

NOTES FOR CONDENSED MATTER PHYSICS

TRANSCRIBED BY NING TANG INSTRUCTOR: PROFESSOR MACIEJ ZWORSKI

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1. PRELIMINARIES AND DERIVATION OF LANDAU'S HAMILTONIAN

1.1. **Classical dynamics.** Newton's equation is of the form $\ddot{x} = \vec{F}(x, \dot{x})$. Classical electrons in a magnetic/electric field satisfy the Maxwell's equations

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

where $\vec{E} = \vec{E}(x)$ and $\vec{B} = \vec{B}(x)$. Then by Poincaré's lemma for forms, divergence of \vec{B} is zero implies $\vec{B} = \nabla \times \vec{A}$ for some A and curl of \vec{E} is zero implies $\vec{E} = -\nabla V(x)$. By Lorentz law, we know that the force is

$$\vec{F} = -\nabla V(x) + \dot{x} \times \vec{B}. \quad (1.1)$$

Now we review some basic knowledge about Hamiltonian formalism that is covered in [17].

Let $(x, \xi) \in \mathbb{R}^n \times \mathbb{R}^n \simeq T^*\mathbb{R}^n$ denotes position-momentum, where we can think of ξ as belonging to $T_x^*\mathbb{R}^n$, the cotangent space of \mathbb{R}^n at x . The symplectic form $\sigma = \sum d\xi_j \wedge dx_j = d(\sum \xi_j dx_j)$ is a bilinear antisymmetric closed form such that

$$\sigma((X, \Xi), (X', \Xi')) = \langle \Xi, X' \rangle - \langle \Xi', X \rangle.$$

For $p \in C^\infty(\mathbb{R}^{2n})$, the corresponding Hamiltonian vector field H_p is defined by $\sigma(Z, H_p) = dp(Z)$, where $Z = (X, \Xi) \in \mathbb{R}^{2n}$. Suppose $H_p = V_1 \partial_x + V_2 \partial_\xi$, then by explicit computation,

$$\langle \Xi, V_1 \rangle - \langle X, V_2 \rangle = \sigma((X, \Xi), (V_1, V_2)) = dp(X, \Xi) = \langle p'_x, X \rangle + \langle p'_\xi, \Xi \rangle,$$

which implies $H_p = \sum \frac{\partial p}{\partial \xi_j} \partial_{x_j} - \frac{\partial p}{\partial x_j} \partial_{\xi_j}$.

Definition 1.1 (Classical flow). *Classical flow is defined as $\varphi_t = \exp tH_p$, that is, $\varphi_t(x, \xi) = (x(t), \xi(t))$, and $x(t), \xi(t)$ solve the equations*

$$\dot{x}(t) = \frac{\partial p}{\partial \xi}(x(t), \xi(t)), \quad \dot{\xi}(t) = -\frac{\partial p}{\partial x}(x(t), \xi(t))$$

with initial conditions $(x(0), \xi(0)) = (x, \xi)$. And here we assume that the solution of the flow exists and is unique for all times $t \in \mathbb{R}$.

A crucial property is that the flow preserves the symplectic form, that is, in fancy words, $\varphi_t^* \sigma = \sigma$. And in practical, this means that

$$\sigma(\partial \varphi_t(X, \Xi), \partial \varphi_t(X', \Xi')) = \sigma((X, \Xi), (X', \Xi')).$$

The proof of this result can be found in [17, Section 5]. Obviously, the volume form $dV = \frac{1}{n!} \sigma^{\wedge n}$ is also preserved by φ_t^* , where $\sigma^{\wedge n}$ denotes the wedge of n copies of σ .

For any classical observables $a = a(x, \xi)$, we define $a_t := \varphi_t^* a = a(\varphi_t(x, \xi))$. Then by simple calculus,

$$\frac{d}{dt} a_t = H_p a_t = \{p, a_t\},$$

where $H_a b = \{a, b\}$.

If we take our Hamiltonian to be

$$p(x, \xi) = \frac{1}{2}\xi^2 + V(x),$$

then

$$\varphi_t^* p = p(\varphi_t(x, \xi)) = p(x, \xi),$$

where the last equality comes from the fact $H_p(p) = 0$, which implies that p does not change along the flow. Then

$$\dot{x} = \frac{\partial p}{\partial \xi} = \xi, \quad \dot{\xi} = -\nabla V(x) \quad \Rightarrow \quad \ddot{x} = -\nabla V(x),$$

which is the Newton's equation if only electric field exists and there is no magnetic field, thanks to (1.1).

Now we want to find a Hamiltonian $p(x, \xi)$ such that the Hamiltonian flow gives the classical motion of electron in a magnetic field.

Theorem 1.2. *The Hamiltonian flow for the classical motion of electron in a magnetic field $p(x, \xi) = \frac{1}{2} \sum (\xi_j - A_j(x))^2 + V(x)$.*

Proof. By a direct computation,

$$\dot{x}_j = \frac{\partial p}{\partial \xi_j} = \xi_j - A_j(x),$$

$$\dot{\xi}_j = \sum_{k=1}^3 \partial_{x_j} A_k(x) (\xi_k - A_k(x)) - \partial_j V(x) = \sum_{k=1}^3 \partial_{x_j} A_k(x) \dot{x}_k - \partial_j V(x),$$

$$\ddot{x}_j = \dot{\xi}_j - \sum_k \partial_{x_k} A_j(x) \dot{x}_k = \sum_k (\partial_{x_j} A_k(x) - \partial_{x_k} A_j(x)) \dot{x}_k - \partial_j V(x) = (\dot{x} \times \vec{B} - \nabla V(x))_j,$$

where $\vec{B} = \nabla \times \vec{A}$. □

1.2. Review for functional analysis. Let H be a (complex) Hilbert space and $A : H \rightarrow H$ is a linear operator. If A is bounded, it is easy to find the adjoint A^* by Riesz representation theorem such that $\langle Au, v \rangle = \langle u, A^*v \rangle$.

Definition 1.3. *We say $A : H \rightarrow H$ is an unbounded operator if there exists a dense subset $\mathcal{D}(A) \subset H$ such that $A : \mathcal{D}(A) \rightarrow H$ is a linear operator.*

If $u, v \in \mathcal{S}(\mathbb{R}^n)$, then the magnetic Schrödinger operator P is formally self-adjoint in the sense that

$$\langle Pu, v \rangle_{L^2(\mathbb{R}^n)} = \langle u, Pv \rangle_{L^2(\mathbb{R}^n)},$$

where $\langle u, v \rangle = \int u \bar{v} dx$.

Definition 1.4. *Here is a list of definitions.*

- A is densely defined if $\overline{\mathcal{D}(A)}^H = H$.

- A is closed if $G(A) := \{(u, Au) : u \in \mathcal{D}(A)\}$ is closed in $H \times H$ in the norm $\|(u, v)\| = \|u\| + \|v\|$.
- $A \subset B$ if $\mathcal{D}(A) \subset \mathcal{D}(B)$ and $B|_{\mathcal{D}(A)} = A$.
- A is closable if there exists a closed operator \bar{A} such that $A \subset \bar{A}$. (Since the closure of a graph may not be a graph, so not every operator is closable, but if it is, \bar{A} is uniquely defined.)
- The domain of the adjoint A^* of A is

$$\mathcal{D}(A^*) := \{u : \exists C = C(u), \forall v \in \mathcal{D}(A), |\langle u, Av \rangle| \leq C\|v\|\}.$$

Then by Riesz representation theorem, A^* is well-defined on $\mathcal{D}(A^*)$.

- A is symmetric if $A \subset A^*$.
- A is self-adjoint if $A = A^*$.
- If A is symmetric, then A is essentially self-adjoint if $\bar{A} = A^*$.

Proposition 1.5. *The following facts are easy to check by definitions.*

- A^* is closed.
- If A^* is densely defined, then A is closable and $\bar{A} = (A^*)^*$.
- A is symmetric if and only if $\langle Au, v \rangle = \langle u, Av \rangle$ for all $u, v \in \mathcal{D}(A)$.

Theorem 1.6 (Spectral theorem). *Suppose P is a self-adjoint operator densely defined on a separable Hilbert space H , then there exists a σ -finite measure space (X, \mathcal{M}, μ) , a measurable real-valued function $f : X \rightarrow \mathbb{R}$ and a unitary operator $U : H \rightarrow L^2(X, \mu)$ such that the domain of P satisfies*

$$x \in \mathcal{D}(P) \iff fUx \in L^2(X, \mu)$$

and for $x \in \mathcal{D}(P)$, $U(Px) = fUx$.

Definition 1.7. *The spectrum of P is defined as the complement of the resolvent, that is,*

$$\text{Spec}(P) := \mathbb{C} \setminus \{z \in \mathbb{C} : (P - z)^{-1} : H \rightarrow H \text{ bounded}\}.$$

From the Spectral theorem, we actually see that the spectrum of a self-adjoint operator is $\text{Spec}(P) = \overline{f(X)} \subset \mathbb{R}$.

One standard and concrete example we will see later is that $U = \mathcal{F}$, $X = \mathbb{R}^n$, $P = D_x$.

Example 1.8. *Let $H = \mathbb{C}^n$, $P = P^*$ be a unitary matrix. Then $X = \mathbb{Z}_n = \mathbb{Z}/n\mathbb{Z}$ and hence $L^2(X) = \mathbb{C}^n$. Since for all $\psi \in L^2(X) = \mathbb{C}^n$, $(UPU^{-1}\psi)(n) = f(n)\psi(n)$, where $\psi(n)$ means the n -th entry in \mathbb{C}^n , this implies that for all $\psi \in \mathbb{C}^n$, $UPU^{-1}\psi = \text{diag}(f(0), \dots, f(n-1))\psi$, that is, $UPU^{-1} = \text{diag}(f(0), \dots, f(n-1))$.*

Example 1.9. *Using the Spectral theorem, for $P : H \rightarrow H$ self-adjoint operator, we can define $U(t) := e^{-itP} : H \rightarrow H$ as a unitary operator. This is simply because we can define by using Spectral theorem that $U(e^{-itP}x) = e^{-itf}Ux$ for $x \in \mathcal{D}(P)$ and note that f is real-valued function. Since $\mathcal{D}(P)$ is dense, we can extend it to H .*

Quantum observables are given by $A : H \rightarrow H$ bounded self-adjoint operators, whose evolution is given by $A_t := U(t)^*AU(t)$ and

$$\frac{d}{dt}A_t = i[P, A_t],$$

which you just use the Spectral theorem and P is a multiplication by function on that side. This is called the Heisenberg picture of quantum mechanics. In the equation above, the differentiation of the operator is defined in the sense of strong operator topology, that is, the operator $\frac{d}{dt}A_t$ is the one such that

$$\left\| \left(\frac{d}{dt}A_t \right) x - \frac{A_{t+s} - A_t}{s} x \right\| \rightarrow 0$$

as $s \rightarrow 0$ for all $x \in \mathcal{D}(A_t)$. Then by writing things explicitly and use the add and subtract trick, it suffices to prove

$$\left\| \left(\frac{e^{-itf} - I}{it} x - M_f x \right) \right\| \rightarrow 0$$

as $t \rightarrow 0$ for $x \in \mathcal{D}(M_f) = \{x \in L^2 : fx \in L^2\}$. Suppose $u \in L^2$, $fu \in L^2$,

$$\frac{\sin tf(y)}{t} - f(y) \quad \text{and} \quad \frac{\cos tf(x) - 1}{it}$$

is uniformly bounded by constant (independent of t, y) multiples of $f(y)$. Hence, by the uniform convergence theorem,

$$\left\| \left(\frac{e^{-itf(y)} - 1}{it} u(y) - f(y)u(y) \right) \right\|_{L_y^2} \rightarrow 0$$

as $t \rightarrow 0$.

For more discussion in depth, see the Hill-Yosida theorem.

1.3. Quantization process. We turn a classical function of position and momentum into an operator. The process of turning $p(x, \xi)$ into P is done by

$$\xi_j \rightsquigarrow \frac{1}{i} \partial_{x_j} = D_{x_j}, \quad x_j \rightsquigarrow \text{multiply by } x_j.$$

Let $a(x, \xi)$ either be a polynomial in the variable ξ or in $\mathcal{S}(\mathbb{R}^n \times \mathbb{R}^n)$. Then $A := a^w(x, D)$ is defined as

$$a^w(x, D)u := \frac{1}{(2\pi)^n} \int a\left(\frac{x+y}{2}, \xi\right) e^{i\langle \xi, x-y \rangle} u(y) dy d\xi$$

for $u \in \mathcal{S}(\mathbb{R}^n)$. Now, by computation,

$$\begin{aligned}
(\xi_j)^w u &= \frac{1}{(2\pi)^n} \int \xi_j e^{i(x-y)\cdot\xi} u(y) dy d\xi = \frac{1}{(2\pi)^n} \int \xi_j e^{ix\cdot\xi} \widehat{u}(\xi) d\xi = D_{x_j} u, \\
(x_j)^w u &= \frac{1}{(2\pi)^n} \int \frac{x_j + y_j}{2} e^{i(x-y)\cdot\xi} u(y) dy d\xi \\
&= x_j \frac{1}{(2\pi)^n} \int e^{i(x-y)\cdot\xi} u(y) dy d\xi + \frac{1}{(2\pi)^n} \int \frac{y_j - x_j}{2} e^{i(x-y)\cdot\xi} u(y) dy d\xi \\
&= x_j u(x) + \frac{i}{2(2\pi)^n} \int \partial_{\xi_j} (e^{i(x-y)\cdot\xi}) u(y) dy d\xi \\
&= x_j u(x) + \frac{i}{2(2\pi)^n} \int \partial_{\xi_j} \left(\int e^{i(x-y)\cdot\xi} u(y) dy \right) d\xi \\
&= x_j u(x) + \frac{i}{2(2\pi)^n} \int \partial_{\xi_j} (e^{ix\cdot\xi} \widehat{u}(\xi)) d\xi = x_j u(x).
\end{aligned}$$

And $a^w(x, D)$ is formally self-adjoint in the sense that for $u, v \in \mathcal{S}, a \in \mathcal{S}$,

$$\begin{aligned}
\langle a^w(x, D)u, v \rangle &= \iiint a\left(\frac{x+y}{2}, \xi\right) e^{i(x-y)\xi} u(y) \overline{v(x)} dy d\xi dx \\
&= \int u(y) \left(\int a\left(\frac{x+y}{2}, \xi\right) e^{i(y-x)\xi} v(x) dx d\xi \right) dy = \int u(y) \overline{a^w(y, D)v} dy = \langle u, a^w(x, D)v \rangle.
\end{aligned}$$

If a is not real, we just need to change a to \bar{a} in the derivation.

Let $p = x_j, q = \xi_k$, then $p^w = x_j, q^w = D_{x_k}$, which implies $H_p = -\partial_{\xi_j}, \{p, q\} = -\delta_{jk}$ and $[p^w, q^w] = [x_j, D_{x_k}] = i\delta_{jk}$. Hence, $\{p, q\} = i[p^w, q^w]$. As you can see, the classical version in some sense corresponds to the quantum version here, that is, the Poisson bracket should correspond to the commutator. But in more cases, there should be some correction terms. Fortunately, in the sense of modulo lower terms, they should be in correspondence.

Here is a simple fact.

Theorem 1.10. *If $a \in \mathcal{S}(\mathbb{R}^n \times \mathbb{R}^n)$, then $a^w(x, D) : L^2 \rightarrow L^2$.*

Proof. For $u \in \mathcal{S}$, it is easy to check $a^w(x, D)u \in \mathcal{S}$. Since $\mathcal{S} \subset L^2$ is dense, one only need to show $\|a^w(x, D)u\|_{L^2} \leq C\|u\|_{L^2}$ for $u \in \mathcal{S}$, then one can extend the operator to act on L^2 by density. For $u \in \mathcal{S}$, we write

$$\mathcal{F}(a^w(x, D)u)(\eta) = \frac{1}{(2\pi)^n} \iiint a\left(\frac{x+y}{2}, \xi\right) e^{i(x-y)\xi} u(y) e^{-i\langle x, \eta \rangle} dy d\xi dx.$$

By writing the phase as follows

$$\langle x - y, \xi \rangle - \langle x, \eta \rangle = -2\left\langle \frac{x+y}{2}, \eta - \xi \right\rangle - \langle y, 2\xi - \eta \rangle,$$

we get

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

where $\widehat{a}_1(\zeta, \xi) = \int a(z, \xi) e^{-i(z, \zeta)} dz$, which is also in \mathcal{S} since $a \in \mathcal{S}$. Then it suffices to show $\|Kv\|_{L^2} \leq C\|v\|_{L^2}$ for all $v \in L^2$, where

$$Kv(\eta) = \int K(\eta, \zeta) v(\zeta) d\zeta, \quad K(\eta, \zeta) = \widehat{a}_1(\eta - \zeta, \frac{\eta + \zeta}{2}).$$

Hence, the kernel $K(\eta, \zeta)$ satisfies

$$\int |K(\eta, \zeta)| d\eta \leq C, \quad \int |K(\eta, \zeta)| d\zeta \leq C$$

for some constant C . Thus, by Schur's criterion for boundedness on L^2 or by Cauchy inequality directly, we have

$$\begin{aligned}\|Kv\|_{L^2}^2 &= \int \left| \int K(\eta, \zeta) v(\zeta) d\zeta \right|^2 d\eta \leq \int \left(\int |K(\eta, \zeta)| d\zeta \right) \left(\int |K(\eta, \zeta)| |v(\zeta)|^2 d\zeta \right) d\eta \\ &\leq C \iint |K(\eta, \zeta)| |v(\zeta)|^2 d\zeta d\eta \leq C \int \left(\int |K(\eta, \zeta)| d\eta \right) |v(\zeta)|^2 d\zeta \leq C^2 \|v\|_{L^2}^2,\end{aligned}$$

which completes the proof. \square

And we present some worth-knowing non-simple facts, though they may not be used in this course.

Theorem 1.11 (Calderon-Vaillancourt Theorem). *Suppose a is a smooth function such that $|\partial_{x, \xi}^\alpha a| \leq C_\alpha$ for all $x, \xi \in \mathbb{R}^n$, then $a^w(x, D) : L^2 \rightarrow L^2$.*

Theorem 1.12 (Beals's theorem). *Suppose $A : L^2 \rightarrow L^2$ is bounded linear and*

$$ad_{x_{j_1}} ad_{\xi_{j_1}} \cdots ad_{x_{j_l}} ad_{\xi_{j_l}} A : L^2 \rightarrow L^2$$

bounded, where $ad_B A = [B, A]$. Then there exists a smooth function a such that $|\partial_{x, \xi}^\alpha a| \leq C_\alpha$ and $A = a^w(x, D)$.

And here is a fact which follows from general theory.

Proposition 1.13. *Suppose $a_j(x, \xi) = \sum_{|\alpha| \leq m_j} a_{j, \alpha}(x) \xi^\alpha$. Then $a_1^w(x, D) \circ a_2^w(x, D) = a_3^w(x, D)$ and*

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

which is actually a finite sum since when k grows, it will eventually kills a_1, a_2 as they are polynomials.

In particular,

$$i[a_1^w(x, D), a_2^w(x, D)] = \{a_1, a_2\}^w + \text{lower order differential operators},$$

where the left hand side is of order $m_1 + m_2 - 1$.

1.4. Quantum dynamics.

Definition 1.14. The magnetic Schrödinger operator is given by

$$P = \frac{1}{2} \sum_{j=1}^3 (D_{x_j} - A_j(x))^2. \quad (1.2)$$

Remark 1.15. One thing to note that is the operator seems to strongly depend on the form of A_j , but A_j is not uniquely determined by the magnetic field \vec{B} . We will come back to this point later.

In order to develop the properties of the magnetic Schrödinger operator P , we assume $A_j(x)$ is linear and hence \vec{B} is constant. Then we study the following operator in a more general form

$$P = p^w(x, D) = \frac{1}{2} \langle AD_x, D_x \rangle + \frac{1}{2} \langle BD_x, x \rangle + \frac{1}{2} \langle x, BD_x \rangle + \frac{1}{2} \langle Cx, x \rangle,$$

where $A = A^T, C = C^T$ are $n \times n$ real matrices and its symbol is

$$p = \frac{1}{2} \langle A\xi, \xi \rangle + \langle B\xi, x \rangle + \frac{1}{2} \langle Cx, x \rangle.$$

The following theorem serves as an example for the general functional analysis stuffs.

Theorem 1.16. Suppose $\mathcal{D}(N_p) = \mathcal{S}$, $N_p u = Pu$ and $\mathcal{D}(M_p) = \{u \in L^2 : Pu \in L^2\}$, $M_p u = Pu$. Then

- (1) M_p is closed;
- (2) $\bar{N}_p = M_p$;
- (3) $N_p^* = M_p^* = \bar{M}_p$.

In the definition of $\mathcal{D}(M_p)$ above, $Pu \in L^2$ can be understood as follows. Since P is a well-defined differential operator, so $Pu \in \mathcal{S}'$ naturally. Furthermore, if $Pu \in L^2$ at the same time, then we say $u \in \mathcal{D}(M_p)$.

Proof. • It suffices to show the graph of M_p is closed. Suppose $\mathcal{D}(N_p) \ni u_j \xrightarrow{L^2} u$, $p^w(x, D)u_j \xrightarrow{L^2} v \in L^2$. Since $u_j \xrightarrow{L^2} u$ implies $u_j \xrightarrow{\mathcal{S}'} u$ and hence $p^w(x, D)u_j \xrightarrow{\mathcal{S}'} p^w(x, D)u$. Hence, $v = p^w(x, D)u$ as \mathcal{S}' and since $v \in L^2$, they are identical as L^2 functions. Thus, $u \in \mathcal{D}(M_p)$.

- Note that $\bar{N}_p = M_p$ if and only if for all $u \in \mathcal{D}(M_p)$, there exists $\mathcal{D}(N_p) = \mathcal{S}$ such that $u_\varepsilon \xrightarrow{L^2} u$ and $p^w(x, D)u_\varepsilon \xrightarrow{L^2} p^w(x, D)u$.

Take $\chi \in C_c^\infty(\mathbb{R}^n; [0, 1])$, $\chi \equiv 1$ in $B(0, 1)$. Let $\Psi_\varepsilon := \chi(\varepsilon x)\chi(\varepsilon D_x)$, then $\Psi_\varepsilon : L^2 \rightarrow \mathcal{S}$. Now we prove $\Psi_\varepsilon u \xrightarrow{L^2} u$ as follows.

$$\begin{aligned} \|\chi(\varepsilon x)\chi(\varepsilon D_x)u - u\|_{L^2} &\leq \|(\chi(\varepsilon x) - 1)\chi(\varepsilon D_x)u\|_{L^2} + \|(\chi(\varepsilon D_x) - 1)u\|_{L^2} \\ &\leq \|(\chi(\varepsilon x) - 1)(\chi(\varepsilon D_x) - 1)u\|_{L^2} + \|(\chi(\varepsilon x) - 1)u\|_{L^2} + \|(\chi(\varepsilon D_x) - 1)u\|_{L^2} \end{aligned}$$

By the bounded convergence theorem, $\|(\chi(\varepsilon D_x) - 1)u\|_{L^2} \rightarrow 0$ and $\|(\chi(\varepsilon x) - 1)u\|_{L^2} \rightarrow 0$. Moreover, $(\chi(\varepsilon x) - 1)$ is bounded on L^2 . Hence, $\|\chi(\varepsilon x)\chi(\varepsilon D_x)u - u\|_{L^2} \rightarrow 0$.

Put $u_\varepsilon := \Psi_\varepsilon u$. Now it suffices to show $p^w u_\varepsilon \xrightarrow{L^2} p^w u$. We write

$$p^w u_\varepsilon = \Psi_\varepsilon p^w u + [p^w, \Psi_\varepsilon]u = (p^w u)_\varepsilon + [p^w, \Psi_\varepsilon]u.$$

As we have seen before, $(p^w u)_\varepsilon \xrightarrow{L^2} p^w u$, so we need to show $[p^w, \Psi_\varepsilon]u \rightarrow 0$ as $\varepsilon \rightarrow 0$.

We cheat a little bit to replace $\Psi_\varepsilon(x, D) = (\chi(\varepsilon x)\chi(\varepsilon \xi))^w$ and then we will have $[p^w, \Psi_\varepsilon(x, D)] = \{p, \Psi_\varepsilon\}^w(x, D)$.

Since

$$\begin{aligned} \{\Psi_\varepsilon, p\}^w &= \sum_{j=1}^n (\partial_{x_j} p(x, \xi) \partial_{\xi_j} \Psi_\varepsilon - \partial_{\xi_j} p(x, \xi) \partial_{x_j} \Psi_\varepsilon)^w \\ &= \varepsilon \chi(\varepsilon x) A x \partial_\xi \chi(\varepsilon D) + \text{terms of analogous form,} \end{aligned} \tag{1.3}$$

which shall be bounded on L^2 uniformly with respect to ε since terms like $\varepsilon \chi(\varepsilon x) A x$ is uniformly bounded. Take $\tilde{\chi} \in C_c^\infty(B(0, 1); [0, 1])$ and $\tilde{\chi} \equiv 1$ near 0, and $\tilde{\Psi}_\varepsilon := \tilde{\chi}(\varepsilon x)\tilde{\chi}(\varepsilon D_x)$. By the support conditions of $\Psi_\varepsilon, \tilde{\Psi}_\varepsilon$, we know that $\tilde{\chi}(\varepsilon x)\partial\chi(\varepsilon x) = 0$ and $\tilde{\chi}(\varepsilon D)\partial\chi(\varepsilon D) = 0$. Hence, by the explicit formula (1.3),

$$\begin{aligned} \|[p^w, \Psi_\varepsilon(x, D)]\tilde{\Psi}_\varepsilon\|_{L^2 \rightarrow L^2} &= \|\varepsilon \chi(\varepsilon x) A x \partial_\xi \chi(\varepsilon D) \tilde{\chi}(\varepsilon x) \tilde{\chi}(\varepsilon D)\|_{L^2 \rightarrow L^2} + \text{terms of analogous form} \\ &\leq \|\varepsilon \chi(\varepsilon x) A x \partial_\xi \chi(\varepsilon D) \tilde{\chi}(\varepsilon x) \tilde{\chi}(\varepsilon D)\|_{L^2 \rightarrow L^2} + \text{terms of analogous form,} \end{aligned}$$

and using the support conditions and the commutator estimates $\|[\tilde{\chi}(\varepsilon x), \tilde{\chi}(\varepsilon D)]\|_{L^2 \rightarrow L^2} = \mathcal{O}(\varepsilon^2)$ like $\|[x, \tilde{\chi}(\varepsilon x)]\|_{L^2 \rightarrow L^2} = \mathcal{O}(\varepsilon)$ and so on on different terms appropriately, which implies

$$\|[p^w, \Psi_\varepsilon(x, D)]\tilde{\Psi}_\varepsilon\|_{L^2 \rightarrow L^2} = \mathcal{O}(\varepsilon).$$

We write

$$\|[p^w, \Psi_\varepsilon(x, D)]u\| \leq \|[p^w, \Psi_\varepsilon(x, D)]\tilde{\Psi}_\varepsilon u\| + \|[p^w, \Psi_\varepsilon(x, D)](1 - \tilde{\Psi}_\varepsilon)u\| \leq \mathcal{O}(\varepsilon)\|u\| + C\|(1 - \tilde{\Psi}_\varepsilon)u\|,$$

where the last term tends to 0 as $\varepsilon \rightarrow 0$, which completes the proof.

- We claim $M_p^* \subset M_{\bar{p}}$. It suffices to show $\mathcal{D}(M_p^*) \subset \mathcal{D}(M_{\bar{p}})$. For each $v \in \mathcal{D}(M_p^*)$, there exists $C(v)$ such that for all $u \in \mathcal{D}(M_p) \supset \mathcal{S}$, $|\langle M_p u, v \rangle| \leq C(v)\|u\|$. Then for all $u \in \mathcal{S}$, $v \in L^2$, M_p acts on u as a differential operator, the pairing $\langle M_p u, v \rangle$ is just the distributional pairing $\langle v, M_p u \rangle_{\mathcal{S}' \times \mathcal{S}}$ and hence by the definition of the distributional derivative, we have

$$\langle v, M_p u \rangle_{\mathcal{S}', \mathcal{S}} = \langle M_{\bar{p}} u, v \rangle_{\mathcal{S}', \mathcal{S}}.$$

Thus,

$$|\langle u, M_{\bar{p}} v \rangle| \leq C(v)\|u\|_{L^2}$$

holds for all $u \in \mathcal{S}$, which implies $M_{\bar{p}}v \in L^2$. Hence, $v \in \mathcal{D}(M_{\bar{p}})$, that is, the claim is true.

Then it follows from $\mathcal{D}(N_{\bar{p}}) = \mathcal{S}$ that $N_{\bar{p}} \subset N_p^*$. And then N_p^* is densely defined and hence by Proposition 1.5,

$$N_{\bar{p}} \subset N_p^* = \overline{N_p^*} = M_p^*. \quad (1.4)$$

On the other hand,

$$M_{\bar{p}} = \overline{N_{\bar{p}}} \subset M_p^*,$$

where the first step follows from the second property we have proved and the last step from (1.4) and Proposition 1.5. Hence, $M_{\bar{p}} = M_p^* = N_p^*$. \square

The theorem we proved can be applied to show $-\Delta - |x|^2$ is essentially self-adjoint if the domain is Schwartz functions. And now we go back to discuss the magnetic Schrödinger operator.

2. MAGNETIC SCHRÖDINGER OPERATOR

Without loss of generality, we assume $\vec{B} = (0, 0, B)$. As noted before, \vec{A} is not uniquely determined by \vec{B} since modifying \vec{A} by a gradient will not change \vec{B} .

Now we choose the Landau gauge $A = (0, Bx_1, 0)$ such that the magnetic Schrödinger operator defined in (1.2) is of the form

$$P_B = D_{x_1}^2 + (D_{x_2} + Bx_1)^2 + D_{x_3}^2 = (\xi_1^2 + (\xi_2 + Bx_1)^2 + \xi_3^2)^w. \quad (2.1)$$

Here are two central examples of operators.

2.1. Spectrum of Laplacian. Let $P = -\Delta$, $\mathcal{D}(P) = \{u \in L^2 : \Delta u \in L^2\}$. And we define $U : L^2 \rightarrow L^2$ by

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

where the integral is meant as the distributional Fourier transform, which is unitary on L^2 . Therefore,

$$(UPU^*v)(\xi) = |\xi|^2v(\xi).$$

If $z \notin [0, \infty)$, then $(|\xi|^2 - z)^{-1} \in L^\infty$ and serves as a bounded inverse of $UPU^* - z$. And one can show $\text{Spec}(P) = [0, +\infty)$.

Then we can look at the propagators. For the Schrödinger equation $(i\partial_t - P)u = 0$, it is easy to solve by using Fourier transform that $v(t, \xi) = e^{-it|\xi|^2}v(0, \xi)$. We call $\lambda = |\xi|^2$ to be the dispersion relation for P and the Schrödinger equation.

If one want to find solution to the eigenvalue equation $-\Delta u = \lambda u$, then $\text{supp}\hat{u}(\xi) \subset \{|\xi|^2 - \lambda = 0\}$, which implies that $\hat{u} \notin L^2$.

For $P = |D| = \sqrt{-\Delta}$, we have $UPU^*v(\xi) = |\xi|v(\xi)$. The evolution is governed by $(i\partial_t - P)u = 0$ and hence $(i\partial_t - |\xi|)v(\xi) = 0$. In this case, the dispersion relation is $\lambda = |\xi|$.

This equation is a half-wave equation and the Schrödinger equation is a dispersive equation.

2.2. Spectrum of harmonic oscillator. Let

$$P_\omega = -\Delta + \sum_{j=1}^n \omega_j^2 x_j^2 = \sum_{j=1}^n (D_{x_j}^2 + \omega_j^2 x_j^2),$$

where $\omega_j > 0$, which is called the quantum harmonic oscillator.

For $P_\omega = p^w(x, D)$ and $p(x, \xi) = |\xi|^2 + \sum_j \omega_j^2 x_j^2$. We want to find a change of variable $x = \alpha y$ and $D_x = \frac{1}{\alpha} D_y$ such that $D_x^2 + \omega^2 x^2 = \omega(D_y^2 + y^2)$. By comparing the coefficients, we find that $\omega = \frac{1}{\alpha^2}$ works. Moreover, note that if $j \neq k$, then $D_{x_j}^2 + \omega_j^2 x_j^2$ commutes with $D_{x_k}^2 + \omega_k^2 x_k^2$. Then, it suffices to consider this operator on the real line.

Let $P = D_x^2 + x^2$, $A = D_x - ix$ and $A^* = D_x + ix$, where we don't care about the domain here. A direct computation implies

$$A^*A = P - 1, \quad AA^* = P + 1, \quad [A, A^*] = 2.$$

Next we want to find $\ker A$. For $v_0 \in \ker A$, $(\partial_x + x)v_0 = 0$, which can be solved explicitly that $v_0(x) = e^{-x^2/2} \in L^2$. Then $(P-1)v_0 = A^*Av_0 = 0$ and hence $Pv_0 = v_0$, that is, $v_0 \in L^2$ is a very nice state and also an eigenfunction of P . We notice $PA^*v_0 = (A^*A+1)A^*v_0 = 3A^*v_0$, so let $v_1 = A^*v_0$ and then we have $Pv_1 = 3v_1$. By induction,

$$P((A^*)^n v_0) = (2n+1)(A^*)^n v_0,$$

that is, using A^* we create excited states from the state v_0 . This is why we usually call A^* as the creation operator. And A is an annihilation operator because you can check A acting on $(A^*)^n v_0$ will lower your eigenvalue by 2. And induction also implies $v_n = (A^*)^n v_0 \in L^2$. For $m > n$, we write

$$\langle (A^*)^n v_0, (A^*)^m v_0 \rangle = \langle A^m (A^*)^n v_0, v_0 \rangle = \langle A^{m-1} (A^*A + 2)(A^*)^{n-1} v_0, v_0 \rangle = \dots = 0,$$

where the last step is because one have $m > n$, so one can kill all the A^* right before v_0 and then using $Av_0 = 0$ to conclude. In other words, $\left\{ u_n = \frac{v_n}{\|v_n\|} \right\}$ is an orthonormal set.

By induction,

$$u_n = \frac{1}{\|v_n\|} (D_x + ix)^n e^{-\frac{x^2}{2}} = H_n(x) e^{-\frac{x^2}{2}}, \quad (2.2)$$

where $H_n(x)$ is a polynomial of degree n with nonvanishing leading coefficients such that $H_n(-x) = (-1)^n H_n(x)$. These are called the Hermite polynomials.

Now we claim that $\text{span}\{u_n\} = L^2(\mathbb{R})$. Suppose not, then there exists $g \in L^2$ such that

$$0 = \int g(x) \overline{u_n(x)} dx = \int_{\mathbb{R}} g(x) \overline{H_n(x)} e^{-\frac{x^2}{2}} dx,$$

which implies that for all $n \geq 0$,

$$\int g(x) x^n e^{-\frac{x^2}{2}} dx = 0.$$

Put $e^{-ix\xi} = \sum \frac{(-ix\xi)^n}{n!}$. Thanks to the trivial bound independent of N that $\left| \sum_{j=1}^N \frac{(-ix\xi)^j}{j!} \right| \leq \sum_{j=1}^N \frac{|x\xi|^j}{j!} \leq e^{|x\xi|}$ and the dominated convergence theorem, we have

$$\int g(x) e^{-\frac{x^2}{2}} e^{-ix\xi} dx = 0$$

for all ξ . Therefore, $g \equiv 0$. Contradiction! (Another way to show this is by showing $F(\xi) = \int g(x) e^{-\frac{x^2}{2}} e^{-ix\xi} dx$ is holomorphic and using dominated convergence theorem to show $F^{(k)}(0) = 0$ for all k .) Thus, $\{u_n\}$ form an orthonormal basis of $L^2(\mathbb{R})$.

So what we found is a map $U : L^2(\mathbb{R}) \rightarrow \ell^2(\mathbb{N})$ ($\mathbb{N} = \{0, 1, 2, \dots\}$) that turns this differential operator into a multiplication operator defined by

$$Uu(n) = \int u(x) \overline{u_n(x)} dx,$$

where $(UPU^*u)(n) = (2n+1)u(n)$. Moreover, U is unitary since $u(x) = \sum_n \langle u, u_n \rangle u_n$. And the domain for UPU^* is $\{u \in \ell^2 : \{(2n+1)u(n)\}_n \in \ell^2\}$. Thus, $\text{Spec}(P) = \{2n+1 : n \in \mathbb{N}\}$.

Finally, we can conclude for our operator at the beginning that

$$\text{Spec}\left(\sum_{j=1}^d (D_{x_j}^2 + \omega_j^2 x_j^2)\right) = \left\{ \sum_{j=1}^d \omega_j (2n_j + 1) : n_j \in \mathbb{N} \right\}$$

and the eigenfunctions of P_ω will be the product of the eigenfunction for 1-dimensional case.

Now we continue to discuss the magnetic Schrödinger operator (2.1).

2.3. Spectrum of the magnetic Schrödinger operator. Recall $P_B = D_{x_1}^2 + (D_{x_2} + Bx_1)^2 + D_{x_3}^2$. Note that the coefficients in x_2, x_3 variables are constant, it is more like a Laplacian in x_2, x_3 , so it is natural to take the unitary Fourier transform $U_1 : L^2 \rightarrow L^2$ in the last two variable

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

to get

$$U_1 P_B U_1^* v = (D_{x_1}^2 + (Bx_1 + \xi_2)^2 + \xi_3^2) v(x_1, \xi_2, \xi_3),$$

which looks like the form of harmonic oscillator with x_1 shifted by ξ_2 . Let $y_1 = \beta^{-1}(Bx_1 + \xi_2)$ with β to be determined, then $D_{y_1} = \frac{\beta}{B} D_{x_1}$ and hence

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

if we take $\beta = B^{\frac{1}{2}}$. So we set

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

where one can check directly by a change of variable that the coefficient $B^{-\frac{1}{4}}$ makes U_2 unitary and then $U_3 = U_2 U_1$ satisfies

$$U_3 P U_3^* v(y_1, \xi_2, \xi_3) = B(D_{y_1}^2 + y_1^2) + \xi_3^2.$$

Let $U_4 v(n, \xi_2, \xi_3) = \int v(y_1, \xi_2, \xi_3) \overline{u_n(y_1)} dy_1$, where $\{u_n\}$ are the same as those constructed in the example for harmonic oscillators in Section 2.2. Therefore, $U = U_4 U_3$ satisfies

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

where $U : L^2(\mathbb{R}^3) \rightarrow \ell^2(\mathbb{Z}, L^2(\mathbb{R}^2))$. Hence,

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

It is also natural to discuss the 2-dimensional version $P_B = D_{x_1}^2 + (D_{x_2} + Bx_1)^2$. In this case, what we have is much simpler:

$$(Uu)(n, \xi_2) = \frac{1}{\sqrt{2\pi}B^{\frac{1}{4}}} \int u(B^{-\frac{1}{2}}y_1 - B^{-1}\xi_2, x_2) \overline{u_n(y_1)} e^{-ix_2\xi_2} dx_2 dy_1 \quad (2.3)$$

and $UP_B U^* v(n, \xi_2) = (2n+1)Bv(n, \xi)$. Here $B, 3B, 5B, \dots$ in the spectrum are called Landau levels.

In 2-dimensional case,

$$\begin{aligned} H_n &= \{u \in L^2(\mathbb{R}^2) : P_B u = (2n+1)Bu\} = \{U^*(u_n(y)f(\xi_2)) : f \in L^2\} \\ &= \{B^{\frac{1}{4}} \frac{1}{\sqrt{2\pi}} \int u_n(B^{-\frac{1}{2}}y + B^{-1}\xi_2) f(\xi_2) e^{ix_2\xi_2} d\xi_2 : f \in L^2(\mathbb{R})\} \subset L^2. \end{aligned} \quad (2.4)$$

2.4. Instruction to calculate in a different gauge. The symmetric gauge is $A(x) = (-B\frac{x_2}{2}, B\frac{x_1}{2}, 0) = (0, Bx_1, 0) - \frac{B}{2}\nabla(x_1x_2)$. We do in dimension 2 and put $B = 1$. We using the holomorphic differentiation

$$\partial_w = \frac{1}{2}(\partial_x - i\partial_y), \quad \partial_{\bar{w}} = \frac{1}{2}(\partial_x + i\partial_y),$$

$$\mathcal{O}(\mathbb{C}) = \{u : \mathbb{C} \rightarrow \mathbb{C} : \overline{\partial_w} u = 0 \text{ in the sense of distributions}\},$$

then P has a nice characterization

$$\begin{aligned} P &= \left(\frac{1}{i}\partial_{x_1} - \frac{x_1}{2}\right)^2 + \left(\frac{1}{i}\partial_{x_2} + \frac{x_2}{2}\right)^2 = \left(-\Delta + \frac{|x|^2}{4}\right) + \frac{1}{2i}(x_1\partial_{x_2} - x_2\partial_{x_1}) \\ &= -4\partial_w\partial_{\bar{w}} + \frac{|w|^2}{2} + w\partial_w - \bar{w}\partial_{\bar{w}} = (-2\partial_w + \frac{1}{2}\bar{w})(2\partial_{\bar{w}} + \frac{1}{2}w) + 1, \end{aligned}$$

where the first one is like a harmonic oscillator and the second one is like the angular momentum. This allows us to find the ground state $Pu_0 = u_0$ for the magnetic Hamiltonian in this gauge since it suffices to find the kernel of $(-2\partial_w + \frac{1}{2}\bar{w})(2\partial_{\bar{w}} + \frac{1}{2}w)$. Moreover, $-2\partial_w + \frac{1}{2}\bar{w}$ is just the conjugate of $2\partial_{\bar{w}} + \frac{1}{2}w$, so it suffices to consider

$$(2\partial_{\bar{w}} + \frac{1}{2}w)u_0 = 0.$$

We observe that it has a solution $u_0(w, \bar{w}) = e^{-\frac{|w|^2}{4}}$. And using this function, one can find that all the solutions is of the form

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

where f is a function such that $\bar{\partial}f = 0$. (Note that in two dimension, $\bar{\partial}$ is elliptic, so distributional solution $\bar{\partial}f = 0$ would be at least C^2 . And by the theory of complex analysis, we know f is holomorphic.) Moreover, we want $u \in L^2$, so we need

$$f \in \{g \in \mathcal{O}(\mathbb{C}) : \int_{\mathbb{C}} |g|^2 e^{-\frac{|w|^2}{2}} dm(w) < +\infty\}.$$

This space is infinite dimensional, but all the polynomials in w lie in this space. Thus $\{(x_1 + ix_2)^m e^{-\frac{|x|^2}{4}} : m \in \mathbb{N}\}$ is a set of ground states, which form a basis of the eigenspace of 1 in our two dimensional case.

Though the ground states computed in the symmetric gauge look very different from those we derived in the Landau gauge, you have the freedom to take arbitrary $f \in L^2$ in (2.4), which may give you a similar form.

3. DENSITY OF STATES

For $P = -\Delta + \sum_{j=1}^3 \omega_j^2 x_j^2$, we have $\text{Spec}(P) = \{\sum_{j=1}^3 \omega_j(2n_j + 1) : n_j \in \mathbb{N}\}$. From the matrix case $P = U^* \Lambda U$ and $f(P) = U^* f(\Lambda) U$, we expect

$$\text{tr} f(P) = \sum_{\lambda \in \text{Spec}(P)} f(\lambda) = \int f(\lambda) d\mu(\lambda),$$

where $f \in \mathcal{S}(\mathbb{R})$, $\mu = \sum_{\lambda_j \in \text{Spec}(P)} \delta_{x_j}$.

In this section, we introduce the trace class operator to make sense of the trace of operators on Hilbert space. And finally we will show the existence of the limit

$$\tilde{\text{tr}} f(P) = \lim_{L \rightarrow \infty} \frac{\text{tr}(1_{[-L, L]^3} f(P))}{(2L)^3}$$

and explain why we see oscillations for specific functions in the behavior in the density states of the functions.

3.1. Quick introduction to trace class operator.

Theorem 3.1 (Riesz theorem). *For compact operator $A : H \rightarrow H$, the spectrum of A satisfies*

$$\text{Spec}(A) = \mathfrak{C}\{(A - \lambda)^{-1} : H \rightarrow H \text{ bounded}\} = \{\lambda_j(A)\}_{j=0}^J,$$

where $\lambda_j(A) \rightarrow 0$ if $J = \infty$.

If $A = A^*$ is self-adjoint, then by the Spectral theorem

$$Au = \sum_j \lambda_j(A) e_j \otimes e_j,$$

where $(f \otimes g)(u) = f\langle u, g \rangle$, $\{e_j\}$ is an orthonormal basis for H consisting of eigenvectors for A .

Remark 3.2. The convention $(f \otimes g)(u) = f\langle u, g \rangle$ here may look weird, physicists prefer to use the bra-ket notation:

$$\langle u | v \rangle := \langle v, u \rangle, \quad |f\rangle\langle g| := f \otimes g, \quad |f\rangle\langle g | u \rangle := (f \otimes g)(u).$$

Theorem 3.3 (Singular value decomposition). *Let A be a compact operator, then there exists $s_0 \geq s_1 \geq \dots \geq s_j \rightarrow 0$ as $j \rightarrow \infty$ (or just finitely many) and $\{e_j\}, \{f_j\}$ are orthonormal sets such that $A = \sum_j s_j(A) f_j \otimes e_j$. Moreover, the numbers of s_j depending only on this decomposition are called singular values of A . In fact,*

$$\{s_j\} \setminus \{0\} = \text{Spec}((A^*A)^{\frac{1}{2}}) \setminus \{0\} = \text{Spec}((AA^*)^{\frac{1}{2}}) \setminus \{0\}.$$

Proof. We only show the main idea. Note that $A^*A : H \rightarrow H$ be the compact self-adjoint operator and non-negative since $\langle A^*Au, u \rangle = \|Au\|^2 \geq 0$. Then we take $\{e_j\}$ to be an orthonormal set of eigenfunctions of $\lambda_j(A^*A)$, which is defined to be $s_j(A) := \lambda_j(A^*A)$. Let

$$f_j := \begin{cases} s_j^{-1}(A)Ae_j, & s_j \neq 0, \\ 0, & s_j = 0. \end{cases}$$

One can check by a direct computation using self-adjointness that $\langle f_k, f_l \rangle = \delta_{kl}$. \square

Here are a list of properties that can be proved by using the singular value decomposition.

Proposition 3.4. *For compact operators A, B , we have*

- $s_n(A) = \min\{\|A - K\|_{H \rightarrow H} : \text{rank } K \leq n\}$;
- $s_{j+k}(A + B) \leq s_j(A) + s_k(B)$;
- $s_{j+k}(AB) \leq s_j(A)s_k(B)$;
- $s_j(AB) \leq \|A\|s_j(B)$.

One can find the precise statement of these properties in [2, Lecture 23], where the condition of A, B both compact may be loosen a bit.

Example 3.5. *Suppose $A : L^2(\mathbb{T}^n) \rightarrow H^s(\mathbb{T}^n)$ is a bounded operator with $s \geq 0$, $\mathbb{T}^n = \mathbb{R}^n / (2\pi\mathbb{Z})^n$, where*

$$H^s(\mathbb{T}^n) := \left\{ u \in L^2 : (1 + m^2)^{s/2} \widehat{u}(m) \in \ell^2(\mathbb{Z}^n), \widehat{u}(m) = \int_{\mathbb{T}^n} u(x) e^{-ix \cdot m} dx \right\}.$$

*And we assume the spectrum of A^*A is purely discrete such that the singular values are well-defined. (Or we just assume A is compact for simplicity.)*

We claim that $s_j(A) \leq Cj^{-s/n}$. We write

$$s_j(A) = s_j \left((-\Delta + I)^{-s/2} (-\Delta + I)^{s/2} A \right) \leq s_j \left((-\Delta + I)^{-s/2} \right) \left\| (-\Delta + I)^{s/2} A \right\|_{L^2 \rightarrow L^2},$$

where $(-\Delta + I)^{-s/2}$ is a self-adjoint operator given as a multiplier. It suffices to check by counting

$$\#\{j : s_j \leq r\} = \#\{m \in \mathbb{Z}^n : (|m|^2 + 1)^{s/2} \leq r\} \leq r^{n/s},$$

for all $r \in \mathbb{R}$, which implies

$$s_j \geq Cj^{\frac{s}{n}}.$$

Hence,

$$s_j \left((-\Delta + I)^{-s/2} \right) = \frac{1}{s_j \left((-\Delta + I)^{s/2} \right)} \leq \frac{1}{Cj^{\frac{s}{n}}}, \quad (3.1)$$

which proves the claim. Then, since the singular values tends to 0, and using the singular value decomposition, (it's true when we know the spectrum of A^*A is discrete) we know $A = \sum_{j=1}^{\infty} s_j(A) f_j \otimes e_j$. Since $s_j(A) \rightarrow 0$, the finite rank operator

$$A_J = \sum_{j \leq J} s_j(A) f_j \otimes e_j$$

converges to A in operator norm sense, which implies $A : L^2(\mathbb{T}^n) \rightarrow H^s(\mathbb{T}^n)$ is compact.

Note that the proof still works if we consider the operator as $A : L^2(\mathbb{R}^n) \rightarrow H^s(\mathbb{T}^n)$.

3.2. Trace class operators and Hilbert Schmidt operators.

Definition 3.6 (Trace class). We define

$$\mathcal{L}_1(H) = \{A : H \rightarrow H \text{ compact} : \sum_j s_j(A) < \infty\},$$

to be the trace class operators with the norm $\|A\|_1 := \sum_j s_j(A)$.

Definition 3.7. The trace of $A \in \mathcal{L}_1(H)$ is defined as

$$\text{tr}A = \sum_j \langle AE_j, E_j \rangle,$$

where $\{E_j\}$ is any orthonormal basis of H .

The trace is well-defined since one can just write the change of basis explicitly. And there's also another quick way to prove the definition is independent of the choice of the basis. We only need to check by computation that by using the singular value decomposition that

$$\sum_j \langle AE_j, E_j \rangle = \sum_j s_j(A) \langle f_j, e_j \rangle,$$

where $\{e_j\}, \{f_j\}$ are the ones chosen in the singular value decomposition theorem, Theorem 3.3.

Here we present two nontrivial facts.

Theorem 3.8 (Lidskii's theorem). Suppose $A \in \mathcal{L}_1(H)$ and $\text{Spec}(A) = \{\lambda_j(A)\}_{j=0}^{\infty}$, then $\text{tr}(A) = \sum_j \lambda_j(A)$.

Theorem 3.9 (Special case of Weyl inequality). For $A \in \mathcal{L}_1(A)$ and we assume $|\lambda_0| \geq |\lambda_1| \geq \dots$ and $s_0 \geq s_1 \geq \dots$, then

$$\sum_{j=1}^N |\lambda_j| \leq \sum_{j=1}^N s_j, \quad \prod_{j=1}^N (1 + |\lambda_j|) \leq \prod_{j=1}^N (1 + s_j),$$

for all N .

Now let's see an example.

Example 3.10. Let $A : L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)$ such that $A \in \mathcal{L}_1(L^2)$, which is given by an integral kernel

$$Au(x) = \int_{\mathbb{R}^n} K_A(x, y)u(y) dy.$$

Then by Theorem 3.3, we write

$$A = \sum_j s_j(A) f_j \otimes e_j$$

and hence

$$Au(x) = \sum_j s_j(A) f_j(x) \int u(y) \overline{e_j(y)} dy,$$

which implies that

$$K_A(x, y) = \sum_j s_j(A) f_j(x) \overline{e_j(y)}. \quad (3.2)$$

Then by expanding $\{e_j\}$ such that $\{e_j\}$ is an orthonormal basis with $s_j(A)$ possibly zero, we finally find that

$$\text{tr}A = \sum_j \langle Ae_j, e_j \rangle = \sum_j s_j(A) \langle f_j, e_j \rangle = \int_{\mathbb{R}^n} K_A(x, x) dx.$$

Remark 3.11. Note that the integrability of $K_A(x, x)$ will not show the compactness of A . Take $Au(x) = u(ax)$ with $a \neq 1$. Then Schwartz kernel will be $K_A(x, y) = \delta(y - ax)$, then $K_A(x, x) = \delta((1 - a)x) = |1 - a|^{-1} \delta(x)$. Though $\int K_A(x, x) = \frac{1}{|1 - a|}$ is finite, but obviously, A is not compact.

Now let's start with the Laplacian.

Example 3.12. Let U be the unitary Fourier transform, then

$$f(-\Delta)u(x) := Uf(|\xi|^2)U^*u = \frac{1}{(2\pi)^n} \int e^{i\langle x-y, \xi \rangle} f(|\xi|^2)u(y) dy d\xi.$$

Suppose $f \in \mathcal{S}(\mathbb{R})$, then

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

Using the Schur's lemma, we know $A : L^2 \rightarrow L^2$ bounded. For $\chi \in C_c^\infty(\mathbb{R}^n)$, we claim $A = \chi f(-\Delta) \in \mathcal{L}_1$. Now we need to extract the decay property of the kernel

$$K_A(x, y) = \chi(x) \frac{1}{(2\pi)^n} \int f(|\xi|^2) e^{i\langle x-y, \xi \rangle} d\xi \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n).$$

By choosing the support of χ sitting in some torus, that is, $\text{supp}\chi \subset \mathbb{T}^n$, the image is supported in the torus and actually it takes $L^2(\mathbb{R}^n)$ to any Sobolev spaces on torus, namely $H^s(\mathbb{T}^n)$ for all $s > 0$. Using $(1 + |x - y|^2)e^{i\langle x-y, \xi \rangle} = (1 - \Delta_\xi)e^{i\langle x-y, \xi \rangle}$, the integration by parts trick will tell us that $K_A(x, y)$ decays like $\frac{1}{\langle x-y \rangle^N}$ for all N . Hence, $A : L^2(\mathbb{R}^n) \rightarrow H^s(\mathbb{T}^n)$.

Thus, for s sufficiently large, $H^s \subset L^2$ is a compact inclusion and $\sum s_j$ is summable thanks to (3.1), so $A \in \mathcal{L}_1(L^2(\mathbb{R}^n))$.

Note that $1_{[-L,L]^n}$ is bounded and hence $1_{[-L,L]^n}A$ is also a trace class operator. Then, by taking $\chi \equiv 1$ on $[-L, L]^n$, $1_{[-L,L]^n}f(-\Delta) = 1_{[-L,L]^n}\chi f(-\Delta)$ is a trace class operator.

Moreover, we have

$$\text{tr}f(-\Delta) = \int 1_{[-L,L]^n}(x) \frac{1}{(2\pi)^n} \int f(|\xi|^2) d\xi = (2L)^n \frac{1}{(2\pi)^n} \int f(|\xi|^2) d\xi. \quad (3.3)$$

Definition 3.13. A compact operator A is called a Hilbert Schmidt operator if $\sum_j s_j(A)^2 < \infty$.

Proposition 3.14. A bounded operator A is a trace class operator if and only if it can be expressed as the composition of two Hilbert Schmidt operators.

Proof. Suppose A is a trace class operator, then A has the following singular value decomposition

$$A = \sum_j s_j(A) f_j \otimes e_j.$$

Let

$$A_1 := \sum_k s_k(A)^{\frac{1}{2}} e_k \otimes e_k, \quad A_2 := \sum_k s_k(A)^{\frac{1}{2}} f_k \otimes e_k.$$

We compute

$$\begin{aligned} A_2 A_1 u &= \sum_{k,l} s_k(A)^{\frac{1}{2}} s_l(A)^{\frac{1}{2}} (f_k \otimes e_k) \circ (e_l \otimes e_l)(u) = \sum_{k,l} s_k(A)^{\frac{1}{2}} s_l(A)^{\frac{1}{2}} \langle u, e_l \rangle (f_k \otimes e_k)(e_l) \\ &= \sum_{k,l} s_k(A)^{\frac{1}{2}} s_l(A)^{\frac{1}{2}} \langle u, e_l \rangle \delta_{l,k} f_k = \sum_l s_l(A) \langle u, e_l \rangle f_l = Au. \end{aligned}$$

To prove the converse, note that

$$s_{2k}(A_1 A_2) \leq s_k(A_1) s_k(A_2), \quad s_{2k+1}(A_1 A_2) \leq s_k(A_1) s_{k+1}(A_2),$$

and it follows from the Cauchy-Schwartz inequality. \square

Proposition 3.15. Let $A : L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n)$ be a compact operator, which is given by an integral kernel

$$Au(x) = \int_{\mathbb{R}^n} K_A(x, y) u(y) dy.$$

Then A is a Hilbert Schmidt operator if and only if $K_A(x, x) \in L^2$.

Proof. Suppose $A = \sum_j s_j(A) f_j \otimes e_j$ is the singular value decomposition, then by (3.2),

$$\int |K_A(x, x)|^2 dx = \sum_{j,k} s_j(A) s_k(A) f_j(x) \overline{e_j(x) f_j(x) e_k(x)} = \sum_j s_j(A)^2,$$

which completes the proof. \square

3.3. Density of states. In physics, density of states is the number of states per energy interval per unit volume. For $f \in \mathcal{S}(\mathbb{R})$, the following limit

$$\lim_{L \rightarrow +\infty} \frac{\operatorname{tr} (1_{[-L, L]^n} f(P))}{(2L)^n}.$$

turns out to exist for magnetic operators $P = P_B$ and $P = -\Delta$ and determines the density of states. Thanks to (3.3), we know that

$$\frac{\operatorname{tr} (1_{[-L, L]^n} f(P))}{(2L)^n} = \frac{1}{(2\pi)^n} \int f(|\xi|^2) d\xi = \frac{1}{(2\pi)^n} \int f(s) \delta(s - |\xi|^2) ds d\xi = \int f(s) d\rho(s),$$

where the measure

$$d\rho(s) := \frac{1}{(2\pi)^n} \int \delta(s - |\xi|^2) d\xi = \frac{\operatorname{vol}(\mathbb{S}^{n-1})}{(2\pi)^n} \int_0^\infty \delta(s - r^2) r^{n-1} dr = \frac{\operatorname{vol}(\mathbb{S}^{n-1})}{2(2\pi)^n} s_+^{\frac{n-2}{2}}$$

somehow measures the number of states per energy per unit volume.

Now let's do the same calculation to Landau Hamiltonian in dimension 2. As discussed in Section 2.3, $P_B = D_{x_1}^2 + (D_{x_2} + Bx_1)^2$ and $P_B = U^*(B(2n+1))U$, where $U : L^2(\mathbb{R}^2) \rightarrow \ell^2(\mathbb{N}; L^2(\mathbb{R}^2))$ is defined by

$$\begin{cases} Uu(n, \xi_2) = \frac{B^{\frac{1}{4}}}{\sqrt{2\pi}} \int u(x_1, x_2) \overline{u_n(B^{\frac{1}{2}}x_1 + B^{-\frac{1}{2}}\xi_2)} e^{-ix_2\xi_2} dx_2 dx_1, \\ U^*v(x_1, x_2) = \frac{B^{\frac{1}{4}}}{\sqrt{2\pi}} \sum_{n \in \mathbb{N}} \int u_n(B^{\frac{1}{2}}x_1 + B^{-\frac{1}{2}}\xi_2) v(n, \xi_2) e^{ix_2\xi_2} d\xi_2, \end{cases}$$

which is exactly the same formula as in (2.3) if we perform the change of variable $y_1 = B^{\frac{1}{2}}x_1 + B^{-\frac{1}{2}}\xi_2$.

Now, we write

$$f(P_B)u = U^*f((2n+1)B)Uu = \int K(x, x')u(x') dx',$$

where the integral kernel satisfies

$$K(x, x') = \frac{B^{\frac{1}{2}}}{2\pi} \sum_n \int u_n(B^{\frac{1}{2}}x_1 + B^{-\frac{1}{2}}\xi_2) \overline{u_n(B^{\frac{1}{2}}x'_1 + B^{-\frac{1}{2}}\xi_2)} f(B(2n+1)) e^{i(x_2 - x'_2)\xi_2} d\xi_2.$$

Using the same type of argument as in Example 3.12, localizing in space and noting that u_n defined in (2.2), one can show that $f(P_B) \in \mathcal{L}_1(L^2(\mathbb{R}^2))$. Therefore, it follows from Example 3.10 that

$$\begin{aligned} \tilde{\operatorname{tr}} f(P_B) &:= \frac{\operatorname{tr} (1_{[-L, L]^2} f(P_B))}{(2L)^2} = \frac{1}{(2L)^2} \int 1_{[-L, L]^2}(x) K(x, x) dx \\ &= \frac{1}{(2L)^2} \int 1_{[-L, L]^2}(x) \sum_n f(B(2n+1)) dx = \frac{B}{2\pi} \sum_n f(B(2n+1)) = \int f(s) \rho_B(s) ds, \end{aligned}$$

where the density of states is

$$\rho_B(s) = \frac{B}{2\pi} \sum_n \delta(s - (2n+1)B).$$

The same type of argument can be applied to 3 dimensional case and the result should be

$$\begin{aligned}\tilde{\text{tr}}f(P_B) &= \frac{B}{(2\pi)^2} \sum_n \int_{\mathbb{R}} f((2n+1)B + \xi_3^2) d\xi_3 \\ &= \frac{B}{2(2\pi)^2} \int_0^\infty \sum_{n=0}^\infty f(B(2n+1) + y) \frac{dy}{\sqrt{y}} \\ &= \frac{B}{2(2\pi)^2} \int_0^\infty f(s) \sum_{n \in \mathbb{N}} (s - (2n+1)B)_+^{-\frac{1}{2}} ds = \int f(s) \rho_B(s) ds = \rho_B(f).\end{aligned}$$

We only do a sanity check that

$$\tilde{\text{tr}}f(P_B) \rightarrow \tilde{\text{tr}}f(-\Delta)$$

as $B \rightarrow 0$. We write

$$\begin{aligned}\tilde{\text{tr}}f(P_B) &= \frac{B}{(2\pi)^2} \int_{\mathbb{R}} \sum_{n=0}^\infty f(B(2n+1) + \xi_3^2) d\xi_3 \\ &\rightarrow \frac{1}{2} \frac{1}{(2\pi)^2} \int f(s + \xi_3^2) ds d\xi_3 = \frac{1}{(2\pi)^2} \int \rho f(\rho^2 + \xi_3^2) d\rho d\xi_3 = \frac{1}{(2\pi)^3} \int f(|\xi|^2) d\xi\end{aligned}$$

as $B \rightarrow 0$, where the limit follows from the definition of Riemann sum and the last step follows from the cylindrical change of variable.

3.4. Free energy per unit volume.

Definition 3.16. *The free energy per unit volume is defined as*

$$\Omega(z_0, B, N, T) := Nz_0 - \tilde{\text{tr}}f_{z_0, T}(P_B),$$

where

$$f_{z_0, T}(x) := T \log \left(1 + \exp\left(\frac{z_0 - x}{T}\right) \right)$$

for $T > 0$.

This definition is motivated by the Fermi-Dirac distribution in physics. Here, N is the number of particles. Strictly speaking, z_0 is determined by B, T via the equation $\frac{\partial \Omega}{\partial z_0} = 0$. But, we will just fix z_0 as a number such that

$$\begin{cases} z_0 \sim N, & n = 2, \\ z_0^{\frac{3}{2}} \sim N, & n = 3, \end{cases}$$

which is the case that determined by $\frac{\partial \Omega}{\partial z_0} = 0$ when $B = T = 0$ and we omit the calculus here. Note that $f_{z_0, T}(x) \equiv 0$ if $x > z_0$ and decay exponentially like $z_0 - x$ for $x \in (0, z_0)$. This shows that $f_{z_0, T}$ is Schwartz on the positive half real line, which is all we need to justify the definition $f(P_B)$ using the characterization $f((2n+1)B)$. Hence, everything is well-defined and one can check by using the result in preceding subsection.

Definition 3.17. *Here's a concept called magnetization, defined by $m(B, T) = \partial_B \Omega(B, T)$.*

By classical analysis, we want to see that there are oscillations as $T \rightarrow 0$. In the sense of distributions, we have

$$\begin{cases} f_{T,z_0} \rightarrow (z_0 - x)_+^1, \\ f'_{T,z_0} \rightarrow -(z_0 - x)_+^0, \\ f''_{T,z_0} \rightarrow \delta_{z_0}(z), \end{cases}$$

as $T \rightarrow 0$, where $x_+^\gamma = \begin{cases} x^\gamma, & x > 0, \\ 0, & x \leq 0. \end{cases}$

For the two dimensional case,

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

and hence

$$\begin{aligned} \partial_B \Omega(B, T) &= -\frac{1}{2\pi} \sum_n f_{T,z_0}(B(2n+1)) - \sum_n \frac{B(2n+1)}{2\pi} f'_{T,z_0}(B(2n+1)) \\ &\rightarrow \frac{1}{2\pi} \left(-\sum_n (z_0 - B(2n+1))_+^1 + \sum_n B(2n+1)(z_0 - B(2n+1))_+^0 \right) \\ &= \frac{1}{2\pi} \left(-\sum_n (z_0 - B(2n+1))(z_0 - B(2n+1))_+^0 + \sum_n B(2n+1)(z_0 - B(2n+1))_+^0 \right) \\ &= \frac{1}{2\pi} \sum_{2n+1 \leq \frac{z_0}{B}} (-z_0 + 2B(2n+1)) = \frac{M+1}{2\pi} (2(M+1)B - z_0), \end{aligned}$$

where $M = \lfloor \frac{z_0 - B}{2B} \rfloor$. Thus, note that $2BM \sim z_0$ when $B \rightarrow 0$, it is easy to check by a direct computation that

$$m(B, 0) = \frac{M+1}{2\pi} (2(M+1)B - z_0) \sim \frac{z_0}{2\pi} \left(\left\lfloor \frac{z_0/B - 1}{2} \right\rfloor - \frac{z_0/B - 1}{2} + \frac{1}{2} \right) + \mathcal{O}(B),$$

where $\sigma(y) = \lfloor \frac{y-1}{2} \rfloor - \frac{y-1}{2} + \frac{1}{2}$ is a periodic function.

In three dimensional case,

$$\begin{aligned} m(B, 0) &= \partial_B \left(Nz_0 - \frac{4}{3} (2\pi)^{-2} B \sum_n (z_0 - (2n+1)B)_+^{\frac{3}{2}} \right) \\ &= \frac{1}{(2\pi)^2} \sum_{n \in \mathbb{N}} \left(-\frac{4}{3} (z_0 - (2n+1)B)_+^{\frac{3}{2}} + 2(2n+1)B (z_0 - (2n+1)B)_+^{\frac{1}{2}} \right) \\ &= \frac{1}{(2\pi)^2} \sum_{n \in \mathbb{N}} \left(-\frac{10}{3} (z_0 - (2n+1)B)_+^{\frac{3}{2}} + 2z_0 (z_0 - (2n+1)B)_+^{\frac{1}{2}} \right) \\ &= \frac{1}{(2\pi)^2} \left(\left(-\frac{10}{3} z_0^{\frac{3}{2}} r_{\frac{3}{2}}(B/z_0) + 2z_0^{\frac{3}{2}} r_{\frac{1}{2}}(B/z_0) \right) \right), \end{aligned}$$

where in the third step, we write $(2n+1)B$ in the second term as $(2n+1)B - z_0 + z_0$. And we care about small B here and $r_\gamma(h)$ is defined as

$$r_\gamma(h) := \sum_{n \in \mathbb{N}} (1 - (2n+1)h)_+^\gamma.$$

Then we only need to care about the asymptotic expansion of r_γ , which is a classical analysis problem. In the end, we will see that the leading part has a purely oscillatory profile. Now we don't need to care about the physics and only need to do some classical analysis.

3.5. Some classical analysis. In this subsection, we build up the asymptotics of

$$r_\gamma(h) := \sum_{n \in \mathbb{N}} (1 - (2n+1)h)_+^\gamma$$

as $h \rightarrow 0$ when $\gamma > 0$.

Theorem 3.18 (Hankel's formula). *The inverse of $\Gamma(z+1) = \int_0^\infty e^{-t} t^z dt$ can be expressed as*

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

which is called Hankel's formula.

Proof. Let $f(\sigma) := \sigma_+^z e^{-\sigma c}$, which is integrable since $c > 0$. Then taking Fourier transform implies

$$\widehat{f}(s) = \int_0^\infty \sigma^z e^{-\sigma(c+is)} d\sigma.$$

We choose $z \in \mathbb{C} \setminus (-\infty, 0]$, we pick a branch of $(\sigma(c+is))^z$ and make a formal change of variable

$$\widehat{f}(s) = \int_0^\infty \frac{(\sigma(c+is))^z}{(c+is)^{z+1} e^{\sigma(c+is)}} d(\sigma(c+is)) = \frac{1}{(c+is)^{z+1}} \int_0^\infty t^z e^{-t} dt = \frac{\Gamma(z+1)}{(c+is)^{z+1}},$$

which can be made rigorous by contour deformation. Then taking the inverse Fourier transform implies

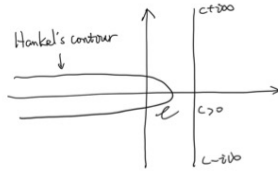
$$\sigma_+^z e^{-\sigma c} \Gamma(z+1)^{-1} = \frac{1}{2\pi} \int_{-\infty}^\infty \frac{e^{i\sigma s}}{(c+is)^{z+1}} ds = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} u^{-z-1} e^{u\sigma} e^{-\sigma c} du. \quad (3.4)$$

Put $\sigma = 1$, we get the Hankel's formula. \square

Remark 3.19. By deforming to the Hankel's contour, one can make sense of the Hankel's formula to all $z \in \mathbb{C}$

$$\frac{1}{\Gamma(z+1)} = \frac{1}{2\pi i} \int_{\mathcal{C}} u^{-z-1} e^u du,$$

where the Hankel's contour is as follows:



Now set $f_\gamma(s) := \sum_{n \in \mathbb{N}} (s - (2n + 1))_+^\gamma$, $r_\gamma(h) = h^\gamma f_\gamma(\frac{1}{h})$. Then what we care about is the asymptotics of f_γ as $s \rightarrow \infty$. By (3.4), we have

$$\sigma_+^\gamma = \frac{1}{2\pi i} \Gamma(\gamma + 1) \int_{c-i\infty}^{c+i\infty} e^{t\sigma} e^{-\gamma-1} dt.$$

Put $\sigma = s - (2n + 1)$ and note that

$$\sum e^{t(s-(2n+1))} = e^{ts} \sum e^{-t(2n+1)} = e^{ts} \frac{1}{2 \sinh(t)},$$

which implies

$$\begin{aligned} f_\gamma(s) &= \frac{1}{4\pi i} \Gamma(\gamma + 1) \int_{c-i\infty}^{c+i\infty} e^{ts} \frac{1}{\sinh t} t^{-\gamma-1} dt \\ &= \sum_{n>0} \Gamma(\gamma + 1) (-1)^n (\pi n)^{-\gamma-1} \cos(n\pi s - \frac{\pi}{2}(\gamma + 1)) + \frac{\Gamma(\gamma + 1)}{2} \frac{1}{2\pi i} \int_{\mathcal{C}} e^{st} (\sinh t)^{-1} t^{-\gamma-1} dt, \end{aligned}$$

where the sum in the last equation is the sum of all residues of $e^{ts} \frac{1}{\sinh t} t^{-\gamma-1}$ at $k\pi i$ for all $k \in \mathbb{Z}_+$. In fact, for $n = 1$, it is pretty good to describe the asymptotics, but as a math class, we need to justify the integral in the last equation is comparably small. We choose the Hankel's contour $\mathcal{C} = \mathcal{C}_1 \cup \mathcal{C}_2 \cup \mathcal{C}_3$ as shown in the graph, where the distances of \mathcal{C}_1 and \mathcal{C}_3 to the real line are less than ε .



We will see that the dominate contribution for this integral comes from \mathcal{C}_2 . The estimate for the integral along $\mathcal{C}_1 \cup \mathcal{C}_3$ is rather easy,

$$\int_{\mathcal{C}_1 \cup \mathcal{C}_3} e^{st} (\sinh t)^{-1} t^{-\gamma-1} dt = \mathcal{O}(\varepsilon^{-\gamma-2} e^{-\varepsilon s}).$$

For the integral along \mathcal{C}_2 , due to the expansion $\frac{t}{\sinh t} = 1 + \sum_{j=1}^{2M} \gamma_j t^{2j} + \mathcal{O}(t^{2M+2})$, we write

$$\int_{\mathcal{C}_2(\varepsilon)} e^{st} (\sinh t)^{-1} t^{-\gamma-1} dt = \mathcal{O}(\varepsilon^{2M+1-\gamma} e^{\varepsilon s}) \frac{\Gamma(\gamma + 1)}{2} \sum_{j=0}^{2M} \gamma_j \frac{1}{2\pi i} \int_{\mathcal{C}_2(\varepsilon)} e^{st} t^{2j-\gamma-2} dt.$$

Since each integrand $e^{st} t^{2j-\gamma-2}$ has exponentially decay on the contour when $t \rightarrow -\infty$, we can open $\mathcal{C}_2(\varepsilon)$ up again to \mathcal{C} up to an error $\mathcal{O}(\varepsilon^{-\gamma-2} e^{-\varepsilon s})$ of the same type as before.

Now, by the Hankel's formula, we have

$$\frac{1}{2\pi i} \int_{\mathcal{C}} e^{st} t^{2j-\gamma-2} dt = \frac{1}{2\pi i} \int_{\mathcal{C}} e^{st} \frac{(st)^{2j-\gamma-2} d(st)}{s^{2j-\gamma-1}} = s^{-2j+\gamma+1} \frac{1}{\Gamma(\gamma+2-2j)}.$$

Combining the formulas above, we get

$$\begin{aligned} f_{\gamma}(s) &= \sum_{n>0} \Gamma(\gamma+1) (-1)^n (\pi n)^{-\gamma-1} \cos(n\pi s - \frac{\pi}{2}(\gamma+1)) \\ &\quad + \frac{\Gamma(\gamma+1)}{2} \sum_{j=0}^{2M} \frac{\gamma_j}{\Gamma(\gamma+2-2j)} s^{-2j+\gamma+1} + \mathcal{O}(\varepsilon^{-\gamma-2} e^{-\varepsilon s} + \varepsilon^{2M+1-\gamma} e^{\varepsilon s}). \end{aligned}$$

Choosing ε such that $\varepsilon^{-\gamma-2} e^{-\varepsilon s} = \varepsilon^{2M+1-\gamma} e^{\varepsilon s}$, that is $\varepsilon = \frac{2M+3}{2s} \log \frac{1}{2}$, then $\mathcal{O}(\varepsilon^{-\gamma-2} e^{-\varepsilon s} + \varepsilon^{2M+1-\gamma} e^{\varepsilon s}) = \mathcal{O}(s^{-\delta M})$, which shows that

$$f_{\gamma}(s) \sim \sum_{n>0} \Gamma(\gamma+1) (-1)^n (\pi n)^{-\gamma-1} \cos(n\pi s - \frac{\pi}{2}(\gamma+1)) + \frac{\Gamma(\gamma+1)}{2} s^{\gamma+1} \sum_{j=0}^{2M} \frac{\gamma_j}{\Gamma(\gamma+2-2j)} s^{-2j}.$$

Here's a final conclusion, stated as a theorem.

Theorem 3.20. *As $B \rightarrow 0$,*

$$B^{-\frac{1}{2}} m(B, 0) = 2(2\pi)^{-2} \left(\sum_{n>0} \Gamma\left(\frac{3}{2}\right) (-1)^n (\pi n)^{\frac{3}{2}} \cos\left(n\pi\left(\frac{z_0}{B}\right) - \frac{3\pi}{4}\right) + \mathcal{O}(B^{\frac{1}{2}}) \right),$$

where the non-oscillatory terms become the lower order terms.

4. BLOCH-FLOQUET THEORY

4.1. Motivation and physics background. So far, we study the free electron in electric/magnetic fields. In this section, we will now consider a bunch of 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 (like a lattice), which we assume do not move or interact with each other.

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

$$-\Delta + V(x), \quad V \in C^{\infty}, \quad V(x + \gamma) = V(x), \quad \gamma \in \gamma_1 \mathbb{Z} \oplus \gamma_2 \mathbb{Z}$$

with $\{\gamma_1, \gamma_2\}$ linearly independent. 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. This approximation is acceptable due to the following reasons.

The transition from physical modeling to non-interacting pseudo-particles modeling of the actual quantum mechanical system is now most frequently done using the density functional theory. It is an approach to study 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. One can consult [5] and [6] for a more detailed discussion and references on density functional theory.

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

$$\langle \widehat{H}\psi, \psi \rangle = \min_{\|\varphi\|=1} \langle \widehat{H}\varphi, \varphi \rangle,$$

In the non-interacting system (especially when considering electrons which are fermions - we will neglect such issues here), a composite ψ can be built 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.

The precise explanation of these things will be explained in the following subsection.

4.2. Honenberg-Kohn theorem and the passage to non-interacting electrons. A very general Hamiltonian describing an N -electron system is given by

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

where the first term is the kinetic energy

$$\widehat{T} = -\frac{1}{2} \sum_{j=1}^N \nabla_{x_j}^2, \quad x_j \in \mathbb{R}^3, j = 1, \dots, N$$

and throughout this subsection, we use x_j to denote a vector in \mathbb{R}^3 for $j = 1, \dots, N$. The repulsive Coulomb potential energy between the electrons given by

$$\widehat{V}_{ee} = \sum_{1 \leq i < j \leq N} \frac{1}{|x_j - x_i|}$$

involves the interactions between different electrons and the external potential \widehat{V} is the potential energy due to external forces, which is given by

$$\widehat{V} = \sum_{j=1}^N v(x_j).$$

Example 4.1. 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

$$v(x) = -\sum_{k=1}^M \frac{Z_k}{|x - X_k|},$$

where X_k is the position of the k th nucleus and Z_k is the number of protons it has.

Once we have the density operator, which is formally from $C^\infty(\mathbb{R}^3)$ to $C^\infty(\mathbb{R}^{3N})$ having the integral kernel $\widehat{n}(x) = \sum_{j=1}^N \delta(x - x_j)$. In other words, we can write

$$\widehat{V}(x_1, \dots, x_N) = \int v(x) \widehat{n}(x) d^3x.$$

From this, starting with a function $\Phi \in L^2(\mathbb{R}^{3N})$ with $\|\Phi\|_{L^2} = 1$, we can define an density function at least formally as

$$n(x) = \langle \widehat{n}(x)\Phi, \Phi \rangle_{L^2} = \sum_{j=1}^N \int_{\mathbb{R}^3} \dots \int_{\mathbb{R}^3} \Phi(x_1, \dots, x_N) \delta_{x-x_j} \overline{\Phi(x_1, \dots, x_N)} d^3x_1, \dots, d^3x_N,$$

where $\langle \widehat{n}(x)\Phi, \Phi \rangle_{L^2}$ is well-defined for $\Phi \in \mathcal{S}$ and then can be extended as functions from L^2 to L^1 by simply using Fubini's theorem.

In particular, if Φ can be expressed by $\Phi(x_1, \dots, x_N) = \varphi_1(x_1) \dots \varphi_N(x_N)$ with $\|\varphi_j\|_{L^2} = 1$, then

$$n(x) = \sum_{j=1}^N |\varphi_j(x)|^2$$

and hence $\int_{\mathbb{R}^3} n(x) dx = N$, which explains why $n(x)$ is called the density function of particles.

For an N -body system, what we are interested in is the ground state, which should be a minimizer of

$$\min_{\|\Phi\|_{L^2}=1} \langle \widehat{H}\Phi, \Phi \rangle.$$

If we start with the domain $\mathcal{D}(\widehat{H}) = C_0^\infty$, then \widehat{H} is essentially self-adjoint, which can be proved using analogous cut-off method as in Theorem 1.16. Like the finite dimensional case, the minimum E is an eigenvalue, which is the Lagrange multiplier of the minimizing problem, and the ground state Ψ will solve $\widehat{H}\Psi = E\Psi$.

In fact, even though Ψ is very complicated as a function in $3N$ variable, you lose no information to by considering $n(x)$ which is only in a single variable $x \in \mathbb{R}^3$. Here, "losing no information" is explained by the Hohenberg-Kohn Theorem in a mathematical way.

Given two Hamiltonians with fixed interparticle interaction (i.e. the interacting parts \widehat{T} and \widehat{V}_{ee} are the same for two Hamiltonians), if the ground states have the same density function, then then the external potential are the same up to a constant. But in physics, you never measure an eigenvalue, you measure differences between eigenvalues. So you lost no information by considering the density functions.

Theorem 4.2 (Hohenberg-Kohn Theorem). *Given a fixed interparticle interaction of N -electron, we suppose $\widehat{H}_1, \widehat{H}_2$ are two N -electron Hamiltonians with external potentials v_1, v_2 , respectively, and each of them has at least one L^2 normalized ground state ψ_1, ψ_2 respectively. If $n_1 = n_2 := n$, where $n_j(x)$ is defined to be*

$$n_j(x) := \langle \widehat{n}(x)\psi_j, \psi_j \rangle,$$

then $v_1 - v_2 = \text{const}$, where $\widehat{n}(x) = \sum_{j=1}^N \delta(x - x_j)$. In other words, the density function completely determines the system of the ground state.

Proof. Let ψ_j be the ground state of \widehat{H}_j , determined by

$$\langle \widehat{H}_j \psi_j, \psi_j \rangle = \min_{\|\psi\|=1} \langle \widehat{H}_j \psi, \psi \rangle,$$

and in particular, $\langle \widehat{H}_1 \psi_1, \psi_1 \rangle \leq \langle \widehat{H}_1 \psi_2, \psi_2 \rangle$. Now we calculate

$$\langle \widehat{V}_1 \psi_j, \psi_j \rangle = \int \langle v_1(x) \widehat{n}(x) \psi_j, \psi_j \rangle dx = \int v_1(x) \langle \widehat{n}(x) \psi_j, \psi_j \rangle dx = \int_{\mathbb{R}^3} v_1(x) n(x) dx,$$

which follows from $\widehat{V}(x_1, \dots, x_n) = \int v(x) \widehat{n}(x) dx$. Hence,

$$\langle \widehat{H}_1 \psi_1, \psi_1 \rangle = \langle (\widehat{T} + \widehat{V}_{ee}) \psi_1, \psi_1 \rangle + \int v_1(x) n(x) dx, \quad \langle \widehat{H}_1 \psi_2, \psi_2 \rangle = \langle (\widehat{T} + \widehat{V}_{ee}) \psi_2, \psi_2 \rangle + \int v_1(x) n(x) dx$$

and therefore,

$$\langle (\widehat{T} + \widehat{V}_{ee}) \psi_1, \psi_1 \rangle \leq \langle (\widehat{T} + \widehat{V}_{ee}) \psi_2, \psi_2 \rangle.$$

Moreover, exchange the subscripts 1 and 2 in all the derivation above, we get

$$\langle (\widehat{T} + \widehat{V}_{ee}) \psi_1, \psi_1 \rangle = \langle (\widehat{T} + \widehat{V}_{ee}) \psi_2, \psi_2 \rangle.$$

Thus, ψ_1, ψ_2 are ground states of both Hamiltonians and the theorem follows from the lemma below. (Since $\psi = \psi_1$ satisfies the assumption of the lemma below.) \square

Lemma 4.3. *If $\widehat{H}_j \psi = E_j \psi$ for $j = 1, 2$, then this implies $\widehat{V}_1 - \widehat{V}_2 = \text{const}$ and hence $v_1 - v_2 = \text{const}$.*

Proof. By subtracting, we get $(\widehat{V}_1 - \widehat{V}_2 - E_1 + E_2) \psi = 0$. Then we claim that

$$W(x_1, \dots, x_N) \psi(x_1, \dots, x_N) = 0$$

implies $W = 0$. Then we only need to rule out the possibility that for some (x_1, \dots, x_N) , $\psi(x_1, \dots, x_N) = 0$ and $W(x_1, \dots, x_N) \neq 0$.

One of the properties of the second order equation $\widehat{H} \psi = E \psi$ is the unique continuation property, which states as follows. If you have a L^2 normalized solution ψ to a second order PDE vanishes, then for any open set $U \subset \mathbb{R}^{3N}$, $\int_U |\psi|^2 > 0$. This is a mathematical explanation of tunneling and the proof uses Carleman estimates, where we don't go into details during the lecture. Some related materials can be found at [18, Chapter 7].

Now we go back to the Euler-Lagrange equation for the minimizing system, this means that $\widehat{H}_j \psi = E_j \psi$ for both $j = 1, 2$. If $W \psi = 0$, then $W |\psi|^2 = 0$ and hence

$$0 = \int W |\psi|^2 \leq \max_U W \int |\psi|^2, \quad 0 = \int W |\psi|^2 \geq \min_U W \int |\psi|^2,$$

which implies $\min_U W \leq 0 \leq \max_U W$. Take some neighborhood U of an arbitrary fixed point $(x_1, \dots, x_N) \in \mathbb{R}^{3N}$, $W(x_1, \dots, x_N) \leftarrow \min_U W \leq 0 \leq \max_U W \rightarrow W(x_1, \dots, x_N)$ as U shrinking to the single point set $\{(x_1, \dots, x_N)\}$. Thus, $W(x_1, \dots, x_N) = 0$.

Recall that

$$\widehat{V}_1(x_1, \dots, x_N) = \sum_{j=1}^N v_1(x_j),$$

then by taking $x_2, \dots, x_N = 0$, we derive from $\widehat{V}_1 - \widehat{V}_2 = \text{const}$ that $v_1 - v_2 = \text{const}$. \square

And there is an algorithm called the Kohn-Sham method [11] using the idea of the same philosophy.

4.3. Periodic structure and the Bloch transform. Now we consider $\Gamma = \gamma_1\mathbb{Z} + \gamma_2\mathbb{Z}$, where $\gamma_j \in \mathbb{R}^2$ and $\{\gamma_1, \gamma_2\}$ is linearly independent. We identify $\mathbb{R}^2 \simeq \mathbb{C}$, then $\gamma_k = 4\pi i\omega_k$ with $\omega = e^{\frac{2\pi i}{3}}$ produces a triangular lattice and this lattice can also be generalized to higher dimensions.

The general Hamiltonian should be a differential operator $P(x, D_x)$ of order 2 which has the property $P(x + \gamma, D_x) = P(x, D_x)$.

Example 4.4. (1) *The first example of such Hamiltonians is related to the mathematical model of crystals, which is given by $-\Delta + V(x)$ with $V \in C^\infty(\mathbb{R}^n; \mathbb{R})$ and $V(x + \gamma) = V(x)$.*

(2) *A second example is the periodic magnetic Schrödinger operator with potential*

$$P = \sum_{j=1}^2 (D_{x_j} + A_j(x))^2 + V(x), \quad A_k(x + \gamma) = A_k(x), V(x + \gamma) = V(x), \quad A_k, V \in C^\infty(\mathbb{R}^n; \mathbb{R}).$$

Remark 4.5. For $A = \sum_{j=1}^2 A_j dx_j$, there exists some scalar function $B(x)$ such that $B = dA = B(x)dx_1 \wedge dx_2$, where B is perpendicular to the (x_1, x_2) -plane. The condition to find periodic A if and only if $\int_{\mathbb{C}^2/\Gamma} B(x) dx_1 dx_2 = 0$, where in fancy language, it is equivalent to requiring the homology class of the form B is equal to zero. Here, \mathbb{C}^2/Γ is called the fundamental cell and we can think it as a torus.

It is easy to prove this equivalence by simply expressing the equality $B(x) = \partial_{x_1} A_2(x) - \partial_{x_2} A_1(x)$ by Fourier series if you are not a topologist.

A further remark is that by adding the assumption that A_j are periodic, it rules out the possibility of making B a constant magnetic field. Later, we will have something different to cover this case, which is more complicated.

In fact, there is a fundamental difference between the two examples in Example 4.4, which is described as follows. In the first example, $P\bar{u} = \overline{Pu}$. In other words, P commutes with complex conjugate in the first example, which is the time reversal symmetry for Schrodinger equation. However, in the second example,

$$\overline{Pu} = \sum_{j=1}^2 \overline{\left(\frac{1}{i}\partial_{x_j} + A_j(x)\right)^2 u + Vu} = \sum_{j=1}^2 \left(\frac{1}{i}\partial_{x_j} - A_j(x)\right)^2 \bar{u} + V\bar{u} = P_{-A}\bar{u},$$

where we use the subscript $-A$ to indicate the potential. This also relates to the topology of eigenspace, which we will discuss later.

Recall that we diagonalize the harmonic oscillator and one particle magnetic Schrödinger operator in the previous sections to study them. As before, we expect to diagonalize the Hamiltonian with periodic structure here.

Put $T_\gamma u(x) = u(x - \gamma)$ with $\gamma \in \Gamma$, which commutes with P , that is, $PT_\gamma = T_\gamma P$. A direct computation shows that $T_\gamma^* = T_{-\gamma} = T_\gamma^{-1}$. Recall that if we have a unitary matrix U and another matrix commutes with this one A , then one can diagonalize them simultaneously, namely, we can look for joint spectrum of A and U .

Heuristically, we will look the joint spectrum of P and T_γ . Let's find the spectrum of T_γ first. To find eigenvectors, we want to solve $u(x - \gamma) = a(\gamma)u(x)$, for all $\gamma \in \mathbb{Z}^n$. If we

consider tempered solutions, we can take the Fourier transform and that gives

$$(a(\gamma) - e^{-i\gamma\xi})\widehat{u}(\xi) = 0,$$

so support of \widehat{u} is on the set where $a(\gamma) - e^{-i\gamma\xi} = 0$. That implies that $|a| = 1$ so if $a(\gamma) = e^{i\alpha(\gamma)}$ and the support of u is on the set where $\sin((\gamma\xi - \alpha(\gamma))/2) = 0$ but this is supposed to be true for all γ and that forces \widehat{u} to be a combination of delta functions. Then one can see $\alpha(\gamma) = -\langle \gamma, k \rangle$ and $u(x) = e^{ikx}$ would work. This somehow motivates the way we diagonalize the operator.

Before we move on, we introduce some notations for lattices.

Definition 4.6. *The reciprocal lattice Γ^* of Γ is defined by*

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

Example 4.7. *If $\Gamma = \mathbb{Z}^2$, then $\Gamma^* = (2\pi\mathbb{Z})^2$.*

Now here is another better motivation for the Bloch transform.

Theorem 4.8. *For $u \in C^\infty(\mathbb{R}^n)$ such that for all $\gamma \in (2\pi\mathbb{Z})^n := \Gamma$, $u(x + \gamma) = u(x)$, we define the Fourier coefficients by*

$$\widehat{u}(k) = \frac{1}{(2\pi)^{\frac{n}{2}}} \int_{\mathbb{R}^n/\Gamma} u(x) e^{-i\langle x, k \rangle} dx,$$

Then

$$|\widehat{u}(k)| \leq C_N (1 + |k|)^{-N}.$$

Moreover, the Fourier series

$$u(x) = \frac{1}{(2\pi)^{\frac{n}{2}}} \sum_{k \in \mathbb{Z}^n} \widehat{u}(k) e^{i\langle k, x \rangle}$$

converges, where $\mathbb{Z}^n = ((2\pi\mathbb{Z})^n)^*$. And $\|u\|_{L^2}^2 = \|\widehat{u}\|_{\ell^2}^2 = (\sum |\widehat{u}(k)|^2)^{\frac{1}{2}}$.

Proof. Since u is smooth, $|\widehat{u}(k)| \leq C_N (1 + |k|)^{-N}$ follows from integration by parts by using $e^{-i\langle x, k \rangle} = \frac{(-\Delta_x + 1)}{1 + |k|^2} e^{-i\langle x, k \rangle}$.

The following proof of the Fourier inversion formula is due to Paul Chernoff, which is fairly neat. For $n = 1$, it suffices to show the formula at $x = 0$ since we can use the Fourier inversion formula for $v(x) = u(x_0 - x)$ at $x = 0$ with $\widehat{v}(k) = -e^{-i\langle x_0, k \rangle} \widehat{u}(-k)$. Moreover, it is enough to show if $u(0) = 0$, then $\sum_{k \in \Gamma^*} \widehat{u}(k) = 0$ since subtracting a constant from u will only contribute to a change of $\widehat{u}(0)$.

If $u(0) = 0$, then $u(2\pi k) = 0$ by periodicity and hence there exists some $f \in C^\infty$ such that $u(x) = (x - 2\pi k)f(x)$ near $x = 2\pi k$. Since $e^{ix} - 1$ is a periodic function with simple zeros of $2\pi k$, we can write $u(x) = (e^{ix} - 1)g(x)$ with $g \in C^\infty$. Now we compute the Fourier coefficients as follows. From

$$\frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{ix} g(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int g(x) e^{-i(k-1)x} dx = \widehat{g}(k-1),$$

it is obvious that $\widehat{u}(k) = \widehat{g}(k-1) - \widehat{g}(k)$, which completes the proof.

In higher dimensions, we complete the proof by applying the 1-dimensional case to it successively in each variable. \square

As a generalization, we have the following Fourier theories for arbitrary lattices. This motivates the definition of dual lattice (reciprocal lattice).

Theorem 4.9. *Now we assume $\Gamma = \gamma_1\mathbb{Z} \oplus \cdots \oplus \gamma_n\mathbb{Z}$ is an arbitrary lattice in \mathbb{R}^n with $\{\gamma_i\}_{i=1}^n$ linearly independent. The dual basis $\Gamma^* = \gamma_1^*\mathbb{Z} \oplus \cdots \oplus \gamma_n^*\mathbb{Z}$ is defined to satisfy $\langle \gamma_j^*, \gamma_j \rangle = 2\pi\delta_{ij}$. For $u(x + \gamma) = u(x), \gamma \in \Gamma$, we write*

$$\widehat{u}(k) = \frac{1}{|\mathbb{R}^n/\Gamma|^{\frac{1}{2}}} \int_{\mathbb{R}^n/\Gamma} u(x) e^{-i\langle x, k \rangle} dx, \quad k \in \Gamma^*,$$

then we have the inversion formula

$$u(x) = \frac{1}{|\mathbb{R}^n/\Gamma|^{\frac{1}{2}}} \sum_{k \in \Gamma^*} \widehat{u}(k) e^{i\langle k, x \rangle},$$

and $\|u\|_{L^2(\mathbb{R}^n/\Gamma)}^2 = \sum_{k \in \Gamma^*} |\widehat{u}(k)|^2$.

Sometimes we will view $\mathbb{R}^n/\Gamma^* = \mathbb{R}^n/\sim$ as a smooth manifold, where $x \sim y \iff x - y \in \Gamma^*$. We will use two kinds of manifolds in this course, which are torus and spheres.

Now we start to develop tools to diagonalize the periodic magnetic Schrödinger operator in Example 4.4, which satisfies $P(x + \gamma, D) = P(x, D)$.

For $\theta \in \mathbb{R}^n/\Gamma^* = \mathbb{R}^n/\sim$, there exists a Hilbert space \mathcal{H}_θ defined as

$$\theta \mapsto \mathcal{H}_\theta := \{u \in L_{loc}^2(\mathbb{R}^n) : u(x - \gamma) = e^{i\langle \gamma, \theta \rangle} u(x)\}. \quad (4.1)$$

In fancy language, this is the Hilbert bundle over a torus, namely for each $\theta \in \mathbb{R}^n/\Gamma^*$, you attach a Hilbert space.

Definition 4.10. *The Hilbert space $L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)$ is defined as follows. For any smooth function $g = g(\theta, x)$, $g \in L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)$ if the following facts hold:*

- (1) $g(\theta + k, x) = g(\theta, x), \quad \forall k \in \Gamma^*$;
- (2) $g(\theta, x - \gamma) = e^{i\langle \gamma, \theta \rangle} g(\theta, x), \quad \forall \gamma \in \Gamma$;
- (3) $\|g\|_{L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)}^2 := \int_{\mathbb{R}^n/\Gamma} \int_{\mathbb{R}^n/\Gamma^*} |g(\theta, x)|^2 d\theta dx < \infty$.

The space $L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)$ is actually the direct integral $\int_{\mathbb{R}^n/\Gamma^*}^{\oplus} \mathcal{H}_\theta d\theta$ just by definition. See [9, Chapter 7] for an introduction of direct integrals.

Definition 4.11. *For $u \in \mathcal{S}(\mathbb{R}^n)$, the Bloch transform of u is defined by*

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

One can check directly that $\mathcal{B}u(\theta, \cdot) \in \mathcal{H}_\theta$ by writing

$$\mathcal{B}u(\theta, x - \gamma) = \sum_{\alpha \in \Gamma} e^{-i\langle \alpha, \theta \rangle} u(x - \gamma - \alpha) = \sum_{\gamma' \in \Gamma} e^{-i\langle \gamma' - \gamma, \theta \rangle} u(x - \gamma') = e^{i\langle \gamma, \theta \rangle} \mathcal{B}u(\theta, x).$$

Theorem 4.12. *The Bloch transform \mathcal{B} defined in Definition 4.11 can be extended to a unitary operator $\mathcal{B} : L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)$. And $B^* = B^{-1} := \mathcal{C}$ satisfies*

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

Proof. We calculate, for $u \in \mathcal{S}$,

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

where we use the fact

$$\frac{1}{|\mathbb{R}^n/\Gamma^*|} \int_{\mathbb{R}^n/\Gamma^*} e^{-i\langle \gamma - \gamma', \theta \rangle} d\theta = \delta_{\gamma\gamma'}.$$

And now we check \mathcal{C} is an inverse. We also do for $u \in \mathcal{S}$ at first and then extend.

$$\mathcal{C}\mathcal{B}u(x) = \frac{1}{|\mathbb{R}^n/\Gamma^*|} \int_{\mathbb{R}^n/\Gamma^*} \left(\sum_{\gamma \in \Gamma} e^{-i\langle \gamma, \theta \rangle} u(x - \gamma) \right) d\theta = u(x),$$

since $\int_{\mathbb{R}^n/\Gamma^*} e^{-i\langle \gamma, \theta \rangle} d\theta = 0$ for all $\gamma \neq 0$. And it's more or less the same to check $\mathcal{B}\mathcal{C}v(\theta, x) = v(\theta, x)$. Finally, thanks to $\|\mathcal{B}u\|^2 = \|u\|^2$, we have $\langle \mathcal{B}^* \mathcal{B}(u+v), u+v \rangle = \langle u+v, u+v \rangle$, which implies $\langle \mathcal{B}^* \mathcal{B}u, v \rangle = \langle u, v \rangle$. Thus $\mathcal{B}^{-1} = \mathcal{B}^*$. \square

Here is a map from \mathcal{H}_θ to $L^2(\mathbb{R}^n/\Gamma)$ defined by $f \mapsto e^{i\langle x, \theta \rangle} f(x)$. In other words, $e^{i\langle x, \theta \rangle} f(x)$ is periodic. We check by writing $e^{i\langle x - \gamma, \theta \rangle} f(x - \gamma) = e^{i\langle x - \gamma, \theta \rangle} e^{i\langle \gamma, \theta \rangle} f(x) = e^{i\langle x, \theta \rangle} f(x)$. This motivates the definition of modified Bloch transform.

Definition 4.13. *For $u \in L^2(\mathbb{R}^n)$, we define the modified Bloch transform as*

$$(\tilde{B}u)(\theta, x) = e^{i\langle x, \theta \rangle} \mathcal{B}u(\theta, x).$$

Note that we gain periodicity of x but we lose the periodicity of θ , that is,

$$(\tilde{B}u)(\theta + k, x - \gamma) = e^{i\langle x, k \rangle} (\tilde{B}u)(\theta, x),$$

while $\mathcal{B}u(\theta + k, x) = \mathcal{B}u(\theta, x)$.

We claim that for $v = v(\theta, x) \in L^2(\mathbb{R}^n/\Gamma^*, \mathcal{H}_\theta)$,

$$\mathcal{B}P(x, D)\mathcal{B}^*v = P(x, D_x)v(\theta, x). \quad (4.2)$$

The key thing is $P(x, D)u(x - \gamma) = P(x - \gamma, D)u(x - \gamma)$ because we assume the coefficients of $P(x, D)$ to be periodic. This follows from $\mathcal{B}P(x, D)u = P(x, D)\mathcal{B}u$, which can be checked

directly by

$$\begin{aligned} P(x, D)\mathcal{B}u &= \frac{1}{|\mathbb{R}^n/\Gamma^*|^{\frac{1}{2}}} \sum_{\gamma \in \Gamma} e^{-i\langle \gamma, \theta \rangle} P(x, D)u(x - \gamma) \\ &= \frac{1}{|\mathbb{R}^n/\Gamma^*|^{\frac{1}{2}}} \sum_{\gamma \in \Gamma} e^{-i\langle \gamma, \theta \rangle} P(x - \gamma, D)u(x - \gamma) = \mathcal{B}P(x, D)u. \end{aligned}$$

Note that the operator $P(x, D_x)$ given by this equation above, which is not the same operator as $P(x, D)$, but we will abuse notation henceforth. Rigorously speaking, the domain of $P(x, D)$ is $H^2(\mathbb{R}^n)$ and the domain of $P(x, D_x)$ is $L^2(\mathbb{R}^n/\Gamma^*; H_{loc}^2(\mathbb{R}^n) \cap \mathcal{H}_\theta)$.

Moreover,

$$\tilde{\mathcal{B}}P(x, D)\tilde{\mathcal{B}}^*v(\theta, x) = e^{i\langle x, \theta \rangle} P(x, D_x) \left(e^{-i\langle x, \theta \rangle} v(\theta, x) \right) = P(x, D_x - \theta)v(\theta, x),$$

where we use

$$e^{i\langle x, \theta \rangle} D_x e^{-i\langle x, \theta \rangle} = D_x - \theta.$$

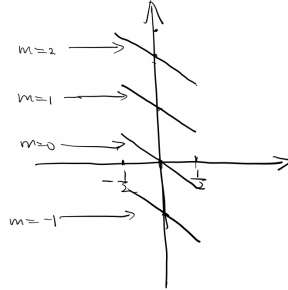
Note that $\tilde{\mathcal{B}}$ and \mathcal{B} are unitarily equivalent since $e^{i\langle x, \theta \rangle}$ is a unitary transformation. Now let's do a trivial example.

Example 4.14. Suppose $n = 1$ and $P = D_x$ with $\Gamma = 2\pi\mathbb{Z}$. On the Fourier side, $\widehat{P}u(\xi) = \xi\widehat{u}$. Here, Fourier transform is a unitary operator which diagonalize this operator, turning the operator into a multiplication. Then $\text{Spec}_{L^2(\mathbb{R})}(P)$ is the whole real line.

On the other hand, we can look at this operator on the modified Bloch side. By the previous discussion, for any fixed $\theta \in \mathbb{R}/\mathbb{Z}$, $\tilde{\mathcal{B}}P\tilde{\mathcal{B}}^* = D_x - \theta$ acts on periodic functions on the circle $H^1(\mathbb{R}/2\pi\mathbb{Z})$, which can be diagonalized by the transform $U : L^2(\mathbb{R}/2\pi\mathbb{Z}) \rightarrow L^2(\mathbb{R}/\mathbb{Z}; \ell^2(\mathbb{Z}))$, where

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

that is, we project things into eigenspaces, since $(D_x - \theta)e^{ixm} = (m - \theta)e^{ixm}$. So we can diagonalize our operator by $U\tilde{\mathcal{B}}P\tilde{\mathcal{B}}^*U^*u(\theta, m) = (m - \theta)u(\theta, m)$ for $\theta \in \mathbb{R}/\mathbb{Z}$. If we choose the fundamental cell to be $[-\frac{1}{2}, \frac{1}{2})$, then the spectrum looks like



Thus, as shown in the figure, we recover our result that $\text{Spec}(P) = \mathbb{R}$.

In general, we want to study the spectrum of $\text{Spec}_{L^2(\mathbb{R}^n/\Gamma)}(P(x, D_x - \theta))$ with the domain $\mathcal{D}(P(x, D_x - \theta)) = H^2(\mathbb{R}^n/\Gamma)$, where $P(x, D)$ is of the form $-\Delta + \langle a(x), D_x \rangle + b(x)$ with

periodic coefficients which satisfies $P = P^*$, then for each $\theta \in \mathbb{R}^2/\Gamma^*$, $P(x, D_x - \theta)$ is self-adjoint on $L^2(\mathbb{R}^2/\Gamma)$.

Definition 4.15. *The Sobolev spaces on the torus is defined by*

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

An easy exercise is that for $p \in \mathbb{N}$,

$$H^p(\mathbb{R}^n/\Gamma) = \{u \in L^2(\mathbb{R}^n/\Gamma) : D_x^\alpha \in L^2(\mathbb{R}^n/\Gamma), \forall |\alpha| \leq p\},$$

which is proved by using $\widehat{D_x^\alpha u}(k) = k_1^{\alpha_1} \dots k_n^{\alpha_n} \widehat{u}(k)$.

Lemma 4.16. *For $P(x, D) = -\Delta + \langle a(x), D_x \rangle + b(x)$ with periodic coefficients, there exists some constant C such that*

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

Proof. For $u \in C^\infty(\mathbb{R}^n/\Gamma)$, u periodic as a function on torus, then

$$\begin{aligned} \langle Pu, u \rangle &= - \int_{\mathbb{R}^n/\Gamma} \Delta u \bar{u} + \int \langle a(x), D_x \rangle u \bar{u} + \int b(x) u \bar{u} \\ &\geq \int |Du|^2 dx - \varepsilon \int |Du|^2 - \frac{C}{\varepsilon} \int |u|^2 - C \int |u|^2 \geq \frac{1}{2} \int |Du|^2 dx - \frac{C}{\varepsilon} \int |u|^2 - C \int |u|^2, \end{aligned}$$

Hence,

$$\int |Du|^2 \leq \int |Pu|^2 + \int |u|^2.$$

Furthermore, writing

$$\begin{aligned} |\langle Pu, Pu \rangle| &\geq \int \Delta u \overline{\Delta u} - \left| \int \langle a, D \rangle u \overline{\Delta u} \right| - \dots \geq \sum_{i,j} \int u_{x_i x_i} \bar{u}_{x_j x_j} - \int |D^2 u| |Du| - \dots \\ &\geq \sum_{i,j} \int |u_{x_i x_j}|^2 - \varepsilon \int |D^2 u|^2 - \frac{C}{\varepsilon} \int |Du|^2 - \frac{C}{\varepsilon} \int |u|^2, \end{aligned}$$

where $\sum_{i,j} |u_{x_i x_j}|^2 = |D^2 u|^2$ and hence

$$\int |D^2 u|^2 \leq \int |Pu|^2 + \int |u|^2.$$

The lemma follows by combining the two inequalities we get. \square

We also have self-adjointness, note that

$$P(x, D - \theta) = -\Delta + \langle a_\theta(x), D_x \rangle + b_\theta(x)$$

is self-adjoint, which implies $(P(x, D - \theta) + i)^{-1} : L^2(\mathbb{R}^n/\Gamma) \rightarrow L^2(\mathbb{R}^n/\Gamma)$. And actually, we can have something better. From the preceding lemma, if we solve

$$(P(x, D_x - \theta) + i) u = f \in L^2,$$

then we have

$$\|u\|_{H^2} \leq C \|f\|_{L^2} + C \|u\|_{L^2}.$$

And we already know that $P(x, D_x - \theta) + i$ is invertible on L^2 , thus $\|u\|_{L^2} \leq C\|f\|_{L^2}$ and hence the inverse map is bounded from L^2 to H^2 .

Hence, by the compact embedding, we know $(P(x, D - \theta) + i)^{-1}$ is a compact operator on $L^2(\mathbb{R}^n/\Gamma)$ and by Example 3.5, we know that the discrete spectrum of $(P(x, D - \theta) + i)^{-1}$ tends to 0. To be specific, we have

$$\text{Spec}((P(x, D_x - \theta) + i)^{-1}) = \{\mu_j(\theta)\}_{j=1}^{\infty},$$

with $\mu_j(\theta) \rightarrow 0$ as $j \rightarrow \infty$. Suppose the eigenfunction corresponding to μ_j is u_j , we define $U : L^2(\mathbb{R}^n) \rightarrow L^2(\mathbb{R}^n/\Gamma^*; \ell^2(\mathbb{N}))$ as

$$Uu(\theta, j) := \langle \tilde{B}u(\theta, \cdot), u_j(\theta, \cdot) \rangle$$

where

$$P(x, D_x - \theta)u_j(\theta, x) = E_j(\theta)u_j(\theta, x), \quad \frac{1}{E_j(\theta) + i} = \mu_j(\theta).$$

Note that $E_j(\theta)$ are real since they are the eigenvalues of the self-adjoint operator $P(x, D_x - \theta)$. Moreover, $E_j(\theta)$ is continuous in θ .

Then we can diagonalize P as

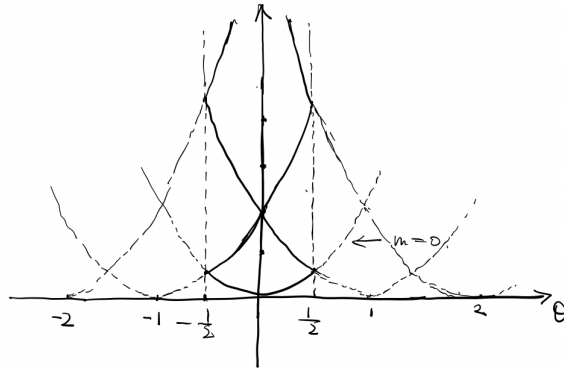
$$UP(x, D_x)U^*v(\theta, j) = E_j(\theta)v(\theta, j)$$

for $v \in L^2(\mathbb{R}^n/\Gamma^*; \ell^2(\mathbb{N}))$. Therefore,

$$\text{Spec}(P) = \bigcup_{j \in \mathbb{N}} I_j, \quad I_j := \bigcup_{\theta \in \mathbb{R}^n/\Gamma^*} E_j(\theta). \quad (4.3)$$

As a final remark, for fixed $\theta \in \mathbb{R}^n/\Gamma^*$, we know that $P(x, D_x - \theta)$ has discrete spectrum with all eigenvalues $\{E_j\}$ and hence the spectrum of $P(x, D_x)|_{\mathcal{H}_\theta}$ is also purely discrete. On the other hand, $\{E_j(\theta)\}$ are in the continuous spectrum of $P(x, D_x)$ on $L^2(\mathbb{R}^n)$.

Example 4.17. Suppose $n = 1$ and $P = D_x^2$, then $P_\theta = (D_x - \theta)^2$ and hence $\text{Spec}(P_\theta) = \{(m - \theta)^2 : m \in \mathbb{Z}\}$. Like in Example 4.14, we choose $[-\frac{1}{2}, \frac{1}{2})$ as the fundamental cell and draw the picture as follows.



4.4. Example: the bands opening up under perturbation. In this subsection, we discuss the following example. Suppose $n = 1$, $P_\lambda = D_x^2 + \lambda \cos x$ with $\Gamma = 2\pi\mathbb{Z}$. When $\lambda = 0$, the bands are continuous as we show in the preceding example. When $\lambda > 0$, the bands can open up, separated with each other. In order to analyze this operator, we need to introduce the Schur's complement formula in linear algebra.

Lemma 4.18 (Schur's complement formula). *If a matrix of operators $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is invertible and its inverse is given by $\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$, then a is invertible if and only if δ is invertible and $a^{-1} = \alpha - \beta\delta^{-1}\gamma$.*

The Schur's complement formula is very useful for the study of the Grushin problem

$$\begin{pmatrix} P - z & R_+ \\ R_- & 0 \end{pmatrix}^{-1} = \begin{pmatrix} E(z) & E_-(z) \\ E_+(z) & E_{-+}(z) \end{pmatrix},$$

where we use notation R, E for historical reasons.

We set up a Grushin problem as follows.

Lemma 4.19. *Given some positive integer k . Suppose*

$$\mathcal{P}(z) = \begin{pmatrix} P - z & R_- \\ R_+ & 0 \end{pmatrix} : H^2(\mathbb{R}^n/\Gamma) \times \mathbb{C}^k \rightarrow L^2(\mathbb{R}^n/\Gamma) \times \mathbb{C}^k,$$

is invertible and $\mathcal{P}(z)^{-1} = \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix}$. For any operator $Q : H^2(\mathbb{R}^n/\Gamma) \rightarrow L^2(\mathbb{R}^n/\Gamma)$, the perturbation $\mathcal{P}_\lambda(z) := \begin{pmatrix} P + \lambda Q - z & R_- \\ R_+ & 0 \end{pmatrix}$ is invertible for $|\lambda| \ll 1$ and

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

In particular,

$$E_{-+}^\lambda = E_{-+} - \lambda E_- Q E_+ + O(\lambda^2). \quad (4.4)$$

Proof. We write

$$\begin{aligned} \mathcal{P}_\lambda &= \mathcal{P} + \lambda \begin{pmatrix} Q & 0 \\ 0 & 0 \end{pmatrix} = \mathcal{P} \left(I + \lambda \mathcal{P}^{-1} \begin{pmatrix} Q & 0 \\ 0 & 0 \end{pmatrix} \right) = \mathcal{P} \left(I + \lambda \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix} \begin{pmatrix} Q & 0 \\ 0 & 0 \end{pmatrix} \right) \\ &= \mathcal{P} \left(I + \lambda \begin{pmatrix} E(z)Q & 0 \\ E_-(z)Q & 0 \end{pmatrix} \right), \end{aligned}$$

which implies

$$\begin{aligned} \begin{pmatrix} E_-^\lambda & E_+^\lambda \\ E_-^\lambda & E_{-+}^\lambda \end{pmatrix} &= \mathcal{P}_\lambda^{-1} = \left(I + \lambda \begin{pmatrix} E(z)Q & 0 \\ E_-(z)Q & 0 \end{pmatrix} \right)^{-1} \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix} \\ &= \left(1 + \sum_k (-\lambda)^k \begin{pmatrix} E(z)Q & 0 \\ E_-(z)Q & 0 \end{pmatrix}^k \right) \begin{pmatrix} E(z) & E_+(z) \\ E_-(z) & E_{-+}(z) \end{pmatrix}. \end{aligned}$$

□

Now we apply these to analyze our operator $P(x, D_x) = -\Delta + \langle a(x), D_x \rangle + b(x)$, and we assume P to have discrete spectrum and compact resolvent as the discussions in previous subsections.

Suppose z_0 is a simple eigenvalue of P with $Pu_0 = z_0u_0$ and $\|u_0\| = 1$. Then our goal now is to find $R_- : \mathbb{C} \rightarrow L^2(\mathbb{R}^2/\Gamma)$ and $R_+ : H^2(\mathbb{R}^n/\Gamma) \rightarrow \mathbb{C}$ so that for z near z_0 , $\mathcal{P}(z)$ is invertible.

We consider

$$\begin{cases} (P - z)u + R_-u_- = v, \\ R_+u = v_+, \end{cases}$$

and we choose

$$R_-u_- := u_-u_0, \text{ and } R_+u = R_-^*u = \langle u, u_0 \rangle.$$

Since $u = \sum_j u_j \langle u, u_j \rangle$, we have

$$\sum_{j=0}^{\infty} (z_j - z)u_j \langle u, u_j \rangle + u_-u_0 = \sum_{j=0}^{\infty} u_j \langle v, u_j \rangle.$$

By direct observation, $R_+E_+ = I, E_-R_- = I$. Then $E_- = R_+, E_+ = R_-$ by the choice of R_-, R_+ . Moreover, since $v = (P - z)Ev + R_-E_-v = (P - z)Ev + u_0 \langle v, u_0 \rangle$, which implies

$$E(z)v = \sum_{j \neq 0} \frac{1}{z - z_j} \langle v, u_j \rangle u_j.$$

Finally, $0 = (P - z)E_+v_- + R_-E_-v_- = (z_0 - z)v_-u_0 + E_-v_-u_0$, which implies $E_-v_- = z - z_0$. Hence, for $|\lambda| \ll 1$, we apply (4.4) to get

$$E_{-+}^\lambda(z) = E_{-+} - \lambda E_-QE_+ + O(\lambda^2) = z - z_0 - \lambda \langle Qu_0, u_0 \rangle + O(\lambda^2).$$

By Schur's lemma, $z(\lambda)$ is the eigenvalue of $P(\lambda) = P + \lambda Q$ if and only if $E_{-+}^\lambda(z) = 0$. Since $\frac{d}{dz}(z - z_0 - \lambda \langle Qu_0, u_0 \rangle + O(\lambda^2)) = 1 + O_z(\lambda^2) > 0$, we use the implicit function theorem to get

$$z(\lambda) = z_0 + \lambda \langle Qu_0, u_0 \rangle + O(\lambda^2),$$

which varies in a smooth way as λ changes and the eigenvalue moves if λ is nonzero.

As a by-product, we derive the Hellmann-Feynman formula $\dot{z}(0) = \langle Qu_0, u_0 \rangle$ from above. If we know that $\lambda \mapsto z(\lambda)$ is differentiable, then we can derive the Hellmann-Feynman formula as follows. For $P(\lambda) = P + \lambda Q$, we have the following implication

$$\begin{aligned} \frac{d}{d\lambda} (P(\lambda)u(\lambda) = z(\lambda)u(\lambda))|_{\lambda=0} &\Rightarrow Qu_0 + P\dot{u} = \dot{z}u_0 + z_0\dot{u}, \\ \Rightarrow \langle Qu_0, u_0 \rangle + \langle \dot{u}, Pu_0 \rangle &= \langle \dot{z}u_0 + z_0\dot{u}, u_0 \rangle = \dot{z}(0) + z_0 \langle \dot{u}, u_0 \rangle, \Rightarrow \langle Qu_0, u_0 \rangle = \dot{z}(0). \end{aligned}$$

Now we can apply these to $P_{\theta, \lambda} = (D_x - \theta)^2 + \lambda \cos x$ and we restrict our fundamental cell as $-\frac{1}{2} \leq \theta < \frac{1}{2}$. For $\lambda = 0$, we derive in Example 4.17 that $\text{Spec}(P_{\theta, 0}) = \{(m - \theta)^2 : m \in \mathbb{Z}\}$. From the picture in Example 4.17, there are two kinds of double points (intersections), which are the two type of solutions to

$$(m_1 - \theta)^2 = (m_2 - \theta)^2 \iff m_1 - \theta = \pm(m_2 - \theta).$$

The two cases are

$$\begin{cases} \theta = 0, & m_1 = m, & m_2 = -m, \\ \theta = \frac{1}{2}, & m_1 = m, & m_2 = -m_1 + 1. \end{cases}$$

Now we are going to the same thing as before. We consider the second case and show that the bands of $P_\lambda = D_x^2 + \lambda \cos x$ will open up at such points. Using the notations introduced before, the perturbation matrix is $Q = \cos x$. Note that $z_0 = (m - \frac{1}{2})^2$ is a double eigenvalue of $P_{\frac{1}{2}}$ with z near $\frac{1}{2}$. Then our goal is to find $R_- : \mathbb{C}^2 \rightarrow L^2(\mathbb{R}^n/\Gamma)$ and $R_+ : H^2(\mathbb{R}^n/\Gamma) \rightarrow \mathbb{C}^2$ so that $P(z)$ is invertible for z near z_0 . Let

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

and

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

with $e_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$.

As before, one can verify that $E_- = R_+$, $E_+ = R_-$ and

$$E_- Q E_+ = \begin{pmatrix} \langle \cos x e_{-m+1}, e_{-m+1} \rangle & \langle \cos x e_{-m+1}, e_m \rangle \\ \langle \cos x e_m, e_{-m+1} \rangle & \langle \cos x e_m, e_m \rangle \end{pmatrix},$$

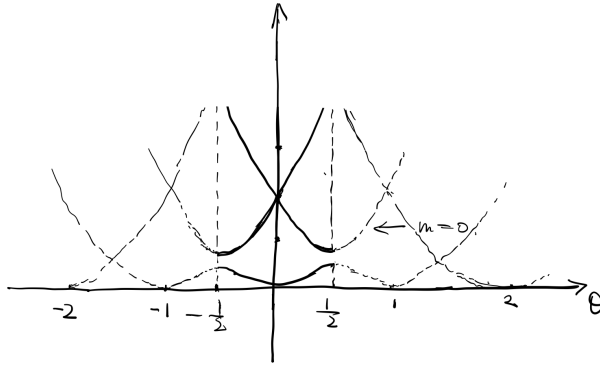
which is nonzero only when $m = 0$. When $m = 0$,

$$E_- Q E_+ = \begin{pmatrix} 0 & \frac{1}{2} \\ \frac{1}{2} & 0 \end{pmatrix}$$

and hence

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

When $\theta = \frac{1}{2}$, $E_{-+}^{\theta, \lambda}$ has an eigenvalue of second order. However, when $\lambda > 0$, the two eigenvalues split. Thanks to Schur's complement formula, it relates to the spectrum of $P_\lambda = D_x^2 + \lambda \cos x$. In other words, for $\lambda > 0$ and $\lambda \ll 1$, the following picture shows that the first band of the spectrum is separated.



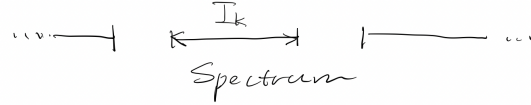
At least in dimension 1 and 2, the bands are all separated, though we only show for $k = 0$ here. See the official notes [19] for more details on this phenomenon and [7, Appendix C] for more details on the general Grushin problem.

4.5. Isolated bands for time reversible operators: trivial topology. Recall that we have derived the following things in the previous discussion:

$$\begin{aligned} P(x, D_x - \theta)u_j(\theta, x) &= E_j(\theta)u_j(\theta, x), \quad u_j(\theta, \cdot) \in L^2(\mathbb{R}^n/\Gamma), \\ e^{i\langle x, \theta \rangle} P(x, D_x)e^{-i\langle x, \theta \rangle} &= P(x, D_x - \theta), \quad e^{i\langle x, \theta \rangle} : \mathcal{H}_\theta \rightarrow L^2(\mathbb{R}^n/\Gamma), \end{aligned}$$

where the Hilbert space \mathcal{H}_θ is given by (4.1). We denote $\varphi_j(x, \theta) := e^{-i\langle x, \theta \rangle} u_j(\theta, x)$.

In this subsection, we fix k and assume that for any θ , $E_k(\theta)$ is a simple eigenvalue for $P(x, D_x) - E_k(\theta)$ defined on \mathcal{H}_θ such that $I_k \cap \bigcup_{j \neq k} I_j = \emptyset$, where I_k is defined in (4.3). The following figure is a sketch of what the spectrum looks like.



The first thing we want to analyze is the orthogonal projection $\Pi(\theta) : \mathcal{H}_\theta \rightarrow \ker_{\mathcal{H}_\theta}(P - E_k(\theta)) \simeq \mathbb{C}$. We use

$$\tilde{\Pi}(\theta) = e^{i\langle x, \theta \rangle} \Pi(\theta) e^{-i\langle x, \theta \rangle} : L^2(\mathbb{R}^n/\Gamma^*) \rightarrow \ker_{H^2(\mathbb{R}^n/\Gamma^*)}(P(x, D_x - \theta) - E_k(\theta)).$$

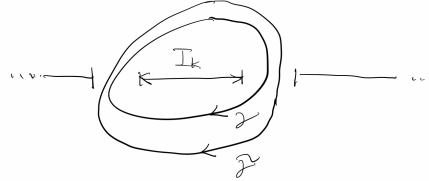
to change the periodicity property such that they are periodic in x , but are no longer periodic in θ . More precisely, for $\psi(x) = \sum_{j=0}^{\infty} \langle \psi(\cdot), \varphi_j(\cdot, \theta) \rangle \varphi_j(\cdot, \theta) \in \mathcal{H}_\theta$, we have

$$(\Pi(\theta)\psi)(x) = \langle \psi(\cdot), \varphi_k(\cdot, \theta) \rangle \varphi_k(\cdot, \theta).$$

Lemma 4.20. *The projection $\Pi(\theta)$ can be also expressed by*

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

where $\gamma \subset \mathbb{C}$ is a simple closed positively oriented contour such that $\gamma \cap \text{Spec}(P) = \emptyset$, as depicted in the figure.



We present two proofs for this lemma.

Proof-Version 1. A quick proof follows from the things we have done. We proved that $P|_{\mathcal{H}_\theta}$ has discrete spectrum with respect to $\{\varphi_j(x, \theta)\}_{k=0}^{\infty} \subset \mathcal{H}_\theta$ and then spectral theorem gives

$$(z - P|_{\mathcal{H}_\theta})^{-1} = \sum_{j=0}^{\infty} \frac{\varphi_j(\cdot, \theta) \otimes \varphi_j(\cdot, \theta)}{z - E_j(\theta)} = \sum_{j=0}^{\infty} \frac{|\varphi_j\rangle \langle \varphi_j|}{z - E_j(\theta)},$$

then we integrate this along γ and it follows from Cauchy's theorem and Residue theorem that

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

which completes the proof. \square

Proof-Version 2. We only show that $\Pi : \frac{1}{2\pi i} \int_{\gamma} (z - P)^{-1} dz$ is a projection. To see this is a projection, we need to check $\Pi^2 = \Pi$. We take another simple closed positively oriented contour $\tilde{\gamma}$ such that $\tilde{\gamma} \cap \text{Spec}(P) = \emptyset$ and γ lie in the interior of $\tilde{\gamma}$. Note that

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

where we use a resolvent identity in the second step. Since $\tilde{\gamma}$ is outside γ , for $\zeta \in \tilde{\gamma}$, $\oint_{\gamma} (\zeta - z)^{-1} dz = 0$ and for $z \in \gamma$, $\oint_{\tilde{\gamma}} (\zeta - z)^{-1} d\zeta = 2\pi i$. Hence,

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

\square

Here, the integral makes sense since $\mathbb{C} \setminus \text{Spec}(P) \ni z \mapsto (z - P)^{-1}$ is a holomorphic function of operator.

Definition 4.21 (holomorphic functions of operator). *Here are three equivalent definitions. Suppose H_1, H_2 are two Hilbert spaces, then we say*

$$\mathbb{C}^n \ni \theta \mapsto B(\theta) \in \mathcal{B}(H_1, H_2)$$

is a holomorphic function of operator if one of the following holds:

- (1) $\bar{\partial}_{\theta_j} B(\theta) = 0$, where $\bar{\partial}$ is taken in the weak sense;
- (2) $\frac{\partial B}{\partial \theta_j}$ exists in norm topology;
- (3) $\theta \mapsto \langle B(\theta)\varphi, \psi \rangle$ is holomorphic for all $\varphi \in H_1, \psi \in H_2$.

The equivalence of these three formulations is nontrivial and one need to use the Banach Steinhaus principle. We will not go into details of these in this course. The third one is easier to verify when we want to check it is a holomorphic function of operator.

Lemma 4.22. $\mathbb{R}^n / \Gamma^* \ni \theta \mapsto \Pi(\theta)$ is a real analytic family of operators, that is, there exists some $\varepsilon > 0$ such that

$$\mathbb{C}^n \supset \mathbb{R}^n + iB(0, \varepsilon) \ni \theta \rightarrow \Pi(\theta)$$

is holomorphic, where

$$\mathbb{R}^n + iB(0, \varepsilon) := \{x + iy : |y| < \varepsilon\}.$$

Proof. Likewise, we have

$$\tilde{\Pi}(\theta) = \frac{1}{2\pi i} \oint_{\gamma} (z - P(x, D_x - \theta)|_{L^2(\mathbb{R}^n/\Gamma)})^{-1} dz.$$

We write

$$\bar{\partial}_{\theta_j} (z - P(x, D_x - \theta))^{-1} = (z - P)^{-1} \bar{\partial}_{\theta_j} P(x, D_x - \theta) (z - P)^{-1}.$$

Since P is a polynomial in the second slot, so $\bar{\partial}_{\theta_j} P(x, D_x - \theta) = 0$, which implies that $\tilde{\Pi}(\theta)$ is holomorphic. \square

Hentforth, we abuse notation as follows. We use φ to denote φ_k and E to denote E_k for the fixed k as we mentioned at the beginning of this subsection. On the other hand, we use subscripts to denote something else.

Theorem 4.23. *Suppose P satisfies the time reversible property $P(x, D)\bar{u} = \overline{P(x, D)u}$, then we can choose $\varphi \in C^\infty(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)$ such that*

$$\mathbb{R}^n/\Gamma^* \ni \theta \mapsto \varphi(\theta) = \varphi(\theta, x),$$

$\varphi(-\theta) = \overline{\varphi(\theta)}$, $\|\varphi(\theta, \cdot)\|_{\mathcal{H}_\theta} = 1$, $\varphi(\theta, \cdot) \in \ker_{\mathcal{H}_\theta}(P - E)$ and real analytic in the sense that $\theta \mapsto \varphi(\theta)$ extends to a holomorphic map from $\mathbb{R}^n + iB(0, \varepsilon)$ to \mathcal{H}_θ as a section.

Remark 4.24. We do not require the two properties to hold after extending θ to the complex numbers.

Proof. The proof consists of two parts:

- topological part: $\theta \mapsto \varphi(x, \theta)$, $\theta \in \mathbb{R}^n/\Gamma^*$ is continuous from torus to smooth functions;
- regularization part: in fact, this is a special case of a general theorem, but we can do it by hand.

Step 1: Without loss of generality, we assume $\Gamma = (2\pi\mathbb{Z})^n$ and $\Gamma^* = \mathbb{Z}^n$. We do induction on n . For $n = 1$, what we intend to prove here is the line bundle $\theta \mapsto \ker(P|_{\mathcal{H}_\theta} - E) \simeq \mathbb{C}$ is trivial. (A vector bundle of rank 1 is called a line bundle.) In fact, any topological line bundle of the circle is trivial, but we will prove this result using a rather elementary method.

For $n = 1$, one can always find

$$\theta \mapsto \tilde{\varphi}(\theta), \quad 0 \leq \theta \leq \frac{1}{2},$$

that is continuous such that $P\tilde{\varphi}(\theta) = E(\theta)\tilde{\varphi}(\theta)$. As long as there is no closing loops, we can find such continuous section by patching up local continuous sections. In fact, a more general statement of this holds: any vector bundle over a compact contractible Hausdorff space is trivial. See [19, Section 2.7] for a proof of the general statement or [4] for general reference. Without loss of generality, we assume $\varphi(0) \in \mathbb{R}$.

Then we define

$$\tilde{\varphi}(-\theta) := \overline{\tilde{\varphi}(\theta)}$$

for $\theta \in [0, \frac{1}{2}]$. This is motivated by the following:

- $\varphi(\theta, \cdot) \in \mathcal{H}_\theta$ implies $\overline{\varphi(\theta, \cdot)} \in \mathcal{H}_{-\theta}$ by the definition of \mathcal{H}_θ ;
- $\varphi(\theta, \cdot) \in \mathcal{H}_\theta \cap \ker(P|_{\mathcal{H}_\theta} - E(\theta))$ implies $\overline{\varphi(\theta, \cdot)} \in \mathcal{H}_{-\theta} \cap \ker(P|_{\mathcal{H}_{-\theta}} - E(\theta))$ thanks to $P\bar{u} = \overline{Pu}$ and E is real;
- by the preceding point, $E(-\theta) = E(\theta)$ thanks to $I_k \cap (\cup_{j \neq k} I_j) = \emptyset$.

Now we want to modify $\tilde{\varphi}$ so that they match at $\pm \frac{1}{2}$. By definition, $|\tilde{\varphi}(-\frac{1}{2})| = |\tilde{\varphi}(\frac{1}{2})|$, which implies $\tilde{\varphi}(-\frac{1}{2}) = e^{-i\alpha} \tilde{\varphi}(\frac{1}{2})$ for some $\alpha \in \mathbb{R}$. Put $\varphi(\theta) = e^{-i\theta\alpha} \tilde{\varphi}(\theta)$, then

$$\varphi(-\frac{1}{2}) = e^{\frac{1}{2}i\alpha} \tilde{\varphi}(-\frac{1}{2}) = e^{-\frac{1}{2}i\alpha} \tilde{\varphi}(\frac{1}{2}) = \varphi(\frac{1}{2}).$$

Step 2: For $n > 1$, by induction hypothesis, we may assume that there exists a continuous section $\varphi' \in C(\mathbb{R}^{n-1}/\mathbb{Z}^{n-1}; \mathcal{H}_{\theta'})$ such that $\varphi'(\theta') \in \ker(P|_{\mathcal{H}_{\theta'}} - E(\theta'))$, $\overline{\varphi'(\theta')} = \varphi'(-\theta')$ and $\|\varphi'(\theta', \cdot)\|_{\mathcal{H}_{\theta'}} = 1$. Analogous to the argument in Step 1, let $\theta = (\theta', \theta_n)$, we can find

$$\Psi(\theta) : (\mathbb{R}^{n-1}/\mathbb{Z}^{n-1})_{\theta'} \times [0, \frac{1}{2}]_{\theta_n} \rightarrow \ker_{\mathcal{H}_\theta}(P|_{\mathcal{H}_\theta} - E(\theta)),$$

such that $\Psi(\theta', 0) = \varphi'(\theta')$. Then define Ψ on $\mathbb{R}^{n-1}/\mathbb{Z}^{n-1} \times [-\frac{1}{2}, \frac{1}{2}]$ by $\Psi(-\theta) = \overline{\Psi(\theta)}$. What we need is $\Psi(\theta', -\frac{1}{2}) = \Psi(\theta', \frac{1}{2})$. We proceed in a similar way. There exists $\alpha(\theta')$ such that

$$\Psi(\theta', \frac{1}{2}) = e^{i\alpha(\theta')} \Psi(\theta', -\frac{1}{2}) \quad (4.5)$$

and $\alpha(\theta')$ is continuous thanks to the continuity of Ψ . Moreover, since $\Psi(\theta', \frac{1}{2})$ and $\Psi(\theta', -\frac{1}{2})$ are both periodic in θ' , there exists $\alpha(\theta' + \gamma) \equiv \alpha(\theta') \pmod{2\pi\mathbb{Z}}$ for $\gamma \in \mathbb{Z}^{n-1}$. Take complex conjugate in (4.5), we get

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

Furthermore, replacing θ' by $-\theta'$ implies

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

Comparing this with (4.5), we find $\alpha(\theta') \equiv \alpha(-\theta') \pmod{2\pi\mathbb{Z}}$. By the continuity of α near $\theta' = 0$, $\alpha(\theta') = \alpha(-\theta')$. Then this implies that for any $1 \leq j \leq n-1$,

$$\alpha(-\frac{1}{2}e_j + e_j) \equiv \alpha(-\frac{1}{2}e_j)$$

becomes an equality, and hence

$$\alpha(\theta' + \gamma) = \alpha(\theta')$$

for all $\gamma \in \mathbb{Z}^{n-1}$.

Like the construction for the one dimensional case, we set

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

then we check

$$\begin{aligned} \varphi(\theta', \frac{1}{2}) &= e^{-i\alpha(\theta')} \Psi(\theta', \frac{1}{2}) = \Psi(\theta', -\frac{1}{2}) = \varphi(\theta', -\frac{1}{2}), \\ \varphi(\theta' + \gamma, \frac{1}{2}) &= e^{-i(\theta_n + \frac{1}{2})\alpha(\theta' + \gamma)} \Psi(\theta' + \gamma, \frac{1}{2}) = \varphi(\theta', \frac{1}{2}), \end{aligned}$$

that is, φ determines a continuous global section over $\mathbb{R}^n/\mathbb{Z}^n$.

Step 3: Let $\chi(\theta) = (2\pi)^{-n/2} e^{-\theta^2/2}$ such that $\int \chi = 1$ and put $\chi_\varepsilon = \varepsilon^{-n} \chi(\theta/\varepsilon)$. Now we view $\varphi(\cdot)$ as a periodic function on \mathbb{R}^n and define

$$\varphi_\varepsilon(\theta, x) = \int_{\mathbb{R}^n} \chi_\varepsilon(\theta - \theta') e^{i(x, \theta' - \theta)} \varphi(\theta', x) d\theta',$$

which stays periodic in θ . Moreover,

$$\begin{aligned}\varphi_\varepsilon(\theta, x - \gamma) &= \int_{\mathbb{R}^n} \chi_\varepsilon(\theta - \theta') e^{i\langle x - \gamma, \theta' - \theta \rangle} \varphi(\theta', x - \gamma) d\theta' \\ &= \int_{\mathbb{R}^n} \chi_\varepsilon(\theta - \theta') e^{i\langle x, \theta' - \theta \rangle} e^{i\langle \gamma, \theta - \theta' \rangle} e^{i\langle \gamma, \theta' \rangle} \varphi(\theta', x) d\theta' = e^{i\langle \gamma, \theta \rangle} \varphi_\varepsilon(\theta, x).\end{aligned}$$

Thus, $\varphi_\varepsilon(\theta, \cdot) \in \mathcal{H}_\theta$. Now $\varphi_\varepsilon(\theta)$ is a real analytic section since the Gaussian is real analytic and $\varphi_\varepsilon(\theta) \rightarrow \tilde{\varphi}(\theta)$ in L^2 as $\varepsilon \rightarrow 0$.

Then for any $\delta > 0$, there exists ε small enough such that $\|\varphi_\varepsilon - \tilde{\varphi}\|_{\mathcal{H}_\theta} < \delta$ and by taking δ small enough (and hence we need to take ε small enough), we know

$$\varphi_0(\theta) := \Pi(\theta)\varphi_\varepsilon(\theta) \in \ker(P|_{\mathcal{H}_\theta} - E)$$

is nonzero since $\tilde{\varphi} \in \ker(P|_{\mathcal{H}_\theta} - E)$ which is a generalization of the basic fact that if two vectors are close enough, then the projection from one to the other is nonzero.

Now thanks to Lemma 4.22, $\varphi_0(\theta)$ is a real analytic section and one can easily check $\overline{\varphi_0(\theta)} = \varphi_0(-\theta)$. Finally, let

$$\varphi(\theta) := \frac{\varphi_0(\theta)}{\left(\int_{\mathbb{R}^n/\Gamma} \varphi_0(\theta, x) dx\right)^{\frac{1}{2}}}$$

then it is obvious that $\|\varphi(\theta)\|_{\mathcal{H}_\theta} = 1$ and $\varphi(-\theta) = \overline{\varphi(\theta)}$, which completes the proof. \square

4.6. Wannier functions and spectral localization to an isolated band. Throughout this subsection, we still assume I_k is an isolated band and all corresponding $E_k(\theta)$'s are simple. Moreover, we still assume P satisfies the time reversibility as we did in Theorem 4.23. We define Π_k be the projection from $L^2(\mathbb{R}^n)$ to the subspace corresponding to $\text{Spec}(P) \cap I_k$, which is given by $\Pi_k = 1_{I_k}(P)$, that is, we plug in P to the characteristic function 1_{I_k} in the sense of functional calculus. Analogous to Lemma 4.20, Π_k is given by

$$\Pi_k = \frac{1}{2\pi i} \oint_\gamma (z - P|_{L^2(\mathbb{R}^n)})^{-1} dz,$$

which is a projection by an analogy of the second proof of Lemma 4.20. To prove the image of the projection corresponds to $\text{Spec}(P) \cap I_k$, it's a bit subtle. From the integral formula, it's easy to see $\Pi_k P = P \Pi_k$. Moreover, one can show that $\text{Spec}(\Pi_k P) = I_k$ and $\text{Spec}((I - \Pi_k)P) \cap I_k = \emptyset$. Suppose φ is the one defined in Theorem 4.23.

Theorem 4.25. *An orthonormal basis of $\Pi_k L^2(\mathbb{R}^n)$ is given by $\{\varphi_\gamma\}_{\gamma \in \Gamma}$, where $\varphi_\gamma(x) := \varphi_0(x - \gamma)$ with*

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

In fact, $\varphi_0 = \mathcal{C}\varphi$ modulo some constant by using the notation $\mathcal{C} : L^2(\mathbb{R}^n/\Gamma^; \mathcal{H}_\theta) \rightarrow L^2(\mathbb{R}^n)$ introduced in Theorem 4.12. Here, φ_γ 's are called Wannier functions.*

Proof. From Theorem 4.23, we know $\varphi_0(x) = \overline{\varphi_0(x)}$. By (4.7), $\varphi_\gamma(x) = \varphi_0(x - \gamma) = \mathcal{C}(e^{i\langle \gamma, \theta \rangle} \varphi)$. Therefore, we compute

$$\begin{aligned} & \langle e^{i\langle \gamma, \theta \rangle} \varphi(x, \theta), e^{i\langle \gamma', \theta \rangle} \varphi(x, \theta) \rangle_{L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)} \\ &= \int_{\mathbb{R}^n/\Gamma^*} e^{-i\langle \gamma' - \gamma, \theta \rangle} \int_{\mathbb{R}^n/\Gamma} |\varphi(x, \theta)|^2 dx d\theta = \int_{\mathbb{R}^n/\Gamma^*} e^{-i\langle \gamma' - \gamma, \theta \rangle} d\theta = \delta_{\gamma\gamma'}. \end{aligned}$$

This implies

$$\langle \varphi_\gamma, \varphi_{\gamma'} \rangle = \langle \mathcal{C}(e^{i\langle \gamma, \theta \rangle} \varphi_0), \mathcal{C}(e^{-i\langle \gamma, \theta \rangle} \varphi_0) \rangle_{L^2} = \delta_{\gamma\gamma'},$$

where we omit all the constants like $\frac{1}{|\mathbb{R}^n/\Gamma^*|}$ in the computation and the final step follows from Theorem 4.12.

Finally, we need to show $\overline{\text{span}\{\varphi_\gamma\}} = \Pi_k L^2(\mathbb{R}^n)$. Note that

$$\widehat{\Pi}_k v(x, \theta) := (\mathcal{B}\Pi_k \mathcal{C}v)(x, \theta) = \langle v(\theta, \cdot), \varphi(\theta, \cdot) \rangle_{\mathcal{H}_\theta} \varphi(\theta, \cdot),$$

then

$$\widehat{\Pi}_k L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta) = \{f(\theta)\varphi(\theta, \cdot) : f \in L^2(\mathbb{R}^n/\Gamma^*)\}.$$

Therefore,

$$\Pi_k L^2(\mathbb{R}^n) = \mathcal{C}\widehat{\Pi}_k L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta) = \left\{ \int_{\mathbb{R}^n/\Gamma^*} f(\theta)\varphi(\theta, \cdot) d\theta : f \in L^2(\mathbb{R}^n/\Gamma^*) \right\}. \quad (4.6)$$

Note that $\Pi_k L^2(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$ by definition. Hence, from (4.6), we can show that for any $f \in L^2(\mathbb{R}^n/\Gamma^*)$,

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

This property can be also checked directly. Since $\varphi \in L^2(\mathbb{R}^n/\Gamma^*; \mathcal{H}_\theta)$, we know $f(\theta)\varphi(\theta, x - \gamma) = f(\theta)\varphi(\theta, x)e^{i\langle \gamma, \theta \rangle}$, which is related to the Fourier transform and convolution, and hence this fact follows by writing these explicitly and apply Young's convolution theorem.

By applying Theorem 4.9 modulo constants, any $f \in L^2(\mathbb{R}^n/\Gamma^*)$ can be expressed by Fourier series

$$f(\theta) = \sum_{\gamma \in \Gamma} \widehat{f}(\gamma) e^{i\langle \gamma, \theta \rangle}, \quad \widehat{f}(\gamma) := \frac{1}{|\mathbb{R}^n/\Gamma^*|} \int_{\mathbb{R}^n/\Gamma^*} f(\theta) e^{-i\langle \gamma, \theta \rangle} d\theta.$$

Recall that $\varphi(x - \gamma, \theta) = \varphi(x, \theta)e^{i\langle \gamma, \theta \rangle}$,

$$\Pi_k L^2(\mathbb{R}^n) = \left\{ \sum_{\gamma \in \Gamma} \widehat{f}(\gamma) \varphi_\gamma(x), f \in L^2(\mathbb{R}^n/\Gamma^*) \right\} = \left\{ \sum_{\gamma \in \Gamma} a_\gamma \varphi_\gamma(x) : \sum_{\gamma} |a_\gamma|^2 < \infty \right\},$$

which completes the proof. \square

Theorem 4.26. *The Wannier function φ_0 constructed above has exponentially decay, that is, there exists c , for all α such that there exists C_α ,*

$$|\partial_x^\alpha \varphi_0(x)| \leq C_\alpha e^{-|x|/c}.$$

Proof. We write

$$\varphi_0(x - \gamma) = \frac{1}{|\mathbb{R}^n/\Gamma^*|} \int_{\mathbb{R}^n/\Gamma^*} \varphi(x - \gamma, \theta) d\theta = \frac{1}{|\mathbb{R}^n/\Gamma^*|} \int_{\mathbb{R}^n/\Gamma^*} \varphi(x, \theta) e^{i\langle \gamma, \theta \rangle} d\theta, \quad (4.7)$$

where the second step is because $\varphi(\cdot, \theta) \in \mathcal{H}_\theta$. By using the analyticity in θ derived in Theorem 4.23, we can deform the contour $\mathbb{R}^n/\Gamma^* \rightsquigarrow \mathbb{R}^n/\Gamma^* - i\frac{\gamma}{|\gamma|}\varepsilon$ and we get $|\varphi_0(x - \gamma)| \leq Ce^{-\varepsilon|\gamma|}$. For higher derivatives, the proof is in the same spirit. \square

5. TOPOLOGY IN PHYSICS

5.1. Line bundles, connection, curvature, the line bundle of projective space $\mathbb{C}P^1$.

Let

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

be the Pauli matrices and $\mathbb{S}^2 = \{x \in \mathbb{R}^3 : |x| = 1\}$. Then there exists a family of operators

$$\mathbb{S}^2 \ni x \mapsto H(x) = \sum_{j=1}^3 x_j \sigma_j = \begin{pmatrix} x_3 & x_1 + ix_2 \\ x_1 - ix_2 & -x_3 \end{pmatrix}, \quad (5.1)$$

and $H(x) : \mathbb{C}^2 \rightarrow \mathbb{C}^2$ is self-adjoint $H(x)^* = H(x)$. It follows from linear algebra that the spectrum of the operator $H(x)$ is $\text{Spec}(H(x)) = \{\pm 1\}$.

The stereographic projection of $x \in \mathbb{S}^2 \subset \mathbb{R}^3$ from the north pole to the complex plane is given by $z(x) = \frac{x_1 + ix_2}{1 - x_3}$ and the stereographic projection of $y \in \mathbb{S}^2 \subset \mathbb{R}^3$ from the south pole to the complex plane is given by $w(y) = \frac{y_1 - iy_2}{1 + y_3}$. And it is easy to check $z(x) = \frac{1}{w(x)}$ for $x \in \mathbb{S}^2 \setminus \{NP, SP\}$. Moreover,

$$\begin{aligned} \mathbb{S}^2 \setminus \{NP\} &: x \rightarrow z(x) \in \mathbb{C}, \\ \mathbb{S}^2 \setminus \{SP\} &: x \rightarrow w(x) \in \mathbb{C} \end{aligned}$$

are nice coordinate charts for the sphere. Since the transition map is given by $z(w) = \frac{1}{w}$ for $w \in \mathbb{C} \setminus \{0\}$, which is holomorphic, then \mathbb{S}^2 is a complex manifold characterized by these two charts.

The eigenspace of $H(x)$ for 1 is given by

$$V_x := \ker(H(x) - 1) = \begin{cases} \mathbb{C} \cdot \begin{pmatrix} z \\ 1 \end{pmatrix}, & x \neq NP, \\ \mathbb{C} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}, & x = NP. \end{cases}$$

The line bundle L of \mathbb{S}^2 is given by $L := \bigcup_{x \in \mathbb{S}^2} \{x\} \times V_x$ and has the following composition of maps

$$L = \bigcup_{x \in \mathbb{S}^2} \{x\} \times V_x \hookrightarrow \mathbb{S}^2 \times \mathbb{C}^2 \rightarrow \mathbb{S}^2$$

denoted by $L \xrightarrow{\pi} \mathbb{S}^2$.

The complex projective line $\mathbb{C}P^1$ is given by

$$\mathbb{C}P^1 := \{[z_0 : z_1] : z_0 \neq 0 \text{ or } z_1 \neq 0, z_j \in \mathbb{C}\} / \simeq$$

by quotienting out the equivalence class given by $[z_0 : z_1] \simeq [z'_0 : z'_1]$ provided $\lambda \in \mathbb{C}$ such that $z_0 = z'_0 \lambda, z_1 = z'_1 \lambda$. In other words, we identify the points on the same line in \mathbb{C}^2 , so we can view $\mathbb{C}P^1$ as lines in \mathbb{C}^2 heuristically.

Moreover, $\mathbb{C}P^1$ is homeomorphic to \mathbb{S}^2 . We only stress the heuristic identification here as follows. The maps

$$[z_0 : z_1] \rightarrow z = \frac{z_1}{z_0}, \forall z_0 \neq 0, \quad [z_0 : z_1] \rightarrow w = \frac{z_0}{z_1}, \forall z_1 \neq 0$$

can be identified with the stereographic projection of the sphere \mathbb{S}^2 . And then in this notation,

$$V_x = V_{[z_0:z_1]} = \left\{ \lambda \begin{pmatrix} z_1 \\ z_0 \end{pmatrix} : \lambda \in \mathbb{C} \right\} \subset \mathbb{C}^2$$

and hence a metaphysical interpretation of the line bundle L for $\mathbb{C}P^1$ is that you associate with each line in $\mathbb{C}P^1$ which it is. In fancy words, this is called a tautological line bundle.

Definition 5.1 (Line bundles). *Let X be a manifold with the charts covering $X = \cup_j U_j$. Then a manifold L is called a line bundle of X if $L \xrightarrow{\pi} X$ satisfies that*

- $\forall x \in X, \pi^{-1}(\{x\})$ is a one-dimensional complex vector space;

$$\pi^{-1}(U_j) \xrightarrow{h_j} U_j \times \mathbb{C}$$

- the diagram
$$\begin{array}{ccc} \pi^{-1}(U_j) & \xrightarrow{h_j} & U_j \times \mathbb{C} \\ \downarrow \pi & \swarrow \text{proj}_1 & \\ U_j & & \end{array}$$
 commutes;

- the transition map $g_{ij} : U_i \cap U_j \rightarrow GL(\mathbb{C})$ between overlapping coordinate patches $U_i \cap U_j$ is given by

$$h_i \circ h_j^{-1}(x, v) = (x, g_{ij}(x)v) : (U_i \cap U_j) \times \mathbb{C} \rightarrow (U_i \cap U_j) \times \mathbb{C}$$

for any $x \in U_i \cap U_j$.

If π, h_j are smooth (resp. holomorphic) and L, X are smooth (resp. holomorphic) manifolds, then we say L is a smooth (resp. holomorphic) line bundle.

Moreover, the transition map satisfies

- for $x \in U_i, g_{ii}(x) = id$.
- for $x \in U_i \cap U_j, g_{ij}(x) \circ g_{ji}(x) = id_{\mathbb{C}}$;
- for $x \in U_i \cap U_j \cap U_k, g_{ij}(x) \circ g_{jk}(x) \circ g_{ki}(x) = id_{\mathbb{C}}$.

One can check that π, h_j are smooth (resp. holomorphic) if and only if all g_{ij} 's are smooth (resp. holomorphic). And we can construct a line bundle provided a bunch of transition maps satisfying these three conditions.

Now let us see our example - the line bundle of projective space. Let $U_j = \{[z_0 : z_1] : z_j \neq 0\}$ for $j = 0, 1$. For $[z_0 : z_1] \in U_0$, the local trivialization map is given by

$$h_0(V_{[z_0:z_1]}) = h_0\left(\left\{\lambda \begin{pmatrix} z_1 \\ z_0 \end{pmatrix}\right\}\right) = ([z_0 : z_1], \lambda z_0)$$

and for $[z_0 : z_1] \in U_1$, the local trivialization map is given by

$$h_1(V_{[z_0:z_1]}) = h_1\left(\left\{\lambda \begin{pmatrix} z_1 \\ z_0 \end{pmatrix}\right\}\right) = ([z_0 : z_1], \lambda z_1).$$

Then the transition maps are

$$\begin{aligned} g_{10}([z_0 : z_1]) : \mathbb{C} &\rightarrow \mathbb{C}, & \lambda z_0 &\mapsto \lambda z_1, \text{ i.e. } \tau \mapsto \tau \frac{z_1}{z_0} = \tau z, \\ g_{01}([z_0 : z_1]) : \mathbb{C} &\rightarrow \mathbb{C}, & \lambda z_1 &\mapsto \lambda z_0, \text{ i.e. } \tau \mapsto \tau \frac{z_0}{z_1} = \tau \frac{1}{z}. \end{aligned}$$

Definition 5.2 (Sections of line bundles). *Suppose $\pi : L \rightarrow X$ is a smooth (resp. holomorphic) line bundle. We say $s \in C^\infty(X; L)$ is a C^∞ (resp. holomorphic) section if $\pi \circ s(x) = x$ for all $x \in X$ and locally, we can trivialize the section s by a family $\{s_j\}$ satisfying some compatibility conditions. More specifically, $h_j \circ s(x) = (x, s_j(x))$ with $s_j \in C^\infty(U_j; \mathbb{C})$ (resp. s_j is holomorphic) locally on U_j and they are compatible in the sense that $g_{ij}(x)(s_j(x)) = s_i(x)$ for $x \in U_i \cap U_j$.*

Then this compatibility result translates into

$$s_1\left(\frac{1}{z}\right) = g_{10}(z)s_0(z) = z s_0(z) \tag{5.2}$$

by composing local coordinate functions and view the sections s_0, s_1 as $s_0, s_1 : \mathbb{C} \setminus \{0\} \rightarrow \mathbb{C} \setminus \{0\}$.

Remark 5.3. Suppose $\pi : L \rightarrow X$ is the holomorphic line bundle with transition map $g_{10}(z) = z$ given as above. Then there are no holomorphic sections except the trivial bundle $s \equiv 0$. Suppose not, then $s_0 : z \mapsto s_0(z)$ holomorphic in \mathbb{C} and $s_1 : w \mapsto s_1(w)$ holomorphic in \mathbb{C} can be expressed using Taylor series

$$s_0(z) = \sum_{j \geq 0} a_j z^j, \quad s_1(w) = \sum_{k \geq 0} b_k w^k.$$

However, the compatibility result (5.2) gives

$$z \sum_{j \geq 0} a_j z^j = \sum_{k \geq 0} b_k z^{-k}$$

has no solutions except $a_j = b_k = 0$ for all j, k , so there are no nontrivial holomorphic sections. So if we expect a holomorphic section, then we need to find some other transition functions such that $s_1(\frac{1}{z}) = z^k s_0(z)$ with $k \leq 0$.

For $f \in C^\infty(X; \mathbb{C})$, then a differential form $df \in C^\infty(X; T^*X)$ is a section of the cotangent bundle, with the formula $df = \sum f_{x_j} dx_j$ in local charts. This leads us to a crucial concept, connection, which is a generalization of differential form to sections.

Definition 5.4 (Connections). *A connection D is a map from smooth sections of L over X to smooth sections of $L \otimes T^*X$ over X*

$$C^\infty(X; L) \rightarrow C^\infty(X; L \otimes T^*X)$$

with the following property that $D(fs) = fDs + s \otimes df$ for all $f \in C^\infty(X; \mathbb{C})$.

Morally speaking, $C^\infty(X; L \otimes T^*X)$ is a differential 1-form with coefficient in sections, that is, if we pair this with a vector field, then we get a section.

Now we give an expression in local coordinates. Suppose the section s is given by $s = (x, s_j(x))$ in local coordinates $x \in U_j$, then we know $s_i(x) = g_{ij}(x)s_j(x)$.

Since any section s can be written as $s(x) = (x, s_j(x)u_j(x))$ locally, where $s_j \in C^\infty(U_j; \mathbb{C})$ as in Definition 5.2 and u_j 's are local sections. Here, the local sections u_j 's correspond to local trivializations h_j 's. Suppose $Du_j = \theta_j u_j$, then we have

$$D(s_j u_j) = s_j Du_j + u_j \otimes ds_j = (s_j \theta_j + ds_j) u_j.$$

Hence,

$$Ds = (x, D_j s_j(x)) = (x, ds_j(x) + \theta_j(x) s_j(x)), \quad (5.3)$$

where $\theta_j \in C^\infty(U_j; T^*X)$ is a one-form.

Conversely, we examine what the compatibility condition of two local representations of the connection shall satisfy. Since $s_j(x) = g_{ji}(x)s_i(x)$, if we expect Ds to be a section with transition function g_{ij} , then

$$\begin{aligned} g_{ij}(x) (ds_j(x) + \theta_j(x) s_j(x)) &= ds_i(x) + \theta_i s_i(x) \\ = d(g_{ij}(x) s_j(x)) + \theta_i(x) g_{ij}(x) s_j(x) &= dg_{ij}(x) s_j(x) + g_{ij}(x) ds_j(x) + \theta_i(x) g_{ij}(x) s_j(x), \end{aligned}$$

which is equivalent to

$$\theta_j(x) = g_{ij}(x)^{-1} dg_{ij}(x) + \theta_i(x) \quad (5.4)$$

by cancelling $g_{ij}(x) ds_j(x)$ from both sides and then cancelling $s_j(x)$.

Proposition 5.5 (Curvature). *A two form Θ defined by $\Theta|_{U_j} = d\theta_j$ is a well-defined closed two form on X .*

Proof. On $U_i \cap U_j$, we have

$$d\theta_i - d\theta_j = d(g_{ij}(x)^{-1} dg_{ij}(x)) = d(d \log g_{ij}) = 0,$$

where $\log g_{ij}$ is only defined locally. Then Θ is a well-defined one form since $d\theta_i|_{U_i \cap U_j} = d\theta_j|_{U_i \cap U_j}$, and it satisfies $d^2 = 0$ locally, so it is closed. \square

Definition 5.6. *The two form Θ given as above is called the curvature form of the connection D .*

The first reason why it is called the curvature is as follows. Suppose we have a curve with holomorphic structure on a Riemann surface, then we identify the tangent space with \mathbb{C} (real 2-dim) as a line bundle of our surface. In this case, the curvature Θ will be the Gaussian curvature of the surface modulo some forms.

The curvature Θ will depend on the choice of connection, but its cohomology class does not.

Proposition 5.7. *Suppose D_1, D_2 are two connections on L with corresponding curvature forms Θ_1, Θ_2 , respectively. Then there exists $\eta \in C^\infty(X; T^*X)$ such that $\Theta_1 = \Theta_2 + d\eta$.*

Proof. On $U_i \cap U_j$, $\Theta_1 - \Theta_2 = d(\theta_{1,i} - \theta_{2,i}) = d(\theta_{1,j} - \theta_{2,j})$. We claim $\theta_1 - \theta_2$ defines a global 1-form η on X . It suffices to check on $U_i \cap U_j$,

$$\theta_{1,i} - \theta_{2,i} = \theta_{1,j} - \theta_{2,j},$$

which follows from

$$\theta_{1,i} - \theta_{1,j} = g_{ij}(x)^{-1} dg_{ij}(x) = \theta_{2,i} - \theta_{2,j}.$$

Hence, we can define a global 1-form η by setting $\eta|_{U_i} = \theta_{1,i} - \theta_{2,i}$ locally. \square

As a corollary, we have a topological invariant called the Chern number.

Definition 5.8. *Suppose X is a 2-dimensional compact smooth manifold with a smooth line bundle L ,*

$$c_1(L) = \frac{i}{2\pi} \int_X \Theta$$

is called the Chern number of the smooth line bundle L and is independent of the choice of the connection.

In fact, in full generality, $c_1(L)$ is a topological invariant for a smooth line bundle. Furthermore, it is the only topological invariant in the sense that if the base manifold and the Chern number are the same for two smooth line bundles, then they are the same. However, we will not cover this general statement in this course. Later, we will show that $c_1(L)$ is an integer.

5.2. Hermitian line bundles through an example: Bloch sphere. Now we come back to the discussion of the line bundle of $\mathbb{C}P^1$. For our tautological line bundle $\pi : L \rightarrow \mathbb{C}P^1$ with a section $s : \mathbb{C}P^1 \rightarrow L$, we compose it with i

$$i \circ s : \mathbb{C}P^1 \xrightarrow{s} L \xrightarrow{i} \mathbb{C}P^1 \times \mathbb{C}^2$$

and then we can differentiate this. Moreover, we have the notion of Hermitian inner product $\langle z, w \rangle = \sum_{j=0}^1 z_j \bar{w}_j$ on \mathbb{C}^2 , so that we can define the orthogonal projection

$$\Pi_x : \mathbb{C}^2 \xrightarrow[\text{w.r.t. } \langle \cdot, \cdot \rangle]{\perp} V_x = \ker(H(x) - 1). \quad (5.5)$$

Now we claim that

$$Ds(x) = \Pi_x(d(i \circ s)) \quad (5.6)$$

is a connection, where the projection Π_x is defined as the projection of each coefficient (which is in \mathbb{C}^2) in the form $d(i \circ s)$. Now we check D is a connection by writing

$$D(fs)(x) = \Pi_x(d(f \cdot i \circ s)) = \Pi_x(df(i \circ s) + f d(i \circ s)) = \Pi_x(df(i \circ s)) + f \Pi_x(d(i \circ s)) = (df)s + fDs,$$

where $f \in C^\infty(\mathbb{C}P^1; \mathbb{C})$. Due to the topological invariance of $c_1(L)$, or say, Proposition 5.7, we are allowed to stick to this connection later to compute the Chern number $c_1(L)$.

Now we choose specific eigenfunctions for $H(x)$ in order to do the computation explicitly. One will see that this will result in a different trivialization, which is non-holomorphic.

Suppose u_0, u_1 are defined on different coordinates respectively such that $H(x)u_0(x) = u_0(x)$, $H(x)u_1(x) = u_1(x)$, $|u_0(x)| = |u_1(x)| = 1$, then they are given by

$$\begin{aligned} u_0(x) &= \frac{1}{(1+|z|^2)^{\frac{1}{2}}} \begin{pmatrix} z \\ 1 \end{pmatrix}, \quad x \in \mathbb{S}^2 \setminus \{NP\}, \quad z = \frac{x_1 + ix_2}{1 - x_3}, \\ u_1(x) &= \frac{1}{(1+|w|^2)^{\frac{1}{2}}} \begin{pmatrix} 1 \\ w \end{pmatrix}, \quad x \in \mathbb{S}^2 \setminus \{SP\}, \quad z = \frac{x_1 - ix_2}{1 + x_3}. \end{aligned} \quad (5.7)$$

Since $i \circ s(x) = s_0(x)u_0(x) = s_1(x)u_1(x)$ on $U_0 \cap U_1$, we have

$$s_0(z) \frac{1}{(1+|z|^2)^{\frac{1}{2}}} \begin{pmatrix} z \\ 1 \end{pmatrix} = s_1\left(\frac{1}{z}\right) \frac{1}{(1+|z^{-1}|^2)^{\frac{1}{2}}} \begin{pmatrix} 1 \\ z^{-1} \end{pmatrix} = s_1\left(\frac{1}{z}\right) \frac{|z|/z}{(1+|z|^2)^{\frac{1}{2}}} \begin{pmatrix} z \\ 1 \end{pmatrix}$$

Hence, $s_0(z) = \frac{|z|}{z} s_1\left(\frac{1}{z}\right)$, which implies $g_{01}(z) = \frac{|z|}{z}$ by Definition 5.2. Since $g_{01}(z)$ is smooth but non-holomorphic on $\mathbb{C} \setminus \{0\}$, $\pi : L \rightarrow X$ is just a smooth line bundle.

Since $d(s_j u_j) = ds_j u_j + s_j du_j$ for $j = 0, 1$, we have

$$\Pi_x(d(s_j u_j)) = \langle ds_j u_j + s_j du_j, u_j \rangle u_j = ds_j + s_j \langle du_j, u_j \rangle, \quad (5.8)$$

and hence $D_j s_j = ds_j + s_j \langle du_j, u_j \rangle$. If we stick to the notation in (5.3), then $\theta_j = \langle du_j, u_j \rangle$. This connection inherited from the Hilbert space and the orthogonal projection is called the Berry connection. And we also have a curvature Θ given by

$$\Theta|_{U_j} = d\theta_j.$$

This line bundle discussed above is called the Bloch sphere.

Now we do a sanity check by showing (5.4) holds. Since $u_1\left(\frac{1}{z}\right) = \frac{|z|}{z} u_0(z)$,

$$\theta_1 = \left\langle d\left(u_0(z) \frac{|z|}{z}\right), u_0(z) \frac{|z|}{z} \right\rangle = \langle du_0, u_0 \rangle + \left\langle d\left(\frac{|z|}{z}\right), \frac{|z|}{z} \right\rangle = \theta_0 + \frac{|z|}{z} d\left(\frac{|z|}{z}\right) = \theta_0 + g_{01}^{-1} dg_{01}.$$

We should note that (5.6) does not rely on the special structure of L , but only on the facts that we have an inclusion from L to the trivial bundle $\mathbb{C}P^1 \times \mathbb{C}^2$ and \mathbb{C}^2 has a Hermitian inner product. If we have an inclusion mapping into a more general trivial bundle $\mathbb{C}P^1 \times H$ with a Hilbert space H , we can still use the definition (5.6).

Definition 5.9. A Hermitian metric on a line bundle $\pi : L \rightarrow X$ is a smooth family of Hermitian inner products $|\cdot|_x$, a way of assigning a length, on each fiber $\pi^{-1}(x)$, $\forall x \in X$. Here, the smoothness is in the sense that for all smooth sections s of L , $\langle s, s \rangle_x$ is smooth on X .

In a trivialization over U_j , $|v|_x$ can be written as

$$|v|_x^2 = h_j(x)|v|^2,$$

where $|v|^2$ is just the norm of \mathbb{C} . Compatibility condition on $x \in U_i \cap U_j$ is given by $|s_j|_x^2 = |s_i|_x^2$, which should be

$$h_j(x)|s_j(x)|^2 = h_i(x)|s_i(x)|^2 = h_i(x)|g_{ij}(x)s_j(x)|^2.$$

Therefore, $h_j(x) = |g_{ij}(x)|^2 h_i(x)$ is the compatibility condition.

Definition 5.10 (Hermitian connection). *Given a connection D on L , we say D is a Hermitian connection if*

$$d(\langle s(x), s'(x) \rangle_x) = \langle Ds(x), s'(x) \rangle_x + \langle s(x), Ds'(x) \rangle_x$$

for all smooth sections $s, s' \in C^\infty(X; L)$.

We can also characterize the Hermitian connection via parallel transport, which will be more natural.

Definition 5.11 (Parallel transport). *Given a connection D on L , a curve $\gamma : [0, 1] \rightarrow X$ and a section s , then we say s is parallel transported along γ if and only if*

$$Ds(\gamma(t))(\dot{\gamma}(t)) = 0.$$

In the definition above, we get $Ds(\gamma(t)) \in C^\infty(X; L \otimes T^*X)$ and we pair it with a tangent vector $\dot{\gamma}(t)$, which will give us a section.

Proposition 5.12. *D is a Hermitian connection on L if and only if for any curve γ , any section s parallel transported along γ , $|s(x)|_x$ is preserved by this parallel transport.*

Proof. Suppose D is a Hermitian connection, then take $s' = s$ be the same section of L , then

$$\dot{\gamma}(t)(|s(\gamma(t))|_x^2) = (d|s(\gamma(t))|_x^2)(\dot{\gamma}(t)) = \langle Ds(\gamma(t))(\dot{\gamma}(t)), s(\gamma(t)) \rangle_{\gamma(t)} + \langle s(\gamma(t)), Ds(\gamma(t))(\dot{\gamma}(t)) \rangle_{\gamma(t)} = 0,$$

which is equivalent to say $|s(\gamma(t))|_x^2$ is constant along γ .

For the other implication, it is easy to use polarization to reverse the argument. \square

In order to discuss what condition would θ_j 's satisfy, we choose a specific trivialization using a frame which has length one. To be specific, we choose a section $u_j \in C^\infty(U_j; L)$ over U_j , respectively, such that $|u_j|_x = 1$, and then we write

$$s(x) = (x, s_j(x)u_j(x)),$$

which gives a local trivialization. Then

$$\langle s_j(x), s'_j(x) \rangle_x = \langle s_j(x), s'_j(x) \rangle$$

is just the usual Hermitian metric on \mathbb{C} .

Now using the Leibniz rule for functions, we have

$$d(\langle s_j, s'_j \rangle) = \langle ds_j, s'_j \rangle + \langle s_j, ds'_j \rangle.$$

On the other hand,

$$d(\langle s_j, s'_j \rangle_x) = \langle Ds_j, s'_j \rangle_x + \langle s_j, Ds'_j \rangle_x = \langle ds_j + \theta_j s_j, s'_j \rangle + \langle s_j, ds'_j + \theta_j s'_j \rangle.$$

Comparing these two identities, we have

$$\langle \theta_j s_j, s'_j \rangle + \langle s_j, \theta_j s'_j \rangle = 0.$$

Since s_j, s'_j are arbitrary, $\theta_j = -\bar{\theta}_j$, that is, θ_j is purely imaginary. What this means is that, in a frame of length one, a Hermitian connection is described by a form that is purely imaginary.

As a sanity check, in our previous example, (5.7) gives a frame of length one. By a direct computation,

$$\theta_0 = \langle du_0, u_0 \rangle = \frac{1}{2(1 + |z|^2)} (\bar{z}dz - z d\bar{z}), \quad (5.9)$$

which is indeed purely imaginary since $\bar{\theta}_0 = -\theta_0$.

Definition 5.13 (Chern connection). *If L is a holomorphic line bundle, we say a connection D is compatible with the holomorphic structure if $D^{0,1} = \bar{\partial}$. There is a unique Hermitian connection D on L given by $\theta_j = \partial h_j$, which is compatible with the holomorphic structure, called the Chern connection.*

See [19, Section 6.2] for a further discussion for the line bundles over tori.

5.3. Holonomy. Now we discuss the parallel transport along a simply closed curve. We start with $|s(\gamma(0))|_{\gamma(0)} = 1$. From Proposition 5.12, $|s(\gamma(t))|_{\gamma(t)} = |s(\gamma(0))|_{\gamma(0)}$.

Definition 5.14 (Holonomy). *For a closed curve γ , $\gamma(1) = \gamma(0)$, $s(\gamma(0)), s(\gamma(1)) \in \pi^{-1}(\gamma(0))$, and hence there exists θ such that $s(\gamma(1)) = e^{i\theta} s(\gamma(0))$. The factor $e^{i\theta}$ is called the holonomy of the connection D over the closed curve γ , denoted by $hol_D(\gamma)$.*

Suppose $\gamma \subset U_j$, then

$$s'_j + \theta_j(\gamma(t))s_j = 0.$$

By solving this ODE explicitly, we get

$$s_j(t) = \exp\left(-\int_0^t \theta_j\right) s_j(0).$$

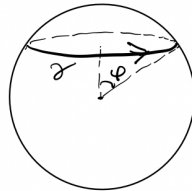
Therefore,

$$hol_D(\gamma) = \exp\left(-\int_\gamma \theta_j\right). \quad (5.10)$$

We write $d = \partial + \bar{\partial}$ with $\partial f = \partial_z f dz$ and $\bar{\partial} f = \partial_{\bar{z}} f d\bar{z}$. A easy algebra calculation leads to $\partial_z = \frac{1}{2}(\partial_x - i\partial_y)$, $\partial_{\bar{z}} = \frac{1}{2}(\partial_x + i\partial_y)$ and $dz = dx + idy$, $d\bar{z} = dx - idy$.

In our previous example introduced at the very beginning of the preceding subsection, from (5.9), we get

$$\Theta = (\partial + \bar{\partial})\theta_0 = \frac{1}{(1 + |z|^2)^2} d\bar{z} \wedge dz.$$



Now we take the curve γ parametrized by $z(t) = \frac{\sin \varphi e^{it}}{1 - \cos \varphi}$, as shown in the picture above.

Then by Stokes' theorem, we compute

$$\begin{aligned} \text{hol}_D(\gamma) &= \exp\left(-\int_{\gamma} \theta_0\right) = \exp\left(\int_{|z| > \frac{\sin \varphi}{1 - \cos \varphi}} \frac{1}{(1 + |z|^2)^2} d\bar{z} \wedge dz\right) \\ &= \exp\left(-4\pi i \int_{\frac{\sin \varphi}{1 - \cos \varphi}}^{\infty} \frac{s}{(1 + s^2)^2} ds\right) = \exp\left(-2\pi i \int_{\left(\frac{\sin \varphi}{1 - \cos \varphi}\right)^2}^{\infty} \frac{ds}{(1 + s^2)^2}\right) = -\exp(\pi i(1 - \cos \varphi)). \end{aligned}$$

On the sphere, take γ to be the equator, then

$$\int_X \Theta = \int_{\gamma} (\theta_0 - \theta_1) = \int_{\gamma} (g_{10}^{-1} dg_{10}) = \int_{\gamma} d \log g_{10} \in 2\pi i \mathbb{Z}$$

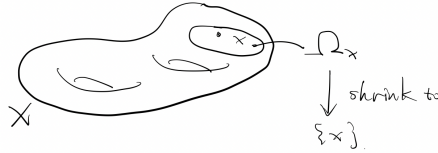
thanks to the Cauchy integral formula. This is also true for the general setting.

Theorem 5.15. *Suppose X is a compact surface, then the Chern number*

$$c_1(L) = \frac{i}{2\pi} \int_X \Theta$$

is an integer.

Proof. For any $x \in X$, take a neighborhood Ω_x , which can shrink to x .



Let $\gamma = \partial\Omega_x$. Then

$$\text{hol}_D(\gamma) = \exp\left(-\int_{\Omega_x} \Theta\right) = \exp\left(\int_{X \setminus \Omega_x} \Theta\right).$$

Let Ω_x shrink to $\{x\}$, then

$$\exp\left(-\int_{\Omega_x} \Theta\right) \rightarrow 1, \quad \exp\left(\int_{X \setminus \Omega_x} \Theta\right) \rightarrow \exp\left(\int_X \Theta\right).$$

Hence, $\int_X \Theta \in 2\pi i \mathbb{Z}$, which completes the proof. \square

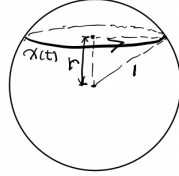
Now we can compute the Chern number for our Bloch sphere example. Since

$$\int_{\mathbb{S}^2} \Theta = \int_{\mathbb{C}} \frac{1}{(1 + |z|^2)^2} d\bar{z} \wedge dz = \int_{\mathbb{C}} \frac{2i \, dx \, dy}{(1 + |z|^2)^2} = 2\pi i \int_0^{\infty} \frac{2r}{(1 + r^2)^2} dr = 2\pi i,$$

the Chern number of the Bloch sphere is given by $c_1(L) = -1$.

5.4. Adiabatic theorem. We will relate what we discussed before with physics via the adiabatic process.

Imagining yourself carrying a box with a swinging pendulum and the pendulum will keep the same frequency as what it starts with if you walk slowly. This phenomenon can be translated into terminologies as follows. Slow movements preserve frequencies of motion, which is called an adiabatic process.



We see a special case of the adiabatic theorem at first.

Theorem 5.16. Let $x(t) = \begin{pmatrix} r \cos t \\ r \sin t \\ \sqrt{1-r^2} \end{pmatrix}$ be the curve shown as above. Suppose w_ε is given by

$$i\varepsilon\partial_t w_\varepsilon = (H(x(t)) - 1)w_\varepsilon, \quad w_\varepsilon|_{t=0} \in V_{x(0)}, \quad |w_\varepsilon|_{t=0}| = 1, \quad (5.11)$$

then $w_\varepsilon(t) = w(t) + \mathcal{O}(\varepsilon)$ for some $w(t) \in V_{x(t)}$, where $V_x := \ker(H(x(t)) - 1)$, $H(x)$ is defined in (5.1). In other words, if we start with an eigenfunction, then it stays in $\ker(H(x(t)) - 1)$ modulo an error.

Proof. Suppose $w_\varepsilon(0) = \frac{1}{(1+|\rho|^2)^{\frac{1}{2}}} \begin{pmatrix} \rho \\ 1 \end{pmatrix} \in V_{x(0)}$, then one can check by a direct computation that

$$\begin{cases} u_1(t) = \frac{1}{(1+|\rho|^2)^{\frac{1}{2}}} \begin{pmatrix} \rho e^{it} \\ 1 \end{pmatrix} \in \ker(H(x(t)) - 1) \\ u_2(t) = \frac{1}{(1+|\rho|^2)^{\frac{1}{2}}} \begin{pmatrix} 1 \\ -\rho e^{-it} \end{pmatrix} \in \ker(H(x(t)) + 1) \end{cases}$$

for all t . We write $w_\varepsilon(t) = c_1(t)u_1(t) + c_2(t)u_2(t)$, then (5.11) is equivalent to

$$\dot{c}_1 = -c_1 \langle \dot{u}_1, u_1 \rangle - \langle \dot{u}_2, u_1 \rangle c_2, \quad \dot{c}_2 = -c_1 \langle \dot{u}_1, u_2 \rangle - c_2 \left(\langle \dot{u}_2, u_2 \rangle - \frac{2i}{\varepsilon} \right).$$

By computing these coefficients explicitly, we get

$$\dot{c}_1 = -ic_1 \frac{\rho^2}{1+\rho^2} + i \frac{\rho e^{-it}}{1+\rho^2} c_2, \quad \dot{c}_2 = -c_1 \frac{\rho e^{it}}{1+\rho^2} + c_2 \left(\frac{i\rho^2}{1+\rho^2} + \frac{2i}{\varepsilon} \right).$$

Furthermore, let $a_1 = c_1$, $a_2 = e^{-it}c_2$, then $\dot{a}_2 = e^{-it}\dot{c}_2 - ia_2$ and hence

$$\dot{c}_1 = -ic_1 \frac{\rho^2}{1+\rho^2} + i \frac{\rho}{1+\rho^2} a_2, \quad \dot{a}_2 + ia_2 = -c_1 \frac{\rho^2}{1+\rho^2} + a_2 \left(\frac{2i}{\varepsilon} + \frac{i\rho^2}{1+\rho^2} \right).$$

Equivalently,

$$\begin{cases} \dot{a}_1 = -i\alpha a_1 + i\beta a_2, \\ \dot{a}_2 = -i\beta a_1 + i\left(\frac{2}{\varepsilon} + \alpha - 1\right)a_2, \\ a_1(0) = 1, a_2(0) = 0. \end{cases}$$

By rescaling, there exists two constants a, b such that

$$\begin{cases} \dot{a}_1 = iaa_1 + iba_2, \\ \dot{a}_2 = -iba_1 + i\varepsilon^{-1}a_2, \end{cases}$$

and then the eigenvalues of the corresponding matrix $A = \begin{pmatrix} a & b \\ -b & \varepsilon^{-1} \end{pmatrix}$ are

$$\lambda_1 = \frac{1}{\varepsilon} + \mathcal{O}(\varepsilon), \quad \lambda_2 = a + \mathcal{O}(\varepsilon).$$

with corresponding eigenvectors

$$v_1 = \begin{pmatrix} b\varepsilon(1 + \mathcal{O}(\varepsilon)) \\ 1 \end{pmatrix}, \quad v_2 = \begin{pmatrix} 1 \\ b\varepsilon(1 + \mathcal{O}(\varepsilon)) \end{pmatrix}.$$

Hence, $A = (v_1 \ v_2) \Lambda (v_1 \ v_2)^{-1}$ implies

$$\exp(itA) = (1 + \mathcal{O}(\varepsilon)) \begin{pmatrix} 1 & b\varepsilon \\ b\varepsilon & 1 \end{pmatrix} \begin{pmatrix} e^{it(a+\mathcal{O}(\varepsilon))} & 0 \\ 0 & e^{\frac{it}{\varepsilon}(1+\mathcal{O}(\varepsilon^2))} \end{pmatrix} \begin{pmatrix} 1 & b\varepsilon \\ b\varepsilon & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} e^{ita} \\ 0 \end{pmatrix} + \mathcal{O}(\varepsilon).$$

Hence,

$$w_\varepsilon(t) = c_1(t)u_1(t) + c_2(t)u_2(t) = e^{ita}u_1(t) + \mathcal{O}(\varepsilon),$$

which completes the proof. \square

Remark 5.17. If we consider a similar problem stated as follows. Suppose w_ε is given by

$$i\partial_t w_\varepsilon = H(x(\varepsilon t))w_\varepsilon, \quad w_\varepsilon|_{t=0} \in V_{x(0)}, \quad (5.12)$$

then $w_\varepsilon(t) = e^{-it}w(\varepsilon t) + \mathcal{O}(\varepsilon)$, which means that the -1 term just affects the phase regardless of modulo some error.

Now we state the general version of the adiabatic theorem, which was first proposed by Born and Fock [3], and later proved mathematically by Kato [10].

Theorem 5.18 (The adiabatic theorem). *Suppose $[0, 1] \ni s \mapsto P(s)$ is a smooth family of bounded self-adjoint operators on H and $s \mapsto \lambda(s)$ is an eigenvalue of $P(s)$ such that*

$$\text{dist}(\lambda(s), \text{Spec}(P(s)) \setminus \{\lambda(s)\}) > \delta > 0, \quad s \in [0, 1].$$

Let u_ε be a solution to the adiabatic process

$$\begin{cases} i\varepsilon\partial_t u_\varepsilon = P(t)u_\varepsilon, \\ u_\varepsilon(0) = u_0 \in \ker(P(0) - \lambda(0)), \end{cases}$$

then

$$u_\varepsilon(t) = \exp\left(-\frac{1}{\varepsilon} \int_0^t \lambda(s) ds\right) u(t) + \mathcal{O}_H(\varepsilon),$$

for some $u(t) \in \ker(P(t) - \lambda(t))$ independent of ε and $\mathcal{O}_H(\varepsilon)$ denotes that its H -norm is of $\mathcal{O}(\varepsilon)$.

Remark 5.19. The adiabatic theorem describes behavior of a system under a slowly varying Hamiltonian. This can be seen from a change of variable, $t = \tau\varepsilon$ as

$$i\varepsilon\partial_t u_\varepsilon = P(t)u_\varepsilon \iff i\partial_\tau u_\varepsilon = P(\varepsilon\tau)u_\varepsilon.$$

Before we give a proof, we make a comment about the relation of this theorem with parallel transport by examining the special case above first. Suppose $s = (x, s_1(x)u_1(x))$ with $|u_1|_H = 1$ is a local trivialization of a section. Then if we choose a local orthonormal frame u_1 such that $Ds = (x, (ds_1 + \langle du_1, u_1 \rangle s_1)u_1)$ as before, then

$$\begin{aligned} Ds(\gamma(t))(\dot{\gamma}(t)) &= (x, (ds_1(\dot{\gamma}(t)) + \langle du_1, u_1 \rangle(\dot{\gamma}(t)))u_1) \\ &= \left\langle \frac{d}{dt} (s_1(\gamma(t))u_1(\gamma(t))), u_1(\gamma(t)) \right\rangle u_1. \end{aligned}$$

Therefore, s is parallel transported along γ if and only if

$$\left\langle \frac{d}{dt} s(t), s(t) \right\rangle = 0,$$

which is equivalent to

$$\langle s(t + \delta), s(t) \rangle = 1 + \mathcal{O}(\delta^2),$$

where s has the localization $s(t) = s_1(\gamma(t))u_1(\gamma(t)) \in H$.

Now we state a theorem due to B.Simon[14].

Theorem 5.20. *Suppose X is a compact surface with $\gamma \subset X$. Set $P(x) = \mathcal{P}(\gamma(x))$, where \mathcal{P} is a family of operators such that $x \mapsto \mathcal{P}(x)$, $\lambda(x) \in \text{Spec}(\mathcal{P}(x))$ and*

$$\text{dist}(\lambda(x), \text{Spec}(P(x)) \setminus \{\lambda(x)\}) > \delta > 0,$$

that is, $\lambda(x)$ is a simple isolated eigenvalue. We define a line bundle $L = \cup_x x \times V_x \subset X \times H$ with $V_x = \ker(\mathcal{P}(x) - \lambda(x)) = \pi^{-1}(x)$ and a Hermitian connection from Hilbert space H . Then suppose $u(t)$ is given by Theorem 5.18, then $u(t)$ is a section parallel transported along γ .

Proof. Without loss of generality, we assume $\lambda(x) \equiv 0$. Otherwise, we consider $\mathcal{P}(x) - \lambda(x)$ instead of \mathcal{P} . Now $u(t)$ satisfies

$$\begin{cases} i\varepsilon\partial_t u_\varepsilon = P(t)u_\varepsilon, \\ u_\varepsilon(0) = u_0 \in \ker(P(0)), \\ u(t) = \lim_{\varepsilon \rightarrow 0} u_\varepsilon(t), \text{ where the limit is meant as converging in } H. \end{cases}$$

A formal argument is as follows. We write

$$\left\langle \frac{d}{dt} u(t), u(t) \right\rangle = \lim_{\varepsilon \rightarrow 0} \left\langle \frac{d}{dt} u_\varepsilon, u \right\rangle = \lim_{\varepsilon \rightarrow 0} \frac{1}{i\varepsilon} \langle P(t)u_\varepsilon(t), u(t) \rangle = \lim_{\varepsilon \rightarrow 0} \frac{1}{i\varepsilon} \langle u_\varepsilon(t), P(t)u(t) \rangle = 0,$$

where in the last step, we apply the result from Theorem 5.18 that $u(t) \in \ker P(t)$.

Unfortunately, the argument above is non-rigorous since we exchange the limit and the differentiation without justification. To make this rigorous, we use mollifications. One should first note that for $u(t) \in \ker(P(x(t))) \subset H$, $\frac{d}{dt}u(t)$ is meant as the element in H .

Now we take $\varphi \in C_c^\infty((0, 1))$, then we compute by using integration by parts that

$$\begin{aligned} \int \varphi(t) \langle \frac{d}{dt}u(t), u(t) \rangle dt &= \lim_{\varepsilon \rightarrow 0} \int \varphi(t) \langle \frac{d}{dt}u(t), u_\varepsilon(t) \rangle dt \\ &= - \lim_{\varepsilon \rightarrow 0} \int \varphi'(t) \langle u(t), u_\varepsilon(t) \rangle dt - \lim_{\varepsilon \rightarrow 0} \int \varphi(t) \langle u(t), \frac{d}{dt}u_\varepsilon(t) \rangle dt, \end{aligned}$$

where

$$\int \varphi'(t) \langle u(t), u_\varepsilon(t) \rangle dt \rightarrow \int \varphi'(t) dt = 0,$$

and

$$\langle u(t), \frac{d}{dt}u_\varepsilon(t) \rangle = \frac{1}{i\varepsilon} \langle u(t), P(t)u_\varepsilon(t) \rangle = \frac{1}{i\varepsilon} \langle P(t)u(t), u_\varepsilon(t) \rangle = 0,$$

which completes the proof. \square

Corollary 5.21. *Suppose $\gamma \subset X$ is a curve on a compact surface such that $\gamma(0) = \gamma(1)$, then $u(1) = \text{hol}_D(\gamma)u(0)$.*

Here are two lemmas prepared for the proof of Theorem 5.18.

Lemma 5.22. *In general, for*

$$i\partial_t V(t) = H(t)V(t), V(0) = I,$$

with $H(t)^* = H(t)$ self-adjoint, then we have $\partial_t(V(t)^*V(t)) = 0$ and hence $V(t)^*V(t) = I$.

Proof. This follows from the computation

$$i\partial_t(V(t)^*V(t)) = V(t)^*(-H(t) + H(t))V(t) = 0$$

since $i\partial_t V(t)^* = -V(t)^*H(t)$. \square

Lemma 5.23. *Given a self-adjoint operator $H(t)^* = H(t)$, then*

$$U(t)^*[Q(t), H(t)]U(t) = i\varepsilon \left(\partial_t(U(t)^*Q(t)U(t)) - U(t)^*\dot{H}(t)U(t) \right).$$

Proof. This is a direct calculation as follows.

$$\begin{aligned} i\varepsilon\partial_t(U(t)^*Q(t)U(t)) &= i\varepsilon U(t)^*\dot{H}(t)U(t) + U(t)^*(-H(t))Q(t)U(t) + U(t)^*\dot{Q}(t)H(t)U(t) \\ &= i\varepsilon U(t)^*\dot{H}(t)U(t) + U(t)^*[Q(t), H(t)]U(t), \end{aligned}$$

\square

Now we prove the adiabatic theorem.

Proof of Theorem 5.18. As in the proof of Theorem 5.20, we assume $\lambda \equiv 0$. The proof is adapted from [1] due to Avron and Elgart.

- Set

$$\begin{cases} i\varepsilon\partial_t U_\varepsilon(t) = P(t)U_\varepsilon(t), \\ U_\varepsilon(0) = id, \end{cases}$$

and we omit the subscript ε in the following proof. One can check that $P(t)^* = P(t)$ implies $U(t)^{-1} = U(t)^*$ thanks to Lemma 5.22.

- Let γ be a contour around the simple isolated eigenvalue $\lambda = 0$ and

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

such that $\Pi(t)H = \ker(P(t))$, $\Pi(t) = \Pi(t)^*$, $\Pi(t)^2 = \Pi(t)$ and the formula for $\Pi(t)$ obviously shows that $\Pi(t)P(t) = P(t)\Pi(t)$.

- We say U_A is given by

$$\begin{cases} i\varepsilon\partial_t U_A(t) = (P(t) + i\varepsilon[\dot{\Pi}(t), \Pi(t)])U_A(t), \\ U_A(0) = I \end{cases}$$

is the adiabatic evolution, where we add a commutator term, which corrects the evolution so that it stays in the zero eigenspace of $P(t)$. Since the commutator, $[\dot{\Pi}(t), \Pi(t)]$ is anti-self-adjoint, and it multiplied by i is again self-adjoint and hence we know $U_A(t)^*U_A(t) = I$ by Lemma 5.22.

- We claim that $\Pi(t)U_A(t) = U_A(t)\Pi(0)$. We compute

$$\begin{aligned} \frac{d}{dt} (U_A(t)^*\Pi(t)U_A(t)) &= U_A^* \left(-P - i\varepsilon[\dot{\Pi}, \Pi] \right) \Pi + \Pi \left(P + i\varepsilon[\dot{\Pi}, \Pi] + i\varepsilon\dot{\Pi} \right) U_A \\ &= i\varepsilon U_A^* \left(\dot{\Pi} - \dot{\Pi}\Pi + \Pi\dot{\Pi}\Pi + \Pi\dot{\Pi}\Pi - \dot{\Pi}\Pi \right). \end{aligned}$$

Since $\dot{\Pi} = \frac{d}{dt}(\Pi^2) = \Pi\dot{\Pi} + \dot{\Pi}\Pi$. If we multiply by Π , we get

$$\Pi\dot{\Pi} = \Pi\dot{\Pi}\Pi + \Pi\dot{\Pi}\Pi = \Pi\dot{\Pi} + \Pi\dot{\Pi}\Pi,$$

which implies $\Pi\dot{\Pi}\Pi = 0$. Thus, $\frac{d}{dt} (U_A(t)^*\Pi(t)U_A(t)) = 0$ and hence the claim holds.

- Now we need to prove

$$\|U(t) - U_A(t)\| \leq C\varepsilon$$

and we write

$$U_A(t) - U(t) = U(t) \int_0^t \frac{d}{ds} (U(s)^*U_A(s)) ds.$$

Let $W(s) = U(s)^*U_A(s)$, then $W(0) = id$ and the same type of argument as in Lemma 5.22 gives

$$\begin{aligned} \partial_s W(s) &= -\frac{i}{\varepsilon} U(s)^* \left(-P(s) + P(s) + i\varepsilon[\dot{\Pi}(s), \Pi(s)] \right) U_A(s) \\ &= U(s)^* [\dot{\Pi}(s), \Pi(s)] U_A(s) = U(s)^* [\dot{\Pi}(s), \Pi(s)] U(s) U(s)^* U_A(s) = U(s)^* [\dot{\Pi}(s), \Pi(s)] U(s) W(s). \end{aligned} \tag{5.13}$$

Motivated by Lemma 5.23 if we could write $U(s)^*[\dot{\Pi}(s), \Pi(s)]U(s)$ as something similar to $U(s)^*[Q(s), H(s)]U(s)$ for some Q, H , then we shall gain an extra ε in the computation.

Now the key thing is to find $X(t)$ such that

$$[\dot{\Pi}(s), \Pi(s)] = [P(s), X(s)]. \quad (5.14)$$

Note that $\Pi(s) = \frac{1}{2\pi i} \oint_{\gamma} (z - P(s))^{-1} dz$, we claim

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

is as desired. We write

$$[P(s), X(s)] = -\frac{1}{2\pi i} \oint (z - P(s))^{-1} \left(P(s) \dot{\Pi}(s) - \dot{\Pi}(s) P(s) \right) (z - P(s))^{-1} dz.$$

The identity

$$(z - P(s))^{-1} P(s) = -(z - P(s))^{-1} (z - P(s)) + z(z - P(s))^{-1}$$

gives

$$\begin{aligned} [P(s), X(s)] &= -\frac{1}{2\pi i} \oint (-I + z(z - P(s))^{-1}) \dot{\Pi}(s) (z - P(s))^{-1} dz \\ &\quad + \frac{1}{2\pi i} \oint (z - P(s))^{-1} \dot{\Pi}(s) (-I + z(z - P(s))^{-1}) dz \\ &= \frac{1}{2\pi i} \oint \left(\dot{\Pi}(s) (z - P(s))^{-1} - (z - P(s))^{-1} \dot{\Pi}(s) \right) dz = [\dot{\Pi}(s), \Pi(s)]. \end{aligned}$$

Combining Lemma 5.23, (5.13) and (5.14), we know

$$\begin{aligned} \dot{W} &= U(s)^*[P(s), X(s)]U(s)W(s) = -i\varepsilon (\partial_s U^* X U + U^* X \partial_s U) W \\ &= -i\varepsilon (\partial_s (U^* X U) - U^* \partial_s X U) W = -i\varepsilon \left(\partial_s (U^* X U W) - U^* X U \dot{W} - U^* \dot{X} U W \right) \\ &= -i\varepsilon \left(\partial_s (U^* X U_A) - U^* X U \partial_s W - U^* \dot{X} U_A \right) = -i\varepsilon \left(\partial_s (U^* X U_A) - U^* X [\dot{\Pi}, \Pi] U_A - U^* \dot{X} U_A \right), \end{aligned}$$

where we use (5.13) in the last step.

Since U^* is unitary, X is bounded, $[\dot{\Pi}, \Pi]$ is bounded and U_A is unitary, we know $U^* X [\dot{\Pi}, \Pi] U_A$ and $U^* \dot{X} U_A$ both bounded. Hence,

$$\begin{aligned} U_A(t) - U(t) &= U(t) \int_0^t \partial_s W(s) ds = -i\varepsilon U(t) \int_0^t \partial_s (U^* X U_A)(s) ds + \mathcal{O}_{H \rightarrow H}(\varepsilon) \\ &= i\varepsilon U(t) (X(0) - U^*(t) X(t) U_A(t)) + \mathcal{O}_{H \rightarrow H}(\varepsilon) = \mathcal{O}_{H \rightarrow H}(\varepsilon), \end{aligned}$$

that is, $\|U_A(t) - U(t)\|_{H \rightarrow H} = \mathcal{O}(\varepsilon)$.

- Set $u(t) = U_A(t)u_0$. Then $u(t) \in \ker P(t)$ since

$$\Pi(t)u(t) = \Pi(t)U_A(t)u_0 = U_A(t)\Pi(0)u_0 = U_A(t)u_0 = u(t).$$

- Moreover, $u(t)$ is independent of ε . We write

$$i\varepsilon\partial_t u = i\varepsilon\partial_t U_A(t)u_0 = \left(P(t) + i\varepsilon[\dot{\Pi}(t), \Pi(t)]\right) U_A(t)u_0 = i\varepsilon[\dot{\Pi}(t), \Pi(t)]u(t),$$

where we use $u \in \ker(P(t))$ in the last step. Hence, u satisfies

$$\partial_t u(t) = [\dot{\Pi}, \Pi]u(t).$$

In particular, $u(t)$ is independent of ε . □

5.5. Floquet band theory revisited, the line bundle of eigenfunctions over \mathbb{R}^2/Γ^* . Let

$$P(x, D) = \sum_{j=1}^2 (D_{x_j} + A_j(x))^2 + V(x), \quad A_j(x+\gamma) = A_j(x), \quad V(x+\gamma) = V(x), \quad \gamma \in \Gamma, x \in \mathbb{R}^2 \quad (5.15)$$

with all things real. For $A_j \neq 0$, it does not satisfy time reversibility as we discussed after presenting Example 4.4. Suppose $P(x, D - \theta)u(\theta, x) = E_k(\theta)u(\theta, x)$ with an isolated band $I_k := \{E_k(\theta) : \theta \in \mathbb{R}^2/\Gamma^*\}$ in the sense that $E_k(\theta)$ is a simple eigenvalue of P on \mathcal{H}_θ and $I_k \cap \cup_{j \neq k} I_j = \emptyset$.

Recall that in the original Bloch-Floquet theory, we introduce some function spaces and operators, say (4.1), Definition 4.11, Definition 4.13 and so on. We look for $v(\theta, \cdot) \in \mathcal{H}_\theta$, that is, $v(\theta, x - \gamma) = e^{i\langle \gamma, \theta \rangle} v(\theta, x)$ such that $Pv(\theta, x) = E_k(\theta)v(\theta, x)$. In order to diagonalize this, we make the Bloch transform

$$\mathcal{B}u(\theta, x) = \sum_{\gamma \in \Gamma} e^{-\langle \gamma, \theta \rangle} u(\theta, x - \gamma), \quad \mathcal{B} : L^2(\mathbb{R}^2) \rightarrow L^2(\mathbb{R}^2/\Gamma^*, \mathcal{H}_\theta),$$

which is periodic in θ . Then we consider the modified Bloch transform

$$\tilde{\mathcal{B}}u(x, \theta) = \sum_{\gamma \in \Gamma} e^{i\langle x - \gamma, \theta \rangle} u(\theta, x - \gamma),$$

which is periodic in x and no longer periodic in θ . This shows that if you want to have periodicity in x , then you will have twist in θ . By introducing the modified Bloch transform, for any θ , we study $v \in L^2(\mathbb{R}^2/\Gamma)$ such that

$$P(x, D - \theta)v(\theta, x) = E_k(\theta)v(\theta, x).$$

Note that $(\tau(p)v)(x) = e^{i\langle x, p \rangle} v(x)$ is a unitary operator on $L^2(\mathbb{R}^2/\Gamma)$, which provides an unitary equivalence

$$P(x, D - \theta - p) = \tau(p)P(x, D - \theta)\tau(p)^*, \quad \theta \in \mathbb{R}^2, \quad p \in \Gamma^*,$$

which motivates the following definition of a line bundle formed by the eigenfunctions. Set

$$L := \{[\theta, v] \in (\mathbb{R}^2 \times L^2(\mathbb{R}^2/\Gamma)) / \sim : v \in \ker_{L^2(\mathbb{R}^2/\Gamma)} (P(x, D - \theta) - E_k(\theta))\}, \quad (5.16)$$

where

$$[\theta, v] = [\theta', v'] \iff (\theta, v) \sim (\theta', v') \iff \exists p \in \Gamma^*, \theta' = \theta + p, v' = \tau(p)v.$$

In the discussion of the Bloch sphere, we associate each point on the sphere a self-adjoint operator. Here, the case is the torus and we would like to associate a self-adjoint operator to each point on the torus. Now we would show that (5.16) is indeed a line bundle given by the equivalence class.

Lemma 5.24. *The set L given by (5.16) gives a C^∞ complex line bundle over \mathbb{R}^2/Γ^* , where*

$$\pi : L \rightarrow \mathbb{R}^2/\Gamma^*, \pi : [\theta, v] \rightarrow [\theta] \in \mathbb{R}^2/\Gamma^*.$$

Proof. By using Lemma 4.16 inductively, we can find $\mathbb{R}^n \ni \theta \mapsto u(\theta, \cdot) \in C^\infty(\mathbb{R}^2/\Gamma)$ to be a smooth family of solutions to $P(x, D - \theta)u(\theta, x) = E_k(\theta)u(\theta, x)$ with $\|u(\theta, \cdot)\|_{L^2(\mathbb{R}^2/\Gamma)} = 1$. (The smoothness in θ can be seen from the analytic formula for the spectral projection $\Pi(\theta)$ or from the Grushin problem.)

Thanks to our assumption that I_k is an isolated simple band, one can check that the action of the discrete group Γ^* , given by

$$p : (\theta, v) \mapsto (\theta + p, \tau(p)v)$$

on the trivial line bundle

$$\tilde{L} := \{(\theta, \tau u(\theta)) : \theta \in \mathbb{C}, \tau \in \mathbb{C}\} \simeq \mathbb{C}_\theta \times \mathbb{C}_\tau$$

is free and proper and the quotient map is given by

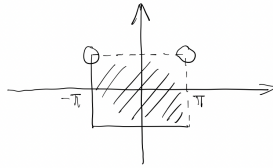
$$(\theta, \tau u(\theta)) \mapsto [\theta, \tau u(\theta)].$$

Hence its quotient by that action, L , is a smooth manifold of dimension two. Moreover, we have

$$\pi^{-1}([\theta]) \simeq \ker_{L^2(\mathbb{R}^2/\Gamma)}(P(x, D - \theta) - E_k(\theta)) \simeq \mathbb{C}$$

has a vector space structure and local coordinates θ provide the needed trivializations. \square

From the dicussion before, we can choose F to be a fundamental domain of $\Gamma^* = (2\pi\mathbb{Z})^2$, given in the figure.



For $F \ni \theta \mapsto u(\theta, x) \in \ker_{L^2(\mathbb{R}^2/\Gamma)}$ over F , a section is written as

$$s : \mathbb{R}^2/\Gamma^* \rightarrow L, \quad s(\theta) = (\theta, \tilde{s}(\theta)u(\theta, x)), \theta \in F, \tilde{s} \in C^\infty(F).$$

As a remark, we just use this single chart here since we only miss a set of measure zero, which will not affect the calculation of Chern number and other properties. When we deal with the Bloch sphere, we do the calculation in \mathbb{C} , which ignore one point (the north/south pole) in the Bloch sphere.

Now we go back to our calculation. Analogous to (5.8), the connection is given by $D(\tilde{s}u) = (d\tilde{s} + \eta\tilde{s})u$, where

$$\eta := \langle d_\theta u(\theta, \cdot), u(\theta, \cdot) \rangle_{L^2(\mathbb{R}^2/\Gamma)} = \langle \partial_{\theta_1} u, u \rangle d\theta_1 + \langle \partial_{\theta_2} u, u \rangle d\theta_2.$$

This gives the following formula for the curvature

$$\Theta = d\eta = -2i\text{Im} \langle \partial_{\theta_1} u(\theta, \cdot), \partial_{\theta_2} u(\theta, \cdot) \rangle_{L^2(\mathbb{R}^2/\Gamma)} d\theta_1 \wedge d\theta_2, \quad \theta \in F.$$

Then the Chern number is given by

$$c_1(L) = \frac{1}{\pi} \int_F \text{Im} \langle \partial_{\theta_1} u(\theta, \cdot), \partial_{\theta_2} u(\theta, \cdot) \rangle_{L^2(\mathbb{R}^2/\Gamma)} d\theta_1 d\theta_2.$$

In particular, if the integral on the right hand side does not vanish then the line bundle is nontrivial. The good side of this is nontrivial topology prevents fast decay of Wannier functions. As we know, Wannier functions give us an orthonormal basis for the spectrum of the original operator P associated to this k -th band.

5.6. Decay of Wannier functions. We again assume I_k is a simple isolated band as we did at the beginning of the preceding subsection. And we denote the spectral projection associated to I_k by $\Pi_k := 1_{I_k}(P)$. In Section 4.6, we discussed the basis of $\Pi_k L^2(\mathbb{R}^2)$ for time reversible operators P , $\overline{Pu} = P\bar{u}$. We now consider a more general case.

Definition 5.25. We say φ_0 is a Wannier function associated to the simple isolated band I_k if $\{\varphi_0(x - \gamma)\}_{\gamma \in \Gamma}$ form an orthonormal basis of $\Pi_k L^2(\mathbb{R}^2)$.

We mimic the discussion in Theorem 4.25. Note that the proof of Theorem 4.25 does not rely on the analyticity in θ derived in Theorem 4.23, so by the same argument, any $\varphi(\theta, x) \in L^2(\mathbb{R}^2/\Gamma^*; \mathcal{H}_\theta)$ satisfying $P\varphi(\theta) = E_k(\theta)\varphi(\theta)$ produces a Wannier function

$$\varphi_0(x) := \frac{1}{|\mathbb{R}^2/\Gamma^*|} \int_{\mathbb{R}^2/\Gamma^*} \varphi(\theta, x) d\theta$$

such that $\{\varphi_0(x - \gamma)\}$ form an orthonormal basis of $\Pi_k L^2(\mathbb{R}^2)$.

On the other hand, set $\varphi(\theta, \cdot) := |\mathbb{R}^2/\Gamma^*|^{\frac{1}{2}} \mathcal{B}\varphi_0(\theta, \cdot)$, then $\varphi \in \ker_{\mathcal{H}_\theta}(P - E_k(\theta))$ thanks to (4.2).

The condition that $\{\varphi_0(x - \gamma)\}_{\gamma \in \Gamma}$ forms an orthonormal basis implies $\|\varphi(\theta, \cdot)\|_{\mathcal{H}_\theta} = 1$ since

$$\begin{aligned} \|\varphi(\theta, \cdot)\|_{\mathcal{H}_\theta}^2 &= \int_{\mathbb{R}^2/\Gamma} \sum_{\gamma, \gamma' \in \Gamma} e^{-i(\gamma - \gamma')\theta} \varphi_0(\theta, x - \gamma) \overline{\varphi_0(\theta, x - \gamma')} dx \\ &= \int_{\mathbb{R}^2/\Gamma} \sum_{\gamma, \gamma'' \in \Gamma} e^{-i\gamma''\theta} \varphi_0(\theta, x - \gamma) \overline{\varphi_0(\theta, x - \gamma + \gamma'')} dx \\ &= \int_{\mathbb{R}^2} \sum_{\gamma'' \in \Gamma} e^{-i\gamma''\theta} \varphi_0(\theta, x) \overline{\varphi_0(\theta, x + \gamma'')} dx = \int_{\mathbb{R}^2} |\varphi_0(x)|^2 dx = 1. \end{aligned}$$

Conversely, from the derivation in Section 4.6, we know any normalized family $\varphi(\theta, x) \in L^2(\mathbb{R}^2/\Gamma^*; \mathcal{H}_\theta)$ such that $P\varphi(\theta) = E_k(\theta)\varphi(\theta)$ produces a Wannier function φ_0 as in Theorem 4.25.

Obviously, our Wannier function is totally non-unique because we can always multiply it by some phase $g(\theta)$ as long as we know it's L^2 norm is 1. But, in the case of trivial line bundle, we can choose a Wannier function analytic in θ , which has exponential decay in x .

And this is closely related to what we discussed in Section 4.6, where we study the special cases that P is time reversible and prove that we can choose a Wannier function with exponential decay in x (Theorem 4.26), using the specific construction of φ with analyticity in θ , obtained in Theorem 4.23.

Theorem 5.26. *Suppose P is given by (5.15) and for some k , I_k is an isolated simple band. Let L be the line bundle over \mathbb{R}^2/Γ^* given by (5.16). 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 and $\varepsilon > 0$ satisfying $\int_{\mathbb{R}^2} |x|^{2(1+\varepsilon)} |\varphi_0(x)|^2 dx < \infty$;*
- (3) $c_1(L) = 0$.

Remark 5.27. In other words, you can only have localized Wannier functions if the line bundle is trivial. Wannier functions cannot decay that fast, which implies that the electrons are not so localized and can interact, which is related to interesting physical phenomena such as superconductivity - see [15].

To show (2) \Rightarrow (3), we need a lemma. Recall the modified Bloch transform \tilde{B} is given by

$$\tilde{B}u(x, \theta) = \frac{1}{|\mathbb{R}^2/\Gamma^*|^{\frac{1}{2}}} \sum_{\gamma \in \Gamma} e^{i\langle x-\gamma, \theta \rangle} u(x-\gamma),$$

which satisfies

$$\tilde{B}u(x-\gamma, \theta+p) = e^{i\langle x, p \rangle} \tilde{B}u(x, \theta) = \tau(p) \tilde{B}u(x, \theta).$$

Lemma 5.28. *Suppose $u \in \mathcal{S}(\mathbb{R}^2)$, we have*

$$D_{\theta_j} \tilde{B}u = \tilde{B}(x_j u),$$

which is somewhat similar to Fourier transform. This motivates the definition of $H_\tau^k(\mathbb{R}^2/\Gamma^ \times \mathbb{R}^2/\Gamma)$, given by*

$$\|v\|_{H_\tau^k(\mathbb{R}^2/\Gamma^* \times \mathbb{R}^2/\Gamma)}^2 = \sum_{|\alpha| \leq k} \int_{\mathbb{R}^2/\Gamma} \int_{\mathbb{R}^2/2\Gamma^*} |D_\theta^\alpha v|^2 d\theta dx,$$

where $v \in \mathcal{S}'(\mathbb{R}^2 \times \mathbb{R}^2)$ such that $v(x+\gamma, \theta+p) = \tau(p)v(x, \theta)$. Then we have

$$\|\tilde{B}u\|_{H_\tau^k(\mathbb{R}^2/\Gamma^* \times \mathbb{R}^2/\Gamma)}^2 \simeq \|\langle x \rangle^k u\|_{L^2(\mathbb{R}^2)}^2.$$

Proof. For $u \in \mathcal{S}(\mathbb{R}^2)$, we compute

$$D_{\theta_j} \tilde{B}u = \frac{1}{|\mathbb{R}^2/\Gamma^*|^{\frac{1}{2}}} \sum_{\gamma \in \Gamma} e^{i\langle x-\gamma, \theta \rangle} (x_j - \gamma_j) u(x-\gamma) = \tilde{B}(x_j u).$$

It follows that $\|\tilde{B}u\|_{H_\tau^k(\mathbb{R}^2/\Gamma^* \times \mathbb{R}^2/\Gamma)}^2$ is some constant multiple of $\|\langle x \rangle^k u\|_{L^2(\mathbb{R}^2)}^2$. \square

Remark 5.29. Here, v is not periodic in θ , so we cannot use the definition for Sobolev spaces on periodic functions. To make sense of the derivative on the boundary of the cell, we consider on a larger cell $\mathbb{R}^2/2\Gamma$ instead of just focusing on a fundamental cell of Γ in the definition of $H_\tau^k(\mathbb{R}^2/\Gamma^* \times \mathbb{R}^2/\Gamma)$ and hence

$$H_\tau^k(\mathbb{R}^2/\Gamma^* \times \mathbb{R}^2/\Gamma) \subset H_{loc}^k(\mathbb{R}^2 \times \mathbb{R}^2).$$

Now we prove Theorem 5.26.

Proof of Theorem 5.26. It is obvious that (1) \Rightarrow (2). For (3) \Rightarrow (1), we do the regularization argument like what we did in Theorem 4.23 to get a real analytic section and the existence of wannier functions with exponential decay is then obtained like what we did for Theorem 4.26.

Now we show (2) \Rightarrow (3). First, from Lemma 5.28, we know $\|\tilde{B}u\|_{H^k(\mathbb{R}^2/\Gamma^* \times \mathbb{R}^2/\Gamma)}^2 \simeq \|\langle x \rangle^k u\|_{L^2(\mathbb{R}^2)}$. By an interpolation argument in [13, Appendix A], we can replace $k \in \mathbb{Z}_+$ by any $s \in \mathbb{R}_+$. Then by our assumption, $\varphi_0(\cdot) \in H^{1+\varepsilon}(\mathbb{R}^2)$, which implies

$$\varphi(\theta, x) = |\mathbb{R}^2/\Gamma^*|^{\frac{1}{2}} \mathcal{B}\varphi_0(\theta, x) \in H^{1+\varepsilon}(\mathbb{R}^2 \times \mathbb{R}^2),$$

and hence $\theta \mapsto \varphi(\theta, \cdot)$ is a continuous thanks to the Sobolev embedding $H^{1+\varepsilon}(\mathbb{R}^2) \subset C^0(\mathbb{R}^2)$. This means that our line bundle has a non-vanishing continuous continuous section and hence (3) holds. \square

5.7. Kronig-Penney model and Thouless pumping - computation of Chern number. We provide an example with physical background in which we can compute the Chern number explicitly. The Kronig-Penney model is a simplified model for an electron in a one-dimensional periodic potential. See [16] for a brief account.

We consider

$$P(\lambda) = D_x^2 + V(x - \lambda), \quad V(x) = V(x + 1),$$

where V is a potential, not smooth but enough to do explicit computation. The potential

$$V(x) = \sum_{m \in \mathbb{Z}} q \delta_0(x - m)$$

is called the Kronig-Penney model, where q is a constant. The domain

$$\mathcal{D}(P) = \{u \in H^1(\mathbb{R}) : u \in H^2(\mathbb{R} \setminus \mathbb{Z}), u'(m_+) - u'(m_-) = qu(m), \forall m \in \mathbb{Z}\}$$

where H^1 implies continuity and u is H^2 away from the integers implies that the derivative is continuous away from the integers. At the integers, the first derivative has a jump.

Thus, for $u \in \mathcal{D}(P)$, $\text{supp} u \subset (-1, 1)$, the distribution derivative u'' will be given by

$$\partial_x^2 u = q \delta_0 u.$$

Moreover, one can check $P(0)$ is a self-adjoint operator.

As we did before when discussing the Floquet theory, we look for w such that

$$\begin{aligned} P(0)w(\theta, x) &= E(\theta)w(\theta, x), \\ w(\theta, x + 1) &= e^{i\theta}w(\theta, x), \quad 0 \leq \theta < 2\pi. \end{aligned}$$

Away from integers, $P = P(0) = D_x^2$, making the equation explicitly solvable and we only need to match the boundary conditions about the jumps. The solution is explicitly given by

$$\begin{aligned} w(\theta, x) &= e^{-i\theta x} u(\theta, x), \quad u(\theta, x) = \sum_{m \in \mathbb{Z}} u_1(\theta, x - m), \\ u_1(\theta, x) &= c_1(\theta) (e^{i\theta x} \sin(\alpha(\theta)x) + e^{i\theta(1+x)} \sin(\alpha(\theta)(1-x))) 1_{[0,1]}(x), \\ q \sin \alpha(\theta) + 2\alpha(\theta) \cos \alpha(\theta) &= 2\alpha(\theta) \cos \theta, \quad \text{Im } \alpha(\theta) \geq 0, \quad E(\theta) = \alpha(\theta)^2, \end{aligned}$$

where $c_1(\theta)$ is chosen such that $\|u_1(\theta, \cdot)\|_{L^2([0,1])} = 1$. By solving the transcendental equation for $\alpha(\theta)$ numerically, we find that it has a discrete set of solutions (with imaginary values of α occurring when q is negative). It is easy to check

$$P(0, \theta)u(\theta, x) = \left((D_x - \theta)^2 + \sum_{m \in \mathbb{Z}} a\delta_0(x - m) \right) u(\theta, x) = E(\theta)u(\theta, x)$$

thanks to the property that

$$(D_x - \theta)(e^{i\theta x}w(\theta, x)) = e^{i\theta x}D_x w(\theta, x).$$

Note that even though we assume V is smooth when we discuss the Floquet theory, but in fact this is completely irrelevant and the complete theory is still nice as long as we assume periodicity for V . Suppose that $E(\theta) = E_k(\theta)$ and

$$\{E_k(\theta) : \theta \in [0, 2\pi)\} \cap \{E_j(\theta) : \theta \in [0, 2\pi)\} = \emptyset, \quad \forall j \neq k.$$

Let $\lambda \in \mathbb{Z}$, we now consider the following periodic deformation of $P(\theta)$:

$$P(\lambda, \theta) = (D_x - \theta)^2 + V(x - \lambda),$$

with the same eigenvalues and eigenfunctions given by $u(\theta, x - \lambda)$, that is, $P(\lambda, \theta)u(\theta, x - \lambda) = E(\theta)u(\theta, x - \lambda)$. Then we can consider the following natural line bundle similar to (5.16) given by

$$\begin{aligned} L_{KP} &= \{(\lambda, [\theta, v]) \in \mathbb{R} \times (\mathbb{R} \times L^2(\mathbb{R}/\mathbb{Z})) / \sim : v \in \ker_{L^2(\mathbb{R}/\mathbb{Z})}(P(\lambda, \theta) - E_k(\theta))\}, \\ [\theta, v] = [\theta', v'] &\iff (\theta, v) \sim (\theta', v') \iff \exists p \in \mathbb{Z}, \theta' = \theta + 2\pi p, v' = e^{2\pi i p x} v. \end{aligned} \quad (5.17)$$

Roughly speaking, the operator is not periodic in θ , but if you shift the operator by $2\pi p$ in θ , then it is unitarily equivalent, and the unitarily equivalence is given by multiplication by $e^{2\pi i p x}$. The eigenfunction corresponding to $E(\theta)$ is given by $u(\theta, \lambda, x) = u(\theta, x - \lambda)$ and

$$u(\theta + 2\pi p, x + l) = e^{-2\pi i l p} e^{2\pi i p x} u(\theta, x). \quad (5.18)$$

Now we compute the Chern number. We use a trivialization of our section on $(0, 1)_\lambda \times (0, 2\pi)_\theta$,

$$s(\theta, \lambda) = (\theta, \lambda, s_1(\theta, \lambda)u(\theta, \lambda)).$$

Then like what we did to derive (5.8), we get

$$D_1 s_1 = ds_1 + \langle du, u \rangle_{L^2(\mathbb{R}/\mathbb{Z})} = ds_1 + \langle \partial_\lambda u, u \rangle d\lambda + \langle \partial_\theta u, u \rangle d\theta.$$

Let $\eta = \langle \partial_\lambda u, u \rangle d\lambda + \langle \partial_\theta u, u \rangle d\theta$, then the curvature is given by

$$\Theta = d\eta = \partial_\theta \langle \partial_\lambda u, u \rangle d\theta \wedge d\lambda + \partial_\lambda \langle \partial_\theta u, u \rangle d\lambda \wedge d\theta = 2i \operatorname{Im} \langle u_\lambda, u_\theta \rangle d\theta \wedge d\lambda. \quad (5.19)$$

On the other hand, we compute

$$\begin{aligned} c_1(L_{KP}) &= \frac{i}{2\pi} \int_{\mathbb{T}^2_{(\lambda, \theta)}} d\eta = \frac{1}{\pi} \int_0^1 \int_0^{2\pi} \int_0^1 \operatorname{Im} \left(\partial_\lambda u(\theta, x - \lambda) \overline{\partial_\theta u(\theta, x - \lambda)} \right) d\lambda d\theta dx \\ &= -\frac{1}{\pi} \int_0^1 \int_0^{2\pi} \int_0^1 \operatorname{Im} \left(\partial_x u(\theta, x) \overline{\partial_\theta u(\theta, x)} \right) d\lambda d\theta dx = -\frac{1}{\pi} \int_0^1 \int_0^{2\pi} \operatorname{Im} \left(\partial_x u(\theta, x) \overline{\partial_\theta u(\theta, x)} \right) d\theta dx, \end{aligned} \quad (5.20)$$

where in the second step we use the periodicity in x and in the third step we use $\partial_\lambda u(\theta, x - \lambda) = -\partial_x u(\theta, x - \lambda)$. Using (5.19),

$$\operatorname{Im} \left(\partial_x u(\theta, x) \overline{\partial_\theta u(\theta, x)} \right) d\theta \wedge dx = \frac{1}{2i} d(u_\theta \bar{u} d\theta + u_x \bar{u} dx)$$

Hence, by Stokes' theorem,

$$\begin{aligned} c_1(L_{KP}) &= \frac{i}{2\pi} \int_0^1 \int_0^{2\pi} d(u_\theta \bar{u} d\theta + u_x \bar{u} dx) \\ &= \frac{i}{2\pi} \int_0^{2\pi} (u_\theta \bar{u})(\theta, 2\pi) - (u_\theta \bar{u})(\theta, 0) d\theta + \frac{i}{2\pi} \int_0^{2\pi} (u_x \bar{u})(1, x) - (u_x \bar{u})(0, x) dx. \end{aligned}$$

Now we derive from (5.18) that

$$u(\theta, 1) = u(\theta, 0), \quad u(2\pi, x) = e^{2\pi i x} u(0, x),$$

and hence the first integrand is 0 and the second is $2\pi i |u(0, x)|^2$, which implies that

$$c_1(L_{KP}) = -1.$$

5.8. Landau Hamiltonian in dimension 2 revisited. Now we go back to Section 2.4 and consider the two dimensional Landau Hamiltonian

$$P_B = (D_x + A)^2 = (D_{x_1} + A_1(x))^2 + (D_{x_2} + A_2(x))^2,$$

where $d(A_1(x) dx_1 + A_2(x) dx_2) = B dx_1 \wedge dx_2$. We choose the symmetric gauge $A = (A_1, A_2)$,

$$A_1(x) = -\frac{B}{2} x_2, \quad A_2(x) = \frac{B}{2} x_1.$$

Let $w = x_1 + ix_2$, then

$$P_B = A_B^* A_B + B, \quad A_B = 2D_{\bar{w}} - \frac{1}{2} i B w,$$

with $\operatorname{Spec}(P_B) = \{(2n+1)B\}_{n \in \mathbb{N}}$, $D_{\bar{w}} = \frac{1}{i} \partial_{\bar{w}} = \frac{1}{2i} (\partial_{\operatorname{Re} w} + i \partial_{\operatorname{Im} w})$, where each eigenvalue has infinite multiplicity.

And the interesting point is that it has explicit flat bands. As we discussed in Section 2.4,

$$A_B = e^{-B|w|^2/4} (2\partial_{\bar{w}}) e^{B|w|^2/4},$$

$$\ker_{L^2(\mathbb{C})}(P_B - B) = \ker_{L^2(\mathbb{C})}(A_B) = \left\{ f(w) e^{-\frac{B|w|^2}{4}} : f \in \mathcal{O}(\mathbb{C}), \int |f|^2 e^{-\frac{B|w|^2}{4}} dm(w) < \infty \right\}. \quad (5.21)$$

Definition 5.30. Let $\Gamma \subset \mathbb{C}$ be a lattice with $\gamma \in \Gamma$. Analogous to the usual translation $T_\gamma u(w) = u(w - \gamma)$, a magnetic translation by γ is given by

$$T_\gamma^B u(w) = e^{\frac{1}{4} B (w \bar{\gamma} - \bar{w} \gamma)} u(w - \gamma).$$

It is easy to check that $(T_\gamma^B)^* = T_{-\gamma}^B$, $A_B T_\gamma^B = T_\gamma^B A_B$, $P_B T_\gamma^B = T_\gamma^B P_B$ and

$$T_\gamma^B T_{\gamma'}^B = e^{\frac{1}{2} B (\gamma' \bar{\gamma} - \bar{\gamma}' \gamma)} T_{\gamma' + \gamma}^B T_\gamma^B, \quad (5.22)$$

where $\frac{1}{2}(\gamma' \bar{\gamma} - \bar{\gamma}' \gamma)$ is the parallelogram formed by $\bar{\gamma}, \gamma'$.

The problem for generalizing the Bloch-Floquet theory to this case is that the magnetic translations do not commute, as shown in (5.22). However, since there is no potential term in our operator P_B , we have the freedom to choose our lattice. If one choose Γ such that

$$\frac{1}{2}B(\gamma'\bar{\gamma} - \bar{\gamma}'\gamma) \in 2\pi i\mathbb{Z}, \quad \forall \gamma, \gamma' \in \Gamma, \quad (5.23)$$

which is called the rational flux condition, that is, the flux through the fundamental cell, the parallelogram formed by $\bar{\gamma}, \gamma'$, is $2\pi\mathbb{Z}$, then $[T_\gamma^B, T_{\gamma'}^B] = 0$.

Suppose $\gamma = \mathbb{Z} \oplus \tau\mathbb{Z}$ for simplicity with $\text{Im } \tau > 0$. Then the rational flux condition (5.23) is simply

$$N_B := \frac{B}{2\pi} \text{Im } \tau \in \mathbb{Z}. \quad (5.24)$$

Note that if $N_B \in \mathbb{Q}$, say $N_B = \frac{p}{q}$, then we consider in a larger lattice fundamental cell spanned by $q, q\tau$, which would satisfy (5.24). This is why we call this the rational flux condition.

Due to the missing periodicity for the gauge, we shall define a new space \mathcal{H}_k^B instead of using $L^2(\mathbb{R}^2/\Gamma)$. Now we define

$$\mathcal{H}_k^B := \left\{ u \in L_{loc}^2(\mathbb{C}) : T_\gamma^B u(w) = e^{i\text{Re}(\bar{k}\gamma)} u(w), \forall \gamma \right\}, \quad k \in \mathbb{C}.$$

The condition in the definition above is similar to the Floquet condition since $\text{Re}(\bar{k}\gamma) = \langle k, \gamma \rangle$ if we view $k, \gamma \in \mathbb{C} \simeq \mathbb{R}^2$. Moreover, the space \mathcal{H}_k^B is the same for k modulo Γ^* and hence we can just assume $k \in \mathbb{C}/\Gamma^*$. When (5.24) holds, $\{T_\gamma^B\}_{\gamma \in \Gamma}$ is an abelian group, which is isomorphic to the lattice Γ . By Schur's lemma from representation theory, all irreducible complex representations of abelian groups one-dimensional. And note that for all $k \in \mathbb{C}/\Gamma^*$, $\pi_k(\gamma) : \mathbb{C} \rightarrow \mathbb{C}$ given by

$$\pi_k(\gamma)z := e^{i\text{Re}(\bar{k}\gamma)} z = e^{\frac{i}{2}(\bar{k}\gamma + k\bar{\gamma})} z$$

are all unitary irreducible representations of Γ . Note that if $\Gamma = \mathbb{Z} \oplus \tau\mathbb{Z}$, $\Gamma^* = \frac{2\pi i}{\text{Im } \tau} \Gamma$.

For $u \in \mathcal{S}(\mathbb{C})$, the magnetic Bloch transform is given by

$$\mathcal{B}^B u(k, x) := \frac{1}{|\mathbb{C}/\Gamma^*|^{\frac{1}{2}}} \sum_\gamma e^{-i\text{Re}(\bar{k}\gamma)} T_\gamma^B u(x) \in L^2(\mathbb{C}/\Gamma^*; \mathcal{H}_k^B).$$

It extends to a unitary operator as for $u \in \mathcal{S}(\mathbb{C})$, we have

$$\begin{aligned} & \sum_{\gamma \in \Gamma} \sum_{\gamma' \in \Gamma} \int_{\mathbb{C}/\Gamma} \frac{1}{|\mathbb{C}/\Gamma^*|} \left(\int_{\mathbb{C}/\Gamma^*} e^{-\frac{i}{2}(\bar{k}(\gamma-\gamma') + k(\bar{\gamma}-\bar{\gamma}'))} dm(k) \right) e^{\frac{1}{4}(w(\bar{\gamma}-\bar{\gamma}') - \bar{w}(\gamma-\gamma'))} u(w-\gamma) \overline{u(w-\gamma')} dm(w) \\ &= \sum_{\gamma \in \Gamma} \sum_{\gamma' \in \Gamma} \int_{\mathbb{C}/\Gamma} \delta_{\gamma\gamma'} e^{\frac{1}{4}(w(\bar{\gamma}-\bar{\gamma}') - \bar{w}(\gamma-\gamma'))} u(w-\gamma) \overline{u(w-\gamma')} dm(w) = \int_{\mathbb{C}} |u(w)|^2 dm(w). \end{aligned}$$

Then one can easily compute the inverse of \mathcal{B}^B as in Theorem 4.12, which is given by

$$\mathcal{C}^B v(x) := \frac{1}{|\mathbb{C}/\Gamma^*|^{\frac{1}{2}}} \int_{\mathbb{C}/\Gamma^*} v(k, x) dm(k).$$

Hence, as in Section 4.3, we also have

$$\mathcal{B}^B P_B \mathcal{C}^B v(k, x) = (P_B v(k, \cdot))(x).$$

Then we can study the vector space

$$\ker_{\mathcal{H}_k^B}(P_B - B) = \ker_{\mathcal{H}_k^B} A_B.$$

Theorem 5.31 (Haldane-Rezayi). *Suppose $\Gamma = \mathbb{Z} \oplus \tau\mathbb{Z}$ and (5.24) holds. Then the kernel $\ker_{\mathcal{H}_k^B}(P_B - B) = \ker_{\mathcal{H}_k^B} A_B$ is finite dimensional and*

$$\dim \ker_{\mathcal{H}_k^B}(P_B - B) = N_B.$$

Proof. In view of (5.21), we write $f(w) = g(w) \exp(Bw^2/4)$. (Note that this is w^2 instead of $|w|^2$.) Therefore, for $u \in \ker_{\mathcal{H}_k^B}(P_B - B)$,

$$u(w) = f(w) \exp(-B|w|^2/4) = g(w) \exp\left(\frac{Bw(w - \bar{w})}{4}\right).$$

By a direct computation, we have

$$T_1^B u(w) = e^{\frac{i}{2}B\text{Im} w} u(w - 1) = g(w - 1) e^{\frac{B(w-1)\text{Im} w}{2}} e^{\frac{i}{2}B\text{Im} w} = g(w - 1) \exp\left(\frac{Bw(w - \bar{w})}{4}\right).$$

On the other hand, $u \in \mathcal{H}_k^B$ implies

$$T_1^B u(w) = e^{i\text{Re} k} u(w) = e^{i\text{Re} k} g(w) \exp\left(\frac{Bw(w - \bar{w})}{4}\right).$$

Hence,

$$g(w - 1) = e^{i\text{Re} k} g(w). \quad (5.25)$$

Similarly, by computing $T_\tau^B u(w)$, we get

$$g(w - \tau) = e^{i\text{Re}(k\tau) - i\pi N_B(\tau - 2w)} g(w). \quad (5.26)$$

Thanks to (5.25) and (5.26), one can compute explicitly that the integration of $\frac{g'}{g}$ along the boundary of a fundamental cell is N_B , which implies that g has exactly N_B zeros in any fundamental cell by argument principle. Suppose g_0 is such a holomorphic function satisfying (5.25) and (5.26), with zeros p_1, \dots, p_{N_B} . Then for any g satisfying (5.25) and (5.26), $h = \frac{g}{g_0}$ is a well-defined meromorphic function on \mathbb{C}/Γ since it is periodic. Now, in order to compute

$$\begin{aligned} \dim \ker_{\mathcal{H}_k^B}(P_B - B) &= \dim\{g \in \mathcal{O}(\mathbb{C}) : g \text{ satisfies (5.25) and (5.26)}\} \\ &= \dim\{h \in \mathcal{M}(\mathbb{C}/\Gamma) \setminus \{0\} : \mathcal{D}(h) \geq D^{-1} = (p_1 \cdots p_{N_B})^{-1}\} \cup \{0\}, \end{aligned}$$

where $\mathcal{M}(\mathbb{C}/\Gamma)$ are all the meromorphic functions on \mathbb{C}/Γ and the divisor D is given by $D = p_1 \cdots p_{N_B}$. Now we claim that

$$\dim\{\omega \in \mathcal{M}^1(\mathbb{C}/\Gamma) \setminus \{0\} : D(\omega) \geq D\} \cup \{0\} = 0.$$

We use the fact any the meromorphic 1-form on the torus is of the form $\omega = f(z) dz$ with f being a meromorphic function on \mathbb{C}/Γ . (See [12, Chapter IV].) Since $D(\omega) \geq D$, then ω is a holomorphic 1-form such that $f = 0$ at p_1, \dots, p_{N_B} . Since all holomorphic functions on the torus are constant functions, we know $\omega = 0$. By combining the results above and applying Riemann-Roch theorem ([8, Chapter 3.4], [12]), we know

$$\dim \ker_{\mathcal{H}_k^B}(P_B - B) = \deg(D) + \dim\{\omega \in \mathcal{M}^1(\mathbb{C}/\Gamma) \setminus \{0\} : D(\omega) \geq D\} \cup \{0\} = N_B + 0.$$

□

Now we discuss the specific case $N_B = 1$ for simplicity. Let $\tau_k : \mathcal{H}_k^B \rightarrow \mathcal{H}_0^B$ be given by

$$(\tau_k u)(z) = e^{\frac{i}{2}(\bar{z}k + \bar{k}z)} u(z)$$

so that we can only work on one single space \mathcal{H}_0^B . Moreover, one can check

$$\tau_k P_B \tau_k^* = P_B(k) := (A_B - k)^*(A_B - k) + B.$$

On the other hand, for $p \in \Gamma^*$, we can define a unitary map

$$\tau_p : \mathcal{H}_0^B \rightarrow \mathcal{H}_0^B, \quad \tau_p^* P_B(k) \tau_p = P_B(k + p).$$

As in (5.16) and (5.17), we have a natural line bundle over \mathbb{C}/Γ^*

$$L_B = \left\{ [k, v] \in (\mathbb{C} \times \mathcal{H}_0^B) / \sim : v \in \ker_{\mathcal{H}_0^B}(A_B - k) \right\},$$

$$[k, v] = [k', v'] \iff (k, v) \sim (k', v') \iff \exists p \in \Gamma^*, k' = k + p, v' = \tau_p v.$$

Theorem 5.32. L_B is a holomorphic line bundle and $c_1(L_B) = -1$.

Proof. See [19, Section 8.2, Theorem 11].

□

NOTE TO THE READER

This document consists of lecture notes that Ning Tang took from a topic course given by Maciej Zworski at UC Berkeley in Fall 2022. The official lecture notes [19] is posted on https://math.berkeley.edu/~zworski/Notes_279.pdf. This note mainly covers [19, Section 1-9] and I added some explanation and details when I thought it would be helpful. There are inevitably errors, which should be entirely attributed to me.

Due to the strike, I missed the courses throughout the last four weeks during that semester. Fortunately, I ended up taking this note after we finished a topic and hence in some sense, this document is not incomplete.

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DEPARTMENT OF MATHEMATICS, UNIVERSITY OF CALIFORNIA, BERKELEY, CA 94720, USA
Email address: math_tn@berkeley.edu