$$\widehat{E}(n,m) = \delta_{n,1} + \delta_{n,-1} + \delta_{m,1} + \delta_{m,-1}, \quad (n,m) \in \mathbb{Z}^2,$$

which corresponds to $E(\theta) = 2(\cos\theta_1 + \cos\theta_2)$.

Since $(n,m)\wedge(n\pm1,m) = \pm m$ and $(n,m)\wedge(n,m\pm1) = \mp n$, we see that

$$v(n,m) \xrightarrow{M_B} e^{\frac{i}{2}Bm}v(n-1,m) + e^{-\frac{i}{2}Bm}v(n+1,m) + e^{-\frac{i}{2}Bn}v(n,m-1) + e^{\frac{i}{2}Bn}v(n,m+1).$$

We now introduce a unitary transformation

$$U_B : \ell^2(\Gamma) \to \ell^2(\Gamma), \quad U_B v(n,m) := e^{\frac{i}{2}Bmn}v(n,m),$$

so that

$$v(n,m) \xrightarrow{U_B^* M_B U_B} v(n-1,m) + v(n+1,m) + e^{-iBn}v(n,m-1) + e^{iBn}v(n,m+1).$$

We are interested in the spectrum of M_B which is the same as the spectrum of $\widetilde{M_B} := U_B^* M_B U_B$. We can consider this operator on the Fourier transform side $\theta \in \mathbb{R}^2/\Gamma^*$ where it becomes

$$u(\theta) \longmapsto 2\cos\theta_1\, u(\theta) + 2[\cos(BD_{\theta_1} + \theta_2)u](\theta), \quad u \in L^2(\mathbb{R}^2/\Gamma^*), \quad \Gamma^* = 2\pi\mathbb{Z}^2,$$

or, putting $x = \theta_1 \in \mathbb{R}/2\pi\mathbb{Z}$, $\tau = -\theta_2 \in \mathbb{R}/2\pi\mathbb{Z}$,

$$\begin{gathered} H_B w(x,\tau) := [H_B(\tau)w(\bullet,\tau)](x), \\ H_B(\tau) := \cos x + \cos(BD_x - \tau), \quad H_B(\tau) : L^2(\mathbb{R}/2\pi\mathbb{Z}) \to L^2(\mathbb{R}/2\pi\mathbb{Z}). \end{gathered} \tag{10.19}$$

This is the celebrated *Harper operator*.

We now claim that

$$B \notin 2\pi\mathbb{Q} \implies \operatorname{Spec}_{L^2(\mathbb{R}/2\pi\mathbb{Z})}(H_B(\tau)) = \operatorname{Spec}_{L^2(\mathbb{R}/2\pi\mathbb{Z})}(H_B(0)), \quad \tau \in \mathbb{R}. \tag{10.20}$$

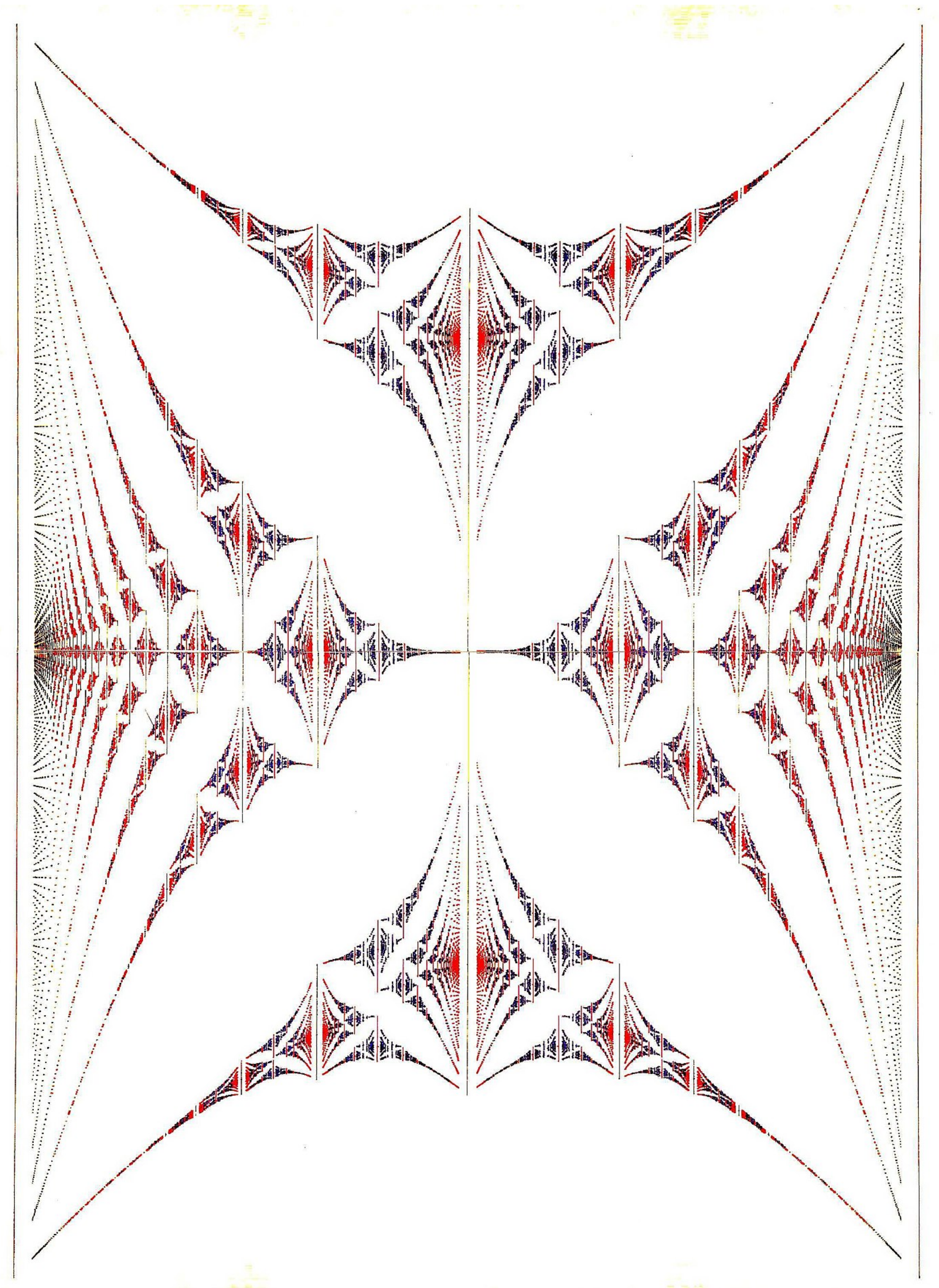


Figure 11. Spectrum of Harper's operator (10.21): the horizontal axis represents magnetic flux through a fundamental domain which for $\Gamma = \mathbb{Z}^2$ is equal to B; the vertical axis is the spectral parameter. The spectrum is a Cantor set when $B/2\pi \notin \mathbb{Q}$ and a union of q disjoint intervals when $B/2\pi = p/q \in \mathbb{Q}$. This picture is known as the *Hofstadter butterfly*. Reproduced from the original figure by Douglas Hofstadter under Creative Commons License CC BY-SA 3.0. The proof of the structure of the spectrum in the general case is due to Avila and Jitomirskaya [AvJi09].

Proof of (10.20). This follows from two observations:

$$
\begin{gathered}
H_B(kB) = U_k H_B(0) U_k^*, \quad k \in \mathbb{Z}, \\
U_k u(x) := e^{ikx} u(x), \quad U_k : L^2(\mathbb{R}/2\pi\mathbb{Z}) \to L^2(\mathbb{R}/2\pi\mathbb{Z}),
\end{gathered}
$$

and, using irrationality of $B/2\pi$ (which implies ergodicity of $\theta \mapsto \theta + B \mod 2\pi$),

$$
\forall\, \varepsilon\, \exists\, k \in \mathbb{Z}\, \forall\, n \in \mathbb{Z} \quad |\cos(B(n+k)) - \cos(Bn - \tau)| < \varepsilon.
$$

In particular $\|\cos(BD_x + Bk) - \cos(BD_x - \tau)\|_{L^2(\mathbb{R}/2\pi\mathbb{Z}) \to L^2(\mathbb{R}/2\pi\mathbb{Z})} < \varepsilon$. But this means that for any $\varepsilon > 0$ there exists $k \in \mathbb{Z}$ such that

$$
\|H_B(\tau) - H_B(kn)\|_{L^2(\mathbb{R}/2\pi\mathbb{Z}) \to L^2(\mathbb{R}/2\pi\mathbb{Z})} = \|H_B(\tau) - U_k H_B(0) U_k^*\|_{L^2(\mathbb{R}/2\pi\mathbb{Z}) \to L^2(\mathbb{R}/2\pi\mathbb{Z})} < \varepsilon.
$$

For bounded self-adjoint operators, A_j, $j = 1, 2$, $\|(A_j - \lambda)^{-1}\| = 1/d(\lambda, \mathrm{Spec}(A_j))$ (which follows from the spectral theorem, Theorem 1), gives

$$
\|A_1 - A_2\| < \varepsilon \implies \mathrm{Spec}(A_1) \subset \mathrm{Spec}(A_2) + (-\varepsilon, \varepsilon).
$$

We apply this this with

$$
A_1 = H_B(\tau), \quad A_2 = U_k H_B(0) U_k^*, \quad \mathrm{Spec}(A_2) = \mathrm{Spec}_{L^2(\mathbb{R}/2\pi\mathbb{Z})}(H_B(0)).
$$

Since ε is arbitrary, (10.20) follows. □

In the notation of (10.19) it follows that, if $B \notin 2\pi\mathbb{Z}$,

$$
\mathrm{Spec}_{L^2(\mathbb{R}^2/2\pi\mathbb{Z}^2)}(H_B) = \mathrm{Spec}_{L^2(\mathbb{R}/2\pi\mathbb{Z})} H_B(\tau), \quad \tau \in \mathbb{R},
$$

as sets. In view of this we can consider (abusing notation slightly) the following operator with the same spectrum:

$$
\begin{gathered}
H_B : L^2((\mathbb{R}/2\pi\mathbb{Z})_x \times (\mathbb{R}/B\mathbb{Z})_\tau) \to L^2((\mathbb{R}/2\pi\mathbb{Z})_x \times (\mathbb{R}/B\mathbb{Z})_\tau), \\
H_B w(x, \tau) = [H_B(\tau) w(\bullet, \tau)](x).
\end{gathered}
$$

We can then define a (modified) Bloch transform in this context (see §5.3)

$$
\begin{gathered}
V_B : L^2(\mathbb{R}) \to \mathscr{H}, \quad \mathscr{H} = \{u \in L^2_{\mathrm{loc}}(\mathbb{R}^2) : u(x + 2\pi m, \tau + kB) = e^{-ixk} u(x, \tau)\}, \\
V_B u(x, \tau) := \sum_{m \in \mathbb{Z}} e^{-\frac{i}{B}\tau(x - 2\pi m)} u(x - 2\pi m), \quad (x, \tau) \in \mathbb{R}/2\pi\mathbb{Z} \times \mathbb{R}.
\end{gathered}
$$

As in §5.4,

$$
\tfrac{1}{2} V_B^* H_B V_B = \cos x + \cos(BD_x) : L^2(\mathbb{R}) \to L^2(\mathbb{R}). \tag{10.21}
$$

This is another version of Harper's operator – see Figure 11. We note that it is given as a semiclassical quantization of the (postulated) Bloch energy, $E(x, \xi)$ where we replace (θ_1, θ_2) by $(x, \xi) \in T^*\mathbb{R}$. The small magnetic field B plays the role of the semiclassical parameter.

10.7. **Smooth dependence on B.** To study smoothness of $B \mapsto f(z, B)$, where f is given in Proposition 10.6, it is natural to differentiate $\mathcal{E}_B(z) = \mathcal{P}_B(z)^{-1}$ with respect to B. The difficulty we encounter is the fact that spaces on which $\mathcal{P}_B(z)$ act (and are invertible on) depend on B. Using weighted estimates from Proposition 10.5 we can however consider these operators as acting on smaller spaces which are independent of B:

Lemma 10.7. *Let*

$$\mathscr{H}^k := \bigcap_N \langle x \rangle^{-N} H^k(\mathbb{R}^2), \quad \mathscr{L} := \bigcap_N \langle \alpha \rangle^{-N} \ell^2(\Gamma),$$

be Fréchet spaces with seminorms $\|u\|_{\mathscr{H}^k, N} := \|\langle \bullet \rangle^N u\|_{H^k}$, $\|v\|_{\mathscr{L}, N} := \|\langle \bullet \rangle^N v\|_{\ell^2}$. *Then, in the notation of* (10.8),

$$\mathcal{P}_B(z) : \mathscr{H}^2 \times \mathscr{L} \to \mathscr{H}^0 \times \mathscr{L}, \quad z \in \mathrm{nbhd}_{\mathbb{C}}(I_k),$$

is a bounded operator, invertible for sufficiently small B, with a uniformly bounded inverse,

$$\mathcal{E}_B(z) : \mathscr{H}^0 \times \mathscr{L} \to \mathscr{H}^2 \times \mathscr{L}, \quad B \in \mathrm{nbhd}_{\mathbb{R}}(0), \quad z \in \mathrm{nbhd}_{\mathbb{C}}(I_k).$$

Proof. We first check that for any B and k, $\mathscr{H}^k = \bigcap_N \langle x \rangle^{-N} H^k_B(\mathbb{R}^2)$. This follows from

$$\|\langle x \rangle^N (D_x + A(x))^\alpha u\|_{L^2} \leq C \|\langle x \rangle^{N+|\alpha|} u\|_{H^{|\alpha|}}$$

and

$$\|\langle x \rangle^N D_x^\alpha u\|_{L^2} = \|\langle x \rangle^N (D_x + A(x) - A(x))^\alpha u\|_{L^2} \leq C \sum_{\beta \leq \alpha} \|\langle x \rangle^{N+|\alpha|} (D_x + A(x))^\beta u\|_{L^2}.$$

To show boundedness and invertibility we then use Proposition 10.5 with

$$f_N(x) = N \chi(\varepsilon_N x) \log\langle x \rangle, \quad \|e^{f_N} u\|_{H^k} \sim \|u\|_{\mathscr{H}^k, N}.$$

Here we take $\chi \in C^\infty(\mathbb{R}^2; [0,1])$ equal to 0 for $|x| < 1$ and equal to 1 for $|x| > 2$. We then choose ε_N so that $N \varepsilon_N \log(\varepsilon_N^{-1})$ is sufficiently small as then $\|f_N'\| + \|f_N''\| \ll 1$ as required by the assumptions of Proposition 10.5. On one hand, we have

$$\begin{aligned} \|\mathcal{P}_B(z) u\|_{\mathcal{H}^0 \times \mathcal{L}, N} &\sim \|e^{f_N} \mathcal{P}_B(z) u\|_{L^2 \times l^2} = \|e^{f_N} \mathcal{P}_B(z) e^{-f_N} e^{f_N} u\|_{L^2 \times l^2} \\ &\leq C \|e^{f_N} u\|_{H^2_B \times l^2} \leq C \|e^{f_{N+2}} u\|_{H^2 \times l^2} \sim \|u\|_{\mathcal{H}^2 \times \mathcal{L}, N+2}. \end{aligned}$$

On the other hand, we have

$$\begin{aligned} \|\mathcal{E}_B(z) u\|_{\mathcal{H}^2 \times \mathcal{L}, N} &\sim \|e^{f_N} \mathcal{E}_B(z) u\|_{H^2 \times l^2} \leq C \|e^{f_{N+2}} \mathcal{E}_B(z) u\|_{H^2_B \times l^2} \\ &= C \|e^{f_{N+2}} \mathcal{E}_B(z) e^{-f_{N+2}} e^{f_{N+2}} u\|_{H^2_B \times l^2} \leq C \|e^{f_{N+2}} u\|_{L^2 \times l^2} \sim \|u\|_{\mathcal{H}^0 \times \mathcal{L}, N+2}, \end{aligned}$$

which completes the proof. $\square$

With this in place we can consider derivatives of $\mathcal{P}_B(z)$:

Proposition 10.8. *For $z \in \mathrm{nbhd}_{\mathbb{C}}(I_k)$,*

$$\mathrm{nbhd}_{\mathbb{R}}(0) \ni B \mapsto \mathcal{P}_B(z) \quad \textit{is in} \quad C^\infty(\mathrm{nbhd}_{\mathbb{R}}(0), \mathcal{B}(\mathscr{H}^2 \times \mathscr{L}, \mathscr{H}^0 \times \mathscr{L})).$$

Consequently, $B \mapsto \mathcal{E}_B(z) : \mathscr{H}^0 \times \mathscr{L} \to \mathscr{H}^2 \times \mathscr{L}$ is also a smooth function of $B \in \mathrm{nbhd}_{\mathbb{R}}(0)$.

Proof. Recall

$$\mathcal{P}_B(z) = \begin{pmatrix} P_B - z & R_-^B \\ R_+^B & 0 \end{pmatrix}, \quad R_-^B u_-(x) = \sum_{\alpha \in \Gamma} u_-(\alpha) T_\alpha^B \varphi_0(x), \quad R_+^B u(\alpha) = \langle u, T_\alpha^B \varphi_0 \rangle.$$

We need to check each individual block is smooth in B. First $P_B = (D_{x_1} - Bx_2/2)^2 + (D_{x_2} + Bx_1/2)^2$ is smooth in B since polynomials are smooth. For $R_-^B : \mathcal{L} \to \mathcal{H}^0$, we note

$$\partial_B T_\alpha \varphi_0(x) = \frac{i}{2} \operatorname{Im}(x\bar{\alpha}) T_\alpha^B \varphi_0(x).$$

Since $|\varphi_0(x)| \le Ce^{-|x|/C}$, the operator

$$\partial_B R_-^B : u_-(\alpha) \mapsto \sum_{\alpha \in \Gamma} u_-(\alpha) \frac{i}{2} \operatorname{Im}(x\bar{\alpha}) T_\alpha^B \varphi_0(x) : \mathcal{L} \to \mathcal{H}^0$$

is bounded by Schur's criterion. Moreover,

$$\begin{aligned}
&(R_-^B - R_-^{B_0} - (B - B_0)\partial_B R_-^{B_0}) u_-(x) \\
&= \sum_{\alpha \in \Gamma} u_-(\alpha) (T_\alpha^B \varphi_0(x) - T_\alpha^{B_0}(x) - \frac{i}{2}(B - B_0) \operatorname{Im}(x\bar{\alpha}) T_\alpha^{B_0} \varphi_0(x)) \\
&= \sum_{\alpha \in \Gamma} u_-(\alpha) e^{-|x-\alpha|/C} \mathcal{O}((B - B_0)^2).
\end{aligned}$$

Thus by Schur's criterion again, $\partial_B R_-^B$ is indeed the derivative of R_-^B. We can iterate this argument to conclude $R_-^B \in C^\infty(\mathrm{nbhd}_{\mathbb{R}}(0), \mathcal{B}(\mathcal{L} \to \mathcal{H}^0))$. The smoothness for R_+^B is similar.

The smoothness of $\mathcal{E}_B(z)$ comes from the identity

$$\mathcal{E}_B \partial_B \mathcal{P}_B + (\partial_B \mathcal{E}_B) \mathcal{P}_B = 0$$

and thus $\partial_B \mathcal{E}_B = -\mathcal{E}_B (\partial_B \mathcal{P}_B) \mathcal{E}_B$. $\square$

As a corollary, $f(z, B, \alpha)$ is smooth in B and we can calculate derivatives $\partial_B^k f(z, B, \alpha)$. By the weighted estimate, for $0 < \delta \ll 1$

$$\begin{aligned}
&\|e^{\delta\langle\bullet\rangle} \partial_B \mathcal{E}_B(z) e^{-\delta\langle\bullet\rangle}\|_{L^2 \times l^2 \to H_B^2 \times l^2} = \|e^{\delta\langle\bullet\rangle} \mathcal{E}_B(z) (\partial_B \mathcal{P}_B(z)) \mathcal{E}_B(z) e^{-\delta\langle\bullet\rangle}\|_{L^2 \times l^2 \to H_B^2 \times l^2} \\
&= \|e^{\delta\langle\bullet\rangle} \mathcal{E}_B(z) e^{-\delta\langle\bullet\rangle} e^{\delta\langle\bullet\rangle} (\partial_B \mathcal{P}_B(z)) e^{-\delta\langle\bullet\rangle} e^{\delta\langle\bullet\rangle} \mathcal{E}_B(z) e^{-\delta\langle\bullet\rangle}\|_{L^2 \times l^2 \to H_B^2 \times l^2} < \infty,
\end{aligned}$$

we conclude $\|e^{\delta\langle\bullet\rangle}\partial_B E^B_{-+}(z)e^{-\delta\langle\bullet\rangle}\|_{l^2\to l^2} < \infty$ and $e^{\delta\langle\alpha\rangle}\partial_B f(z,B,\alpha) \in l^2(\Gamma)$. We can iterate with more derivatives and conclude that

$$|\partial_B^k f(z,B,\alpha)| \leq C_k e^{-c_0|\alpha|}, \qquad B \in \mathrm{nbhd}_{\mathbb{R}}(0), \quad z \in \mathrm{nbhd}_{\mathbb{C}}(I_k). \tag{10.22}$$

10.8. **The algebra of effective Hamiltonians.** Recall the effective Hamiltonian $E^B_{-+}(z)$ is given by operators of the form

$$\mathcal{M}_B(f)u(\alpha) = f\#_B u(\alpha) := \sum_{\beta\in\Gamma} e^{\frac{i}{2}B\alpha\wedge\beta} f(\alpha-\beta)u(\beta), \quad f \in l^1(\Gamma).$$

We study operators of this form in this section. Note $\mathcal{M}_B(f) : l^1(\Gamma) \to l^1(\Gamma)$ is a bounded linear map, we define

$$\mathcal{A}_B := \{\mathcal{M}_B(f) : f \in l^1(\Gamma)\}, \quad \|\mathcal{M}_B(f)\| = \|\mathcal{M}_B(f)\|_{l^1\to l^1} = \|f\|_{l^1}.$$

We claim $\mathcal{A}_B$ has the structure of a *Banach *-algebra*. Recall a Banach *-algebra is a Banach algebra A over $\mathbb{C}$ such that

- There is an involution operator $^* : A \to A$, i.e. $x^{**} = x$.
- $(x+y)^* = x^* + y^*$, $(xy)^* = y^*x^*$ for any $x, y \in A$;
- $(\lambda x)^* = \bar{\lambda}x^*$ for any $\lambda \in \mathbb{C}$, $x \in A$.

If the * operation satisfies the C^* identity $\|x^*x\| = \|x\|^2$ for any $x \in A$, we say A is a *C^*-algebra*. Classical examples of C^*-algebras include continuous functions over a compact Hausdorff space, bounded operators on a Hilbert space and the C^*-enveloping algebra of the convolution algebra of a locally compact group.

The multiplication and * operation is naturally defined on $\mathcal{A}_B$, and we note

$$\mathcal{M}_B(f)^* = \mathcal{M}_B(\tilde{f}), \quad \tilde{f}(\alpha) = \overline{f(-\alpha)}; \qquad\qquad \mathcal{M}_B(f)\mathcal{M}_B(g) = \mathcal{M}_B(\mathcal{M}_B(f)g).$$

On checks

$$\begin{aligned}\langle \mathcal{M}_B(f)u, v\rangle &= \sum_{\alpha,\beta\in\Gamma} e^{\frac{i}{2}B\alpha\wedge\beta} f(\alpha-\beta)u(\beta)\overline{v(\alpha)} \\ &= \sum_{\alpha,\beta\in\Gamma} u(\beta)\overline{e^{\frac{i}{2}B\beta\wedge\alpha}\overline{f(\alpha-\beta)}v(\alpha)} = \langle u, \mathcal{M}_B(\tilde{f})v\rangle\end{aligned}$$

and

$$
\begin{aligned}
\mathcal{M}_B(f)\mathcal{M}_B(g)u(\alpha) &= \sum_{\beta,\rho\in\Gamma} e^{\frac{i}{2}B\alpha\wedge\beta} f(\alpha-\beta) e^{\frac{i}{2}B\beta\wedge\rho} g(\beta-\rho)u(\rho) \\
&= \sum_{\beta,\rho\in\Gamma} e^{\frac{i}{2}B\alpha\wedge(\gamma+\rho)} f(\alpha-\gamma-\rho) e^{\frac{i}{2}B(\gamma+\rho)\wedge\rho} g(\gamma)u(\rho) \\
&= \sum_{\rho\in\Gamma} e^{\frac{i}{2}B\alpha\wedge\rho} \left(\sum_{\gamma\in\Gamma} e^{\frac{i}{2}B(\alpha-\rho)\wedge\gamma} f(\alpha-\rho-\gamma)g(\gamma) \right) u(\rho) \\
&= \mathcal{M}_B(\mathcal{M}_B(f)g)u(\alpha).
\end{aligned}
$$

All the properties of * follows from the definition. For the C^* identity, one checks that

$$
\begin{aligned}
\|\mathcal{M}_B(f)^*\mathcal{M}_B(f)\| = \|\tilde{f}\#_B f\|_{l^1} &= \sum_{\alpha\in\Gamma} \left| \sum_{\beta\in\Gamma} e^{\frac{i}{2}B\alpha\wedge\beta} \overline{f(\beta-\alpha)} f(\beta) \right| \\
&\leq \sum_{\alpha\in\Gamma}\sum_{\beta\in\Gamma} |f(\beta-\alpha)||f(\beta)| = \|f\|_{l^1}^2.
\end{aligned}
$$

The identity will never hold for general $f \in l^1(\Gamma)$, so $\mathcal{A}_B$ is not a C^*-algebra. However, one can define the reduced C^*-enveloping algebra $C_r^*(\mathcal{A}_B)$ as the closure of $\mathcal{A}_B$ inside $B(l^2(\Gamma))$. It is, by definition, a natural C^*-algebra.

One note that if $(B - B')|\mathbb{R}^2/\Gamma| \in 4\pi\mathbb{Z}$, then $\mathcal{A}_B \cong \mathcal{A}_{B'}$. Since $f\#_B g = g\#_{-B} f$, $\mathcal{A}_B$ is commutative if and only if $B|\mathbb{R}^2/\Gamma| \in 2\pi\mathbb{Z}$.

Proposition 10.9. *Suppose $|f(\alpha)| \leq Ce^{-c|\alpha|}$ for $\alpha\in\Gamma$, then $\mathcal{M}_B(f)^{-1} : l^2(\Gamma) \to l^2(\Gamma)$ exists if and only if there exists $g : \Gamma \to \mathbb{C}$ such that $|g(\alpha)| \leq Ce^{-c|\alpha|}$ and*

$$f\#_B g = g\#_B f = \delta_0.$$

Proof. Suppose there exists such g, then it is obvious that $\mathcal{M}_B(f)^{-1} = \mathcal{M}_B(g)$. On the other hand, suppose $\mathcal{M}_B(f)$ is invertible on $l^2(\Gamma)$. Since

$$[\tau_\gamma^B, \mathcal{M}_B(f)] = 0,$$

we know $\mathcal{M}_B(f)^{-1} = \mathcal{M}_B(g)$ for some $g \in l^\infty(\Gamma)$. Moreover,

$$\|g\|_{l^2} = \|\mathcal{M}_B(g)\delta_0\|_{l^2} < \infty.$$

Choose $\varphi : \Gamma \to \mathbb{R}$ such that φ is constant near ∞ and $\|\varphi\|_{\mathrm{Lip}} \ll 1$, then by the exponential decay of f, we have

$$\|e^{\varphi}\mathcal{M}_B(f)e^{-\varphi} - \mathcal{M}_B(f)\|_{l^2\to l^2} \ll 1.$$

This implies that for some $0 < \delta \ll 1$, $\|e^{\delta|\alpha|}g\|_{l^2} < \infty$ and thus

$$|g(\alpha)| \leq Ce^{-\delta|\alpha|}.$$

□

Recall $\tau_\gamma^B f(\alpha) = e^{\frac{i}{2}B\alpha\wedge\gamma} f(\alpha-\gamma) = \mathcal{M}_{-B}(\delta_\gamma) f(\alpha)$. We have the commutator relation

$$\tau_\alpha^{-B}\tau_\beta^{-B} = e^{iB\alpha\wedge\beta}\tau_\beta^{-B}\tau_\alpha^{-B}.$$

This is the *Weyl commutator relation*, which motivates us to give a semiclassical interpretation of the effective Hamiltonian.

10.9. **Semiclassical structure of the effective Hamiltonian.** The effective Hamiltonian E_{-+}^B can be interpreted as a semiclassical pseudodifferential operator, where B is considered as a semiclassical parameter.

Recall for $a(x,\xi) \in C^\infty(\mathbb{R}^2)$ such that $|\partial_{x,\xi}^\alpha a(x,\xi)| \le C_\alpha$, we may define the *Weyl quantization* of a as

$$\mathrm{Op}^w(a)u(x) = a^w(x,D)u(x) = \frac{1}{2\pi}\int_{\mathbb{R}^2} a\left(\frac{x+y}{2},\xi\right) e^{i(x-y)\cdot\xi}u(y)dyd\xi, \quad u \in \mathcal{S}(\mathbb{R}). \tag{10.23}$$

We note that

$$e^{iBD_x}e^{ix}u(x) = e^{i(x+B)}u(x+B), \quad e^{ix}e^{iBD_x}u(x) = e^{ix}u(x+B).$$

So e^{iBD_x}, e^{ix} also satisfy the Weyl commutator relation

$$e^{iBD_x}e^{ix} = e^{iB}e^{ix}e^{iBD_x}.$$

We recall two basic lemmas on the Weyl quantization of exponential of more general linear functions.

Lemma 10.10. *For $a, b \in \mathbb{R}$,*

$$\mathrm{Op}^w(e^{i(ax+b\xi)}) = e^{i(ax+bD_x)}$$

where $v(t,x) = e^{it(ax+bD_x)}u(x)$ is defined by

$$\begin{cases} (i\partial_t + ax + bD_x)v = 0, \\ v(0,x) = u(x). \end{cases}$$

Proof. Let $v(t,x) = e^{it(ax+bD_x)}u(x)$. It is direct to check from the definition that $v(t,x) = e^{itax+\frac{i}{2}t^2ab}u(x+tb)$. On the other hand,

$$\begin{aligned}\mathrm{Op}^w(e^{i(ax+b\xi)})u(x) &= \frac{1}{2\pi}\int e^{i(a\frac{x+y}{2}+b\xi+\xi(x-y))}u(y)dyd\xi = \frac{1}{2\pi}\int e^{i(\frac{ax}{2}+b\xi+\xi x)}\hat{u}\left(\xi-\frac{a}{2}\right)d\xi \\ &= \frac{1}{2\pi}\int e^{i(\frac{ax}{2}+(b+x)(\xi+a/2))}\hat{u}(\xi)d\xi = e^{iax+iab/2}u(x+b) = v(1,x).\end{aligned}$$

□

Lemma 10.11.

$$e^{i(a_1x+b_1D_x)}e^{i(a_2x+b_2D_x)} = e^{\frac{i}{2}(b_1a_2-b_2a_1)}e^{i((a_1+a_2)x+(b_1+b_2)D_x)}.$$

Proof. We check

$$\begin{aligned}
e^{i(a_1x+b_1D_x)}e^{i(a_2x+b_2D_x)}u(x) &= e^{i(a_1x+b_1D_x)}e^{ia_2x+ia_2b_2/2}u(x+b_2) \\
&= e^{ia_1x+ia_1b_1/2}e^{ia_2(x+b_1)+ia_2b_2/2}u(x+b_1+b_2) \\
&= e^{i(a_2b_1-a_1b_2)/2}e^{i(a_1+a_2)x+i(a_1+a_2)(b_1+b_2)/2}u(x+b_1+b_2) \\
&= e^{i(a_2b_1-a_1b_2)/2}e^{i((a_1+a_2)x+(b_1+b_2)D_x)}u(x).
\end{aligned}$$

□

Now for $f \in l^1(\mathbb{Z}^2)$, let

$$\mathcal{R}(f) = \sum_{\alpha\in\mathbb{Z}^2} \operatorname{Op}^w(e^{i\alpha_1 B\xi+i\alpha_2 x})f(\alpha) : L^2(\mathbb{R}) \to L^2(\mathbb{R}).$$

Since the generators satisfy the same Weyl commutator relation, we have

Proposition 10.12. *For $f, g \in \ell^1(\mathbb{Z}^2)$, $\mathcal{R}(f) \circ \mathcal{R}(g) = \mathcal{R}(f\#_B g)$.*

Moreover, if $|f(\alpha)| \le Ce^{-c|\alpha|}$, then $\mathcal{R}(f) = \operatorname{Op}^w(a(x, B\xi))$ where

$$a(x,\xi) = \sum_{\alpha\in\mathbb{Z}^2} e^{i\alpha_1\xi+i\alpha_2 x}f(\alpha) \in C^\omega(\mathbb{R}^2/2\pi\mathbb{Z}^2)$$

is a real analytic periodic function. Similarly, if $|f(\alpha)| \le C_N\langle\alpha\rangle^{-N}$ for any $N \in \mathbb{N}$, then $a(x,\xi)$ is a periodic smooth function.

We can then interpret the spectrum of P_B as a nonlinear spectrum problem for a semiclassical pseudodifferential operator as follows.

Theorem 17. *Suppose $f : \mathbb{Z}^2 \to \mathbb{C}$ such that $|f(\alpha)| \le Ce^{-c|\alpha|}$, then the following are equivalent*

(a) $0 \notin \operatorname{Spec}_{\ell^2(\mathbb{Z}^2)}(\mathcal{M}_B(f))$;
(b) $0 \notin \operatorname{Spec}_{L^2(\mathbb{R})}(\mathcal{R}(f))$;
(c) *$\mathcal{R}(f) : L^2 \to L^2$ is invertible, and there exists $b \in C^\omega(\mathbb{R}^2/2\pi\mathbb{Z}^2)$ such that $\mathcal{R}(f)^{-1} = \operatorname{Op}^w(b(x, B\xi))$.*

Proof. By Proposition 10.12, (a) implies (b). Also it is clear that (c) implies (a), since we can take g to be the Fourier transform of b so that $\mathcal{R}(f)^{-1} = \mathcal{R}(g)$. Proposition 10.12 again tells us $\mathcal{M}_B(f)^{-1}$ is $\mathcal{M}_B(g)$.

We are left with showing (b) implies (c). In order to do this, we need use Beals Lemma (see [Zw12, Theorem 8.3]) which tells us $\mathcal{R}(f)^{-1} = \operatorname{Op}^w(b(x, B\xi))$ for some $b \in C^\infty(\mathbb{R}^2)$ with $|\partial^\alpha_{x,\xi} b(x,\xi)| \le C_\alpha$. In order to show $b(x,\xi)$ is periodic, we introduce $k(x,\xi) = x_0\xi - \xi_0 x$ for $(x_0,\xi_0) \in 2\pi\mathbb{Z}^2/B$ and conjugate using $k^w(x, BD_x)$ by Lemma 10.11:

$$e^{ik^w(x,BD_x)}e^{i(\alpha_2 x+\alpha_1 BD_x)}e^{-ik^w(x,BD_x)} = e^{i(\alpha_2 Bx_0+\alpha_1 B\xi_0)}e^{i(\alpha_2 x+\alpha_1 BD_x)} = e^{i(\alpha_2 x+\alpha_1 BD_x)}.$$

Thus $[e^{ik^w(x,BD_x)}, \mathcal{R}(f)] = 0$ and $[e^{ik^w(x,BD_x)}, \mathcal{R}(f)^{-1}] = 0$. On ther other hand,

$$e^{ik^w(x,BD_x)} b^w(x, BD_x) e^{-ik^w(x,BD_x)} = b^w(x + Bx_0, BD_x + B\xi_0).$$

So $b(x, \xi) \in C^\infty(\mathbb{R}^2/2\pi\mathbb{Z}^2)$ is a periodic function. By Fourier series argument again, $b(x,\xi) = \sum_{\alpha\in\mathbb{Z}^2} g(\alpha) e^{i(\alpha_1\xi+\alpha_2 x)}$ for a rapidly decaying $g : \mathbb{Z}^2 \to \mathbb{C}$. We have $\mathcal{R}(f)^{-1} = \mathcal{R}(g)$ and thus $\mathcal{M}_B(f)^{-1} = \mathcal{M}_B(g)$ by Proposition 10.12. By Proposition 10.9, $|g(\alpha)| \le Ce^{-c|\alpha|}$ has exponential decay. Thus $b \in C^\omega(\mathbb{R}^2/2\pi\mathbb{Z}^2)$ is real analytic. ☐

10.10. **Computation of the semiclassical effective Hamiltonian.** In this section, we want to compute the semiclassical expansion of the symbol $b(x, \xi) \in C^\omega(\mathbb{R}^2/2\pi\mathbb{Z}^2)$ defined via Theorem 17 and Proposition 10.6:

$$b(z, x, \xi; B) = b_0(z, x, \xi) + Bb_1(z, x, \xi) + \mathcal{O}(B^2).$$

By Proposition 10.8, $b(z, x, \xi; B)$ is smooth in B and z. Taking $B = 0$ we conclude $b_0(x, \xi) = z - E(\xi, x)$ from Proposition 10.1. In order to compute b_1, we differentiate in B. Since $\partial_B \mathcal{E}_B(z) = -\mathcal{E}_B(z)(\partial_z \mathcal{P}_B(z))\mathcal{E}_B(z)$, we have

$$\partial_B E^B_{-+}(z)|_{B=0} = -E_-(\partial_B P_B)|_{B=0}E_+ - E_{-+}(z)(\partial_B R^B_+)|_{B=0}E_+ - E_-(\partial_B R^B_-)|_{B=0}E_{-+}(z). \tag{10.24}$$

Recall $P_B = (D_{x_1} - Bx_2/2)^2 + (D_{x_2} + Bx_1/2)^2 + V(x)$, so

$$\partial_B P_B = x_1 D_{x_2} - x_2 D_{x_1} + \tfrac{1}{4}B|x|^2.$$

Moreover, $E_- v(\alpha) = R_+ v(\alpha) = \langle v, \varphi_\alpha\rangle$ and $E_+ v_+(x) = R_- v_+(x) = \sum_{\alpha\in\Gamma} v_+(\alpha)\varphi_\alpha(x)$ and

$$\partial_B R^B_+ v(\alpha) = -\frac{1}{2} i\langle v(\cdot), (\cdot \wedge \alpha) T^B_\alpha \varphi_0(\cdot)\rangle, \quad \partial_B R^B_- v_+(x) = \frac{i}{2}\sum_{\alpha\in\Gamma} v_+(\alpha)(x \wedge \alpha) T^B_\alpha \varphi_0(x).$$

Each term in (10.24) is a convolution operator. The convolution kernel can be computed by its action on $\delta_0(\alpha) \in \ell^2(\Gamma)$. The first term in (10.24) is given by

$$(-E_-(\partial_B P_B)|_{B=0}E_+\delta_0)(\alpha) = -\int_{\mathbb{R}^2} (x_1 D_{x_2} - x_2 D_{x_1})\varphi_0(x)\overline{\varphi_\alpha(x)}dx. \tag{10.25}$$

The second term in (10.24) is

$$(-E_{-+}(z)(\partial_B R^B_+)|_{B=0}E_+\delta_0)(\alpha) = \frac{i}{2}\sum_{\beta\in\Gamma}(z\delta_\beta(\alpha) - \hat{E}(\alpha - \beta)) \int_{\mathbb{R}^2}(x\wedge\beta)\varphi_0(x)\overline{\varphi_\beta(x)}dx \tag{10.26}$$

and the third term in (10.24) is

$$(-E_-(\partial_B R^B_-|_{B=0})E_{-+}(z)\delta_0)(\alpha) = -\frac{i}{2}\sum_{\beta\in\Gamma}\int_{\mathbb{R}^2}(x\wedge\beta)(z\delta_0(\beta) - \hat{E}(\beta))\varphi_\beta(x)\overline{\varphi_\alpha(x)}dx. \tag{10.27}$$

For simplicity of the presentation, we compute for $\Gamma = \mathbb{Z}^2$. Recall

$$b_1(z,x,\xi) = \sum_{\alpha\in\mathbb{Z}^2} (\partial_B E_{-+}^B(z)|_{B=0}\delta_0)(\alpha) e^{i\alpha_1\xi + i\alpha_2 x}.$$

The first term (10.25) gives

$$-\sum_{\alpha\in\mathbb{Z}^2}\int_{\mathbb{R}^2}(y_1D_{y_2}-y_2D_{y_1})\varphi_0(y)\overline{\varphi_\alpha(y)}e^{i\alpha_1\xi+i\alpha_2 x}dy = -\int_{\mathbb{R}^2}(y_1D_{y_2}-y_2D_{y_1})\varphi_0(y)\overline{\varphi((\xi,x),y)}dy.$$

The second term (10.26) gives

$$\begin{aligned}&\frac{i}{2}\sum_{\alpha,\beta\in\mathbb{Z}^2}(z\delta_\beta(\alpha)-\hat{E}(\alpha-\beta))e^{i\alpha_1\xi+i\alpha_2 x}\int_{\mathbb{R}^2}(y\wedge\beta)\varphi_0(y)\overline{\varphi_\beta(y)}dy\\ &=\frac{i}{2}(z-E(\xi,x))\int_{\mathbb{R}^2}\varphi_0(y)\overline{(y_1D_x-y_2D_\xi)\varphi((\xi,x),y)}dy\end{aligned}$$

and the third term (10.27) gives

$$\begin{aligned}&-\frac{i}{2}\sum_{\alpha,\beta\in\mathbb{Z}^2}e^{i\alpha_1\xi+i\alpha_2 x}\int_{\mathbb{R}^2}(y\wedge\beta)(z\delta_0(\beta)-\hat{E}(\beta))\varphi_\beta(y)\overline{\varphi_\alpha(y)}dy\\ &=\frac{i}{2}\sum_{\beta\in\mathbb{Z}^2}\int_{\mathbb{R}^2}(y\wedge\beta)\hat{E}(\beta)\varphi_\beta(y)\overline{\varphi((\xi,x),y)}dy\\ &=\frac{i}{2(2\pi)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2/2\pi\mathbb{Z}^2}E(\theta)(y_1D_{\theta_2}-y_2D_{\theta_1})\varphi(\theta,y)\overline{\varphi((\xi,x),y)}d\theta dy.\end{aligned}$$

We conclude that $b_1(z,x,\xi)$ is given by

$$\begin{aligned}&-\int_{\mathbb{R}^2}(y_1D_{y_2}-y_2D_{y_1})\varphi_0(y)\overline{\varphi((\xi,x),y)}dy\\ &\quad+\tfrac{i}{2}(z-E(\xi,x))\int_{\mathbb{R}^2}\varphi_0(y)\overline{(y_1D_x-y_2D_\xi)\varphi((\xi,x),y)}dy\\ &\quad+\frac{i}{2(2\pi)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2/2\pi\mathbb{Z}^2}E(\theta)(y_1D_{\theta_2}-y_2D_{\theta_1})\varphi(\theta,y)\overline{\varphi((\xi,x),y)}d\theta dy\\ &=\frac{1}{2(2\pi)^2}\int_{\mathbb{R}^2}\int_{\mathbb{R}^2/2\pi\mathbb{Z}^2}(-2(y_1D_{y_2}-y_2D_{y_1})+i(y_1D_{\theta_2}-y_2D_{\theta_1})E(\theta))\varphi(\theta,y)\overline{\varphi(\tau,y)}d\theta dy\\ &\quad+\tfrac{i}{2}(z-E(\xi,x))\int_{\mathbb{R}^2}\varphi_0(y)\overline{(y_1D_x-y_2D_\xi)\varphi((\xi,x),y)}dy.\end{aligned}\tag{10.28}$$

We are interested in the case when $b(z,x,\xi;B)=0$. Then $z=E(\xi,x)+\mathcal{O}(B)$ and the second term on the right hand side of (10.28) is of higher order.

Denote $\tau = (\xi, x)$ and $(a_1, a_2) \wedge (b_1, b_2) = a_2 b_1 - a_1 b_2$. In this notation the y-integral in the first term of (10.28) can be rewritten as

$$\frac{1}{2(2\pi)^2} \sum_{\gamma \in \mathbb{Z}^2} \int_{[0,1)\times[0,1)} (2(y-\gamma) \wedge D_y - i(y-\gamma) \wedge D_\theta E(\theta)) \varphi(\theta, y-\gamma) \overline{\varphi(\tau, y-\gamma)} dy$$

$$= \frac{1}{2(2\pi)^2} \sum_{\gamma \in \mathbb{Z}^2} \int_{[0,1)\times[0,1)} (2(y-\gamma) \wedge D_y - i(y-\gamma) \wedge D_\theta E(\theta)) e^{i\gamma\cdot(\theta-\tau)} \varphi(\theta, y) \overline{\varphi(\tau, y)} dy$$

$$= \tfrac{1}{2} \int_{[0,1)\times[0,1)} (y - D_\theta) \delta(\theta - \tau) \wedge (2D_y - \nabla E(\theta)) \varphi(\theta, y) \overline{\varphi(\tau, y)} dy.$$

Integrating in θ gives

$$\int_{\mathbb{R}^2/\mathbb{Z}^2} (y + D_\tau) \wedge (D_y - \tfrac{1}{2} \nabla E(\tau)) \varphi(\tau, y) \overline{\varphi(\tau, y)} dy$$

$$= \tfrac{1}{2} \nabla E(\tau) \wedge \int_{\mathbb{R}^2/\mathbb{Z}^2} (y + D_\tau) \varphi(\tau, y) \overline{\varphi(\tau, y)} dy + \int_{\mathbb{R}^2/\mathbb{Z}^2} (y + D_\tau) \wedge D_y \varphi(\tau, y) \overline{\varphi(\tau, y)} dy$$

$$= \tfrac{1}{2} \nabla E(\tau) \wedge \langle D_\tau u(\tau, \bullet), u(\tau, \bullet) \rangle + \langle D_\tau \wedge (-\tau + D_y) u(\tau, \bullet), u(\tau, \bullet) \rangle,$$

where $u(\tau, y) = e^{i\langle \tau, y \rangle} \varphi(\tau, y)$ – see §8.3. The term wedged with $\nabla E(\tau)$ is essentially the Berry connection (8.12). We conclude

$$\begin{aligned} b_1(x, \xi, z)|_{b_0(z,x,\xi)=0} = \tfrac{1}{2} \nabla E(\tau) \wedge \langle D_\tau u(\tau, \bullet), u(\tau, \bullet) \rangle \\ + \langle (\tau - D_y) \wedge D_\tau u(\tau, \bullet), u(\tau, \bullet) \rangle, \quad \tau = (\xi, x). \end{aligned} \tag{10.29}$$

Here we used the fact that $\tau \wedge D_\tau = -D_\tau \wedge \tau$. Let $P(\tau) := e^{i\tau\cdot y} P_0 e^{-i\tau\cdot y}$, we note that

$$0 = \nabla_\tau((P(\tau) - E(\tau))u(\tau)) = (P(\tau) - E(\tau))\nabla_\tau u(\tau) + (\nabla_\tau P(\tau))u(\tau) - \nabla_\tau E(\tau) u(\tau)$$

and that

$$\nabla_\tau P(\tau) = 2(\tau - D_y).$$

Hence, we can rewrite (10.29) as follows

$$\begin{aligned} b_1(x, \xi, z)|_{b_0(z,x,\xi)=0} = -\tfrac{i}{2} \int_{\mathbb{R}^2/\Gamma} (P(\tau) - E(\tau)) \nabla_\tau u(\tau, y) \wedge \overline{\nabla_\tau u(\tau, y)} dy \\ + \nabla E(\tau) \wedge \langle D_\tau u(\tau, \bullet), u(\tau, \bullet) \rangle. \end{aligned} \tag{10.30}$$

Remark 23. *Under the symmetry assumption $V(x) = V(-x)$ (see Proposition 8.5) the first term in (10.30) vanishes:*

$$\int_{\mathbb{R}^2/\Gamma} (P(\tau) - E(\tau)) \nabla_\tau u(\tau, y) \wedge \overline{\nabla_\tau u(\tau, y)} dy = 0. \tag{10.31}$$

This is because $\overline{u}(\tau, y) = \alpha(\tau) u(\tau, -y)$ and

$$\overline{\nabla_\tau u(\tau, y)} = \alpha(\tau) \nabla_\tau u(\tau, -y) + u(\tau, -y) \nabla_\tau \alpha(\tau).$$

Thus we have

$$
\begin{aligned}
&\int_{\mathbb{R}^2/\Gamma} (P(\tau) - E(\tau))\nabla_\tau u(\tau, y) \wedge \overline{\nabla_\tau u(\tau, y)} dy \\
&= \int_{\mathbb{R}^2/\Gamma} \alpha(\tau)(P(\tau) - E(\tau))\nabla_\tau u(\tau, y) \wedge \nabla_\tau u(\tau, -y) dy \\
&+ \int_{\mathbb{R}^2/\Gamma} (P(\tau) - E(\tau))\nabla_\tau u(\tau, y) \wedge (\nabla_\tau \alpha(\tau)) u(\tau, -y) dy \\
&= 0
\end{aligned}
$$

where the first term vanishes because

$$
\begin{aligned}
&\int_{\mathbb{R}^2/\Gamma} \alpha(\tau)(P(\tau) - E(\tau))\nabla_\tau u(\tau, y) \wedge \nabla_\tau u(\tau, -y) dy \\
&= \int_{\mathbb{R}^2/\Gamma} \alpha(\tau)\overline{(P(\tau) - E(\tau))}\nabla_\tau u(\tau, -y) \wedge \nabla_\tau u(\tau, y) dy \\
&= \int_{\mathbb{R}^2/\Gamma} \alpha(\tau)\nabla_\tau u(\tau, -y) \wedge (P(\tau) - E(\tau))\nabla_\tau u(\tau, y) dy
\end{aligned}
$$

and the second term vanishes because

$$
\begin{aligned}
&\int_{\mathbb{R}^2/\Gamma} (P(\tau) - E(\tau))\nabla_\tau u(\tau, y) \wedge (\nabla_\tau \alpha(\tau)) u(\tau, -y) dy \\
&= \int_{\mathbb{R}^2/\Gamma} \nabla_\tau u(\tau, y) \wedge (\nabla_\tau \alpha(\tau))\overline{(P(\tau) - E(\tau))} u(\tau, -y) dy \\
&= \int_{\mathbb{R}^2/\Gamma} \nabla_\tau u(\tau, y) \wedge \alpha(\tau)^{-1}(\nabla_\tau \alpha(\tau))\overline{(P(\tau) - E(\tau)) u(\tau, y)} dy = 0.
\end{aligned}
$$

Therefore

$$
b_1(x, \xi, z)|_{b_0(z,x,\xi)=0} = \nabla E(\tau) \wedge \langle D_\tau u(\tau, \bullet), u(\tau, \bullet)\rangle.
$$

Remark 24. *The second term in the Bohr–Sommerfeld expansion, relevant to de Haas–van Alphen oscillations, is given by*

$$
\pi - \int_{E(\xi,x)=\mu} b_1(\mu, x, \xi)|dt|, \tag{10.32}
$$

where t corresponds to the parametrization of $E = \mu$ (we assume here that $\nabla E \neq 0$ when $E = \mu$) given by the Hamilton vector field (see (2.2)):

$$
(\dot{x}(t), \dot{\xi}(t)) = H_{b_0}(x(t), \xi(t)) = (\partial_\xi E(\xi(t), x(t)), -\partial_x E(\xi(t), x(t))).
$$

This means that

$$
(\partial_\xi E, \partial_x E) \wedge (a_1, a_2) dt = -\langle (\dot{\xi}(t), \dot{x}(t)), (a_1, a_2)\rangle
$$

or

$$\begin{aligned}\int_{E(\xi,x)=\mu} b_1(\mu,x,\xi)dt &= \int_{E(\xi,x)=\mu} \langle(\tau - D_y)\wedge D_\tau u(\tau,\bullet), u(\tau,\bullet)\rangle |dt| + \tfrac{i}{2}\int_{\gamma_\mu}\eta \\ &= -\tfrac{i}{2}\int_{E(\xi,x)=\mu} \langle (P(\tau)-E(\tau))\nabla_\tau u(\tau,\bullet), \wedge \nabla_\tau u(\tau,\bullet)\rangle + i\int_{\gamma_\mu}\eta.\end{aligned} \tag{10.33}$$

where $\eta = \int_{\mathbb{R}^2/\mathbb{Z}^2} d_\theta u(\theta,y)\overline{u(\theta,y)}dy$ *is the Berry connection* (8.12)*. The cycle* γ_μ *is given by* $E(\theta)=\mu$ *with the orientation determined by the direction of the Hamilton vector field* H_{b_0}*. Under the symmetry assumption* (8.15)*, we have* $d\eta = 0$ *by Proposition 8.5 and the first term in* (10.33) *vanishes by Remark 23. In this case we have*

$$\int_{E(\xi,x)=\mu} b_1(\mu,x,\xi)dt = i\int_{\gamma_\mu}\eta$$

and the last integral only depends on the homology class of γ_μ*.*

11. 2D periodic structures in constant magnetic field: density of states

11.1. **Regularized traces** $B \neq 0$**.** In this section we consider the density of states in the previous model. Now we move to the case that $B \neq 0$ and small. First we show the existence of $\widetilde{\mathrm{tr}} f(P_B)$. Suppose

$$f(P_B)w(x) = \int_{\mathbb{R}^2} K(x,y)w(y)dy.$$

Since $[T^B_\gamma, P_B] = 0$, we have $[T^B_\gamma, f(P_B)] = 0$, i.e. $K(x+\gamma, y+\gamma) = e^{\frac{i}{2}B(x-y)\wedge\gamma}K(x,y)$. This implies that $K(x+\gamma,x+\gamma) = K(x,x)$ for any $\gamma\in\Gamma$, and hence the existence of the limit

$$\widetilde{\mathrm{tr}} f(P_B) = \lim_{L\to\infty}\frac{1}{(2L)^2}\int_{[-L,L]^2} K(x,x)dx = \frac{1}{|\mathbb{R}^2/\Gamma|}\int_{\mathbb{R}^2/\Gamma} K(x,x)dx.$$

Suppose we have an operator $M : l^2(\Gamma)\to l^2(\Gamma)$ defined as

$$M(f)(\alpha) = \sum_{\gamma\in\Gamma} M(\alpha,\gamma)f(\gamma),$$

we can define the modified trace as

$$\widehat{\mathrm{tr}} M = \lim_{L\to\infty}\frac{1}{(2L)^2}\sum_{\alpha\in\Gamma\cap[-L,L]^2} M(\alpha,\alpha).$$

If $M = \mathcal{M}_B(f)$ such that $M(\alpha,\beta) = e^{\frac{i}{2}B\alpha\wedge\beta} f(\alpha-\beta)$, then we have similarly $\widehat{\mathrm{tr}}\mathcal{M}_B(f) = \frac{f(0)}{|\mathbb{R}^2/\Gamma|}$. Moreover, suppose $\mathcal{R}(f) = a^w(x, BD_x)$, then

$$\widehat{\mathrm{tr}}\mathcal{M}_B(f) = \frac{f(0)}{|\mathbb{R}^2/\Gamma|} = \frac{1}{(2\pi)^2}\int_{\mathbb{R}^2/2\pi\mathbb{Z}^2} a(x,\xi;B)dxd\xi.$$

The modified trace has similar properties as a trace:

Proposition 11.1. *Suppose $A_j : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n), j = 1,2$ such that $|A_j(x,y)| \leq Ce^{-c|x-y|}$ for some $C, c > 0$, then (suppose both sides are well-defined)*

$$\widetilde{\mathrm{tr}}(A_1A_2) = \widetilde{\mathrm{tr}}(A_2A_1).$$

Suppose $\Gamma \subset \mathbb{R}^n$ is a lattice and $B : L^2(\mathbb{R}^n) \to l^2(\Gamma), C : l^2(\Gamma) \to L^2(\mathbb{R}^n)$ such that

$$|B(\alpha,x)| \leq Ce^{-c|x-\alpha|}, \quad |C(x,\alpha)| \leq Ce^{-c|x-\alpha|}$$

for some $C, c > 0$, then $\widetilde{\mathrm{tr}}(CB) = \widehat{\mathrm{tr}}(BC)$

Proof. We only prove the first claim, as the second is proved in the same way. By definition,

$$\begin{aligned}\widetilde{\mathrm{tr}}(A_1A_2) &= \lim_{L\to\infty}\frac{1}{(2L)^n}\int_{[-L,L]^n}\int_{\mathbb{R}^n} A_1(x,y)A_2(y,x)dydx \\ &= \lim_{L\to\infty}\frac{1}{(2L)^n}\int_{\mathbb{R}^n}\int_{[-L,L]^n} A_2(y,x)A_1(x,y)dxdy.\end{aligned}$$

By assumption,

$$|A_2\mathbb{1}_{[-L,L]^n}A_1(y,y) - A_2A_1(y,y)| \leq Ce^{-c|L-|y|_\infty|}, \quad y \in [-L,L]^n$$

and

$$|A_2\mathbb{1}_{[-L,L]^n}A_1(y,y)| \leq Ce^{-c|L-|y|_\infty|}, \quad y \notin [-L,L]^n.$$

Thus

$$\int_{\mathbb{R}^n} |A_2\mathbb{1}_{[-L,L]^n}A_1(y,y) - \mathbb{1}_{[-L,L]^n}A_2A_1(y,y)|dy \leq CL^{n-1}$$

and

$$\begin{aligned}\widetilde{\mathrm{tr}}(A_1A_2) &= \lim_{L\to\infty}\frac{1}{(2L)^n}\int_{\mathbb{R}^n} A_2\mathbb{1}_{[-L,L]^n}A_1(y,y)dy \\ &= \lim_{L\to\infty}\frac{1}{(2L)^n}\int_{\mathbb{R}^n} \mathbb{1}_{[-L,L]^n}A_2A_1(y,y)dy = \widetilde{\mathrm{tr}}(A_2A_1),\end{aligned}$$

completing the proof. □

To compute $\widetilde{\mathrm{tr}}f(P_B)$, we will use the Helffer–Sjöstrand formula which is based on the existence of almost analytic continuations:

Proposition 11.2. *Let $f \in C_0^\infty(\mathbb{R})$, then for any δ there exists $\tilde{f} \in C_0^\infty(\mathbb{C})$ such that*

$$\tilde{f}|_{\mathbb{R}} = f, \qquad \partial \tilde{f}(z) = \mathcal{O}(|\operatorname{Im} z|^\infty), \qquad \operatorname{supp} \tilde{f} \subset \operatorname{supp} f + B_{\mathbb{C}}(0,\delta).$$

In particular, we have

$$f(x) = \frac{1}{\pi} \int_{\mathbb{C}} \bar{\partial} \tilde{f}(z)(x-z)^{-1} dm(z), \quad x \in \mathbb{R}. \tag{11.1}$$

Proof. The identity (11.1) comes from the fact that $\frac{1}{\pi z}$ is the fundamental solution of $\bar{\partial}_z$. The function $\tilde{f}$ is constructed as follows. Let $\chi(y) \in C_0^\infty(\mathbb{R})$ be a cutoff function such that $\chi(y) = 1$ near $x = 0$. Let $\psi(x) \in C_0^\infty(\mathbb{R})$ be a cutoff function such that $\psi(x) = 1$ near $\operatorname{supp} f$. We define

$$\tilde{f}(x+iy) = \frac{\psi(x)\chi(y)}{2\pi} \int_{\mathbb{R}} \hat{f}(\xi)\chi(y\xi)e^{i(x+iy)\xi} d\xi.$$

It is clear that $\tilde{f} \in C_0^\infty(\mathbb{C})$ and $\tilde{f}|_{\mathbb{R}} = f$. We consider

$$\begin{aligned}\bar{\partial}\tilde{f}(x+iy) = {} & \frac{\psi'(x)\chi(y)}{4\pi} \int_{\mathbb{R}} \hat{f}(\xi)\chi(y\xi)e^{i(x+iy)\xi} d\xi \\ & + \frac{i\psi(x)\chi'(y)}{4\pi} \int_{\mathbb{R}} \hat{f}(\xi)\chi(y\xi)e^{i(x+iy)\xi} d\xi + \frac{i\psi(x)\chi(y)}{4\pi} \int_{\mathbb{R}} \hat{f}(\xi)\xi\chi'(y\xi)e^{i(x+iy)\xi} d\xi.\end{aligned}$$

The term with $\chi'(y)$ vanishes near the real line. The last term is

$$\begin{aligned}\frac{i\psi(x)\chi(y)}{4\pi} \int_{\mathbb{R}} \hat{f}(\xi)\xi\chi'(y\xi)e^{i(x+iy)\xi} d\xi &= \frac{i\psi(x)\chi(y)y^N}{4\pi} \int_{\mathbb{R}} \hat{f}(\xi)\xi^{N+1}(y\xi)^{-N}\chi'(y\xi)e^{i(x+iy)\xi} d\xi \\ &= \mathcal{O}(|y|^N)\end{aligned}$$

since $(y\xi)^{-N}\chi'(y\xi)e^{i(x+iy)\xi}$ is uniformly bounded and $\hat{f}(\xi)$ is rapidly decreasing.

The first term is

$$\begin{aligned}&\frac{\psi'(x)\chi(y)}{4\pi} \int_{\mathbb{R}} \hat{f}(\xi)\chi(y\xi)e^{i(x+iy)\xi} d\xi \\ &= \frac{\psi'(x)\chi(y)}{4\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} f(\tilde{x})\chi(y\xi)e^{i(x-\tilde{x}+iy)\xi} d\tilde{x} d\xi \\ &= \frac{\psi'(x)\chi(y)}{4\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} f(\tilde{x})\chi(y\xi)\frac{\partial_\xi e^{i(x-\tilde{x}+iy)\xi}}{i(x-\tilde{x}+iy)} d\tilde{x} d\xi \\ &= -\frac{\psi'(x)\chi(y)}{4\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} f(\tilde{x})y\chi'(y\xi)\frac{e^{i(x-\tilde{x}+iy)\xi}}{i(x-\tilde{x}+iy)} d\tilde{x} d\xi \\ &= -\frac{\psi'(x)\chi(y)y^N}{4\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} f(\tilde{x})\xi^{N-1}(y\xi)^{-N+1}\chi'(y\xi)\frac{e^{i(x-\tilde{x}+iy)\xi}}{i(x-\tilde{x}+iy)} d\tilde{x} d\xi \\ &= \mathcal{O}(|y|^N)\end{aligned}$$

since $(y\xi)^{-N+1}\chi'(y\xi)e^{i(x+iy)\xi}$ is uniformly bounded and

$$\begin{aligned}\int_{\mathbb{R}} \frac{f(\tilde{x})}{i(x-\tilde{x}+iy)}e^{-i\tilde{x}\xi}d\tilde{x} &= \int_{\mathbb{R}} \frac{f(\tilde{x})}{i(x-\tilde{x}+iy)}\left(\frac{1-\partial_{\tilde{x}}^2}{1+\xi^2}\right)^N e^{-i\tilde{x}\xi}d\tilde{x}\\ &= \int_{\mathbb{R}} \left(\frac{1-\partial_{\tilde{x}}^2}{1+\xi^2}\right)^N \left(\frac{f(\tilde{x})}{i(x-\tilde{x}+iy)}\right) e^{-i\tilde{x}\xi}d\tilde{x}\\ &= \mathcal{O}((1+\xi^2)^{-N})\end{aligned}$$

is rapidly decreasing in ξ for $|x-\tilde{x}|>c>0$ since $\operatorname{supp} f \cap \operatorname{supp}\psi' = \varnothing$.

We conclude $\bar{\partial}\tilde{f}(x+iy) = \mathcal{O}(|y|^N)$ for any $N>0$. $\square$

Now for the self-adjoint operator P_B we have (by spectral theorem)

$$f(P_B) = \frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{f}(z)(P_B-z)^{-1}dm(z).$$

Recall from (10.16) that

$$(P_B-z)^{-1} = E^B(z) - E_+^B(z)E_{-+}^B(z)^{-1}E_-^B(z).$$

Since $E^B(z)$ is holomorphic, we have

$$f(P_B) = -\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{f}(z)E_+^B(z)E_{-+}^B(z)^{-1}E_-^B(z)dm(z).$$

By Proposition 11.1 and $\partial_z E_{-+}^B(z) = -\partial_z((R_-^B)^{-1}(P_B-z)(R_+^B)^{-1}) = E_-^B(z)E_+^B(z)$,

$$\begin{aligned}\widetilde{\operatorname{tr}} f(P_B) &= -\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{f}(z)\widetilde{\operatorname{tr}} E_+^B(z)E_{-+}^B(z)^{-1}E_-^B(z)dm(z)\\ &= -\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{f}(z)\widehat{\operatorname{tr}} E_-^B(z)E_+^B(z)E_{-+}^B(z)^{-1}dm(z)\\ &= -\frac{1}{\pi}\int_{\mathbb{C}} \bar{\partial}\tilde{f}(z)\widehat{\operatorname{tr}}((\partial_z E_{-+}^B(z))E_{-+}^B(z)^{-1})dm(z).\end{aligned}$$

11.2. **Smoothness of $B \mapsto \widetilde{\operatorname{tr}} f(P_B)$ for $f \in C_c^\infty(\mathbb{R})$.**

11.3. **Bohr–Sommerfeld quantization rule for pseudodifferential operators in 1D.** In this section we introduce the Bohr–Sommerfeld quantization rule. Let $p(x,\xi;h) : T^*\mathbb{R} \to \mathbb{R}$ be a smooth real symbol such that $P = \operatorname{Op}_h^w(p)$ is self-adjoint. Suppose $p(x,\xi;h)$ has an asymptotic expansion

$$p(x,\xi;h) \sim p_0(x,\xi) + hp_1(x,\xi) + h^2p_2(x,\xi) + \cdots .$$

- Let $I = [E_-, E_+] \subset \mathbb{R}$ and suppose there is a topological annulus $\mathcal{A} \subset p_0^{-1}(I)$ such that $\partial\mathcal{A} = \mathcal{A}_+ \cup \mathcal{A}_-$ with $\mathcal{A}_\pm$ a connected component of $p_0^{-1}(E_\pm)$.
- Suppose p_0 has no critical point in $\mathcal{A}$.
- Suppose $\mathcal{A}_-$ is included by the disk W bounded by $\mathcal{A}_+$.
- Suppose $p_0 > E_+$ outside W.

Then we have

Theorem 18. *The spectrum of P inside I is given by*

$$\mathrm{Spec}(P) \cap I = \{E_n\} + \mathcal{O}(h^\infty)$$

where $E_n = E_n(h)$ satisfies the Bohr–Sommerfeld quantization rule:

$$S_h(E_n) \sim \sum_{j=0}^{\infty} S_j(E_n) h^j = 2\pi n h \tag{11.2}$$

and

$$S_0(E) = \int_{\gamma_E} \xi dx, \quad S_1(E) = \pi - \int_{\gamma_E} p_1 |dt|$$

where $\gamma_E = p_0^{-1}(E) \cap \mathcal{A}$.

Proof. Following [CdV05], we suppose the expansion (11.2) holds and try to compute each term by the following trace formula.

$$\mathrm{tr} f(P) = \sum_{n\in\mathbb{Z}} f(S_h^{-1}(2\pi n h)) + \mathcal{O}(h^\infty). \tag{11.3}$$

By Poisson summation formula, the right hand side of (11.3) is given by

$$\sum_{n\in\mathbb{Z}} f(S_h^{-1}(2\pi h)) = \frac{1}{2\pi h} \int_{\mathbb{R}} f(S_h^{-1}(u)) du + \mathcal{O}(h^\infty) = \frac{1}{2\pi h} \int_{\mathbb{R}} f(E) S_h'(E) dE + \mathcal{O}(h^\infty).$$

By Helffer–Sjöstrand formula, the left hand side of (11.3) is given by

$$\mathrm{tr} f(P) = \frac{1}{\pi} \mathrm{tr} \int_{\mathbb{C}} \partial_{\bar z} \tilde f(z) (P-z)^{-1} dm(z)$$

where $\tilde f$ is an almost analytic extension of f. Let us compute

$$(P-z)^{-1} = \mathrm{Op}_h^w \left(\sum_{j=0}^{\infty} h^j q_j(z) \right).$$

Since

$$(p-z) \# \left(\sum_{j=0}^{\infty} h^j q_j(z) \right) = 1 = \left(\sum_{j=0}^{\infty} h^j q_j(z) \right) \# (p-z),$$

we can determine inductively that

$$q_0 = (p_0 - z)^{-1}, \quad q_1 = -\frac{p_1}{(p_0-z)^2}, \quad q_j = \sum_{l=2}^{L(j)} r_{jl} (p_0 - z)^{-l}.$$

Thus if the full symbol of $f(P)$ is $\sigma_h^{\rm full}(f(P))$, then

$$\begin{aligned}\operatorname{tr} f(P) &= \frac{1}{2\pi h}\int_{T^*\mathbb{R}} \sigma_h^{\rm full}(f(P))dxd\xi \\ &= \frac{1}{2\pi h}\int_{T^*\mathbb{R}} \frac{1}{\pi}\int_{\mathbb{C}} \partial_{\bar z}\tilde f(z)\sigma_h^{\rm full}((P-z)^{-1})dm(z)dxd\xi \\ &= \frac{1}{2\pi h}\int_{T^*\mathbb{R}}\left(f(p_0)+hf'(p_0)p_1+\sum_{j=2}^{\infty} h^j\frac{(-1)^{l-1}}{(l-1)!}f^{(l-1)}(p_0)r_{jl}\right)dxd\xi \\ &= \frac{1}{2\pi h}\int_{\mathbb{R}} f(E)\left(\int_{\gamma_E}|dt| - h\frac{d}{dE}\int_{\gamma_E}p_1|dt| + \sum_{j=2}^{\infty}\frac{h^j}{(l-1)!}\left(\frac{d}{dE}\right)^{l-1}\int_{\gamma_E} r_{jl}|dt|\right)dE.\end{aligned}$$

Compare both sides of (11.3), we get

$$S_0(E)=\int_{\gamma_E}\xi dx + C_0,\quad S_1(E)=C_1-\int_{\gamma_E}p_1|dt|.$$

By choosing a Hamiltonian $\tilde p$ which interpolates between $p(x,\xi)$ and the harmonic oscillator $\mathring{p}=x^2+\xi^2$, $\mathring{P}=-h^2\partial_x^2+x^2$, we can see the constants C_j are independent of the operator and can be computed using the harmonic oscillator. One checks directly that for the harmonic oscillator, $\operatorname{Spec}(\mathring{P})=\{(2n+1)h : n\in\mathbb{N}\}$, and

$$\int_{\gamma_E}\xi dx = \pi E.$$

So

$$\pi E + C_0 + C_1 h = 2\pi n h.$$

We conclude $C_0=0$, $C_1=\pi$. □

Remark 25. *The factor $C_1=\pi$ comes from the Maslov index of the circle γ_E. In general, suppose Λ is a Lagrangian submanifold of $T^*\mathbb{R}^n$, then there is an integral cohomological class $\mathcal{M}\in H^1(\Lambda;\mathbb{Z})$ called Maslov class as defined in [Arn67]. Let $\alpha=\sum\xi_j dx_j$ be the contact 1-form, the Bohr sommerfeld quantization condition says*

$$\frac{1}{2\pi h}\alpha+\frac{1}{4}\mathcal{M}\equiv 0 \mod H^1(\Lambda;\mathbb{Z}).$$

In the case $n=1$ and Λ is a circle, $H^1(\Lambda;\mathbb{Z})=\mathbb{Z}$ and $\mathcal{M}=2$. Integrating over the circle would give the first two terms of (11.2).

11.4. **Magnetic oscillations in density of states: topological corrections.**

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