

Mathematical Preliminaries

Definition 1 Let \mathcal{H} be a Hilbert space. The adjoint of an operator $T \in \mathcal{L}(\mathcal{H})$ is an operator T^\dagger that has the property ¹

$$\langle u, Tv \rangle = \langle T^\dagger u, v \rangle$$

Definition 2 Let \mathcal{H} be a Hilbert space. An operator $T \in \mathcal{L}(\mathcal{H})$ is called self adjoint if:

$$T = T^\dagger$$

Definition 3 Let \mathcal{H} be a Hilbert space. An operator $T \in \mathcal{L}(\mathcal{H})$ is called unitary if:

$$\langle Tu, Tv \rangle = \langle u, v \rangle \quad \forall u, v \in \mathcal{H}$$

Definition 4 Let \mathcal{H} be a Hilbert space. An operator $T \in \mathcal{L}(\mathcal{H})$ is called normal if it has the property

$$T^\dagger T = TT^\dagger$$

Corollary 1 Any self adjoint operator is normal.

Theorem 1 Spectral Theorem: Let \mathcal{H} be a Hilbert space (over \mathbb{C}) that is finite dimensional (should also work in countable dimensions). Let $T \in \mathcal{L}$ be a normal operator. Then there exists an orthonormal basis of \mathcal{H} of eigenvectors of T .

Definition 5 Let T be an operator on some Hilbert space \mathcal{H} . The λ eigenspace of T is the subspace²:

$$Eig_T(\lambda) = \left\{ v \in \mathcal{H} \mid Tv = \lambda v \right\}$$

Theorem 2 Let S, T be operators on \mathcal{H} a Hilbert space. Suppose S, T commute meaning that $ST = TS$. Then S can be restricted on $Eig_T(\lambda)$ (meaning that $S(Eig_T(\lambda)) \subseteq Eig_T(\lambda)$)

Proof:

Let $v \in Eig_T(\lambda)$. This means that $Tv = \lambda v$. Now let's consider Sv and show that $Sv \in Eig_T(\lambda)$. In other words, we want to show that Sv is an eigenvector of T with eigenvalue λ . So let's compute $T(Sv)$. Since S and T commute we have:

$$T(Sv) = S(Tv) = S(\lambda v) = \lambda Sv$$

From this we conclude that $Sv \in Eig_T(\lambda)$ as desired.

Corollary 2 If two normal operators $S, T \in \mathcal{L}(\mathcal{H})$ commute for \mathcal{H} some finite (or countable) dimensional Hilbert space then there exists an orthonormal basis of vectors, which are simultaneously eigenvectors of both S and T .

Proof: Consider λ an eigenvalue of T . Since T is normal, we can decompose our Hilbert space, into the eigen subspaces of T .

$$\mathcal{H} = \oplus_{\lambda \in \text{Spectrum}(T)} Eig_t(\lambda)$$

We can then restrict S onto each of the eigenspaces. It will be still normal on this subspace (prove why) and we can get an orthonormal basis of $Eig_T(\lambda)$ of eigenvectors of S . This gives an orthonormal basis of all of \mathcal{H} , where each vector is an eigenvector of both S and T .

Picture.

Corollary 3 If we have some countable collection of normal operators T_i on \mathcal{H} , there exists an orthonormal basis of \mathcal{H} , where each vector is an eigenvector of T_i for all i .

Remark 1 The theorem above, is really the essence of “quantum numbers”. If we have some collection of operators T_i that are self adjoint (hence normal), then we have an orthonormal basis of eigenvectors that diagonalize all of the above simultaneously. We can then hope to label each eigenvector, by what its eigenvalue is for each operator.

If my operators are nice enough with respect to each other, I can hope to label every eigenvector in my basis, just by its

¹If \mathcal{H} is finite dimensional, then for any T its adjoint T^\dagger exists. This is not always true in the infinite dimensional case. But we can often hope that on some subspace $V \subseteq \mathcal{H}$ onto which we can restrict T , we can find an adjoint. Then you can continue working there.

²Convince yourself this set is a subspace

eigenvalues with respect to all of the

For example, suppose we have T, S that are normal and commute. Then we can consider the vector:

$$|\lambda, \mu\rangle - \text{vector in my basis such that}$$

$$T|\lambda, \mu\rangle = \lambda|\lambda, \mu\rangle \quad S|\lambda, \mu\rangle = \mu|\lambda, \mu\rangle$$

If one of these commuting operators is the Hamiltonian, we call these eigenvalues we use to label eigenvectors (states) “quantum numbers”. Since each eigenvector is an eigenstate of the Hamiltonian, we then get that the quantum number of a state is conserved under time evolution (check why yourself).

Translation Invariant System

Let the Hilbert Space $\mathcal{H} = L^2$, the space of square integrable wave functions³ (on either \mathbb{R} , \mathbb{R}^2 or \mathbb{R}^3 depending on the problem). The inner product is given via:

$$\langle f, g \rangle = \int_{\mathbb{R}^n} \bar{f}g$$

Suppose we have some single particle moving in a periodic potential. The Hamiltonian is then:

$$H = \frac{p^2}{2m} + V(x)$$

Where:

$$p^2 : \mathcal{H} \rightarrow \mathcal{H}$$

$$\psi(x) \rightarrow -\hbar^2 \frac{\partial^2 \psi(y)}{\partial y^2} \Big|_x$$

$$V(x) : \mathcal{H} \rightarrow \mathcal{H}$$

$$\psi(x) \rightarrow V(x)\psi(x)$$

We now make the assumption that the potential is invariant under translations by vectors from some lattice. In particular, fix some $a_1, \dots, a_n \in \mathbb{R}^n$. We then assume that:

$$V\left(x + \sum_i m_i a_i\right) = V(x)$$

Where m_i are all integers.

We can then define the following set of translation operators:

$$T_{\vec{m} \cdot \vec{a}} : \mathcal{H} \rightarrow \mathcal{H}$$

$$\psi(x) \rightarrow \psi\left(x + \sum_i m_i a_i\right)$$

It should be easy to notice, that these operators satisfy the property that:

$$T_{\vec{m} \cdot \vec{a}} \circ T_{\vec{m}' \cdot \vec{a}} = T_{(\vec{m} + \vec{m}') \cdot \vec{a}}$$

You can also see that the adjoint of $T_{\vec{m} \cdot \vec{a}}$ is given by (check this by computing the inner product as in the definition):

$$(T_{\vec{m} \cdot \vec{a}})^\dagger = T_{-\vec{m} \cdot \vec{a}}$$

From the two facts above, we can easily see that $T_{\vec{m} \cdot \vec{a}}$ commutes with its adjoint, meaning that $T_{\vec{m} \cdot \vec{a}}$ is normal and has a spectral theorem as above.

³Perhaps it is better to consider Schwartz spaces instead, but this is not essential for this discussion.

Lemma 1 $T_{m \cdot a}$ commutes with the Hamiltonian

Proof: We check this by showing that $T_{m \cdot a}$ commutes with p^2 and V individually. We do this, by checking how they act on wave functions:

$$\begin{aligned}
(p^2 \circ T_{m \cdot a})(\psi(x)) &= p^2(\psi(x + m \cdot a)) \\
&= -\hbar^2 \frac{\partial^2 \psi(y)}{\partial y^2} \Big|_{x+m \cdot a} && \text{by chain rule} \\
&= T_{m \cdot a} \left(-\hbar^2 \frac{\partial^2 \psi(y)}{\partial y^2} \Big|_x \right) \\
&= (T_{m \cdot a} \circ p^2)(\psi(x))
\end{aligned}$$

Now show that $T_{m \cdot a}$ commutes with V

$$\begin{aligned}
(T_{m \cdot a} \circ V)(\psi(x)) &= T_{m \cdot a}(V(x)\psi(x)) \\
&= V(x + m \cdot a)\psi(x + m \cdot a) \\
&= V(x)\psi(x + v \cdot a) && \text{Because we assumed } V \text{ has this periodicity condition} \\
&= V(x)T_{m \cdot a}\psi(x)
\end{aligned}$$

We therefore get that $T_{m \cdot a}$ commutes with the Hamiltonian for any $m \in \mathbb{Z}^n$

Properties of Translation Operators

Lemma 2 The operators $T_{m \cdot a}$ are unitary.

Proof:

$$\langle Tf, Tg \rangle = \int_{-\infty}^{\infty} \bar{f}(x + m \cdot a)g(x + m \cdot a) = \int_{-\infty}^{\infty} \bar{f}(x)g(x) = \langle f, g \rangle$$

Corollary 4 The eigenvalues of $T_{m \cdot a}$ must have norm 1.

Proof:

Suppose v is an eigenvector of $T_{m \cdot a}$ with eigenvalue $Tv = \lambda v$.

$$\langle v, v \rangle = \langle Tv, Tv \rangle = \langle \lambda v, \lambda v \rangle = |\lambda|^2 \langle v, v \rangle$$

We then get $|\lambda|^2 = 1$ as desired.

Lemma 3 Let $v \in \mathcal{H} = L^2(\mathbb{R}^n)$ be simultaneously an eigenvector of $T_{a_1} \dots T_{a_n}$, then v is an eigenvector of $T_{m \cdot a}$ for all m with eigenvalue given by:

$$T_{m \cdot a}v = \exp \left(ik \cdot \left(\sum_i m_i a_i \right) \right) v$$

For some fixed k depending⁴ on v

Proof: See suggested exercise

Bloch's Theorem

Theorem 3 Bloch's Theorem: Let $\mathcal{H} = L^2(\mathbb{R}^n)$. Let H be a Hamiltonian that commutes with the translations operators $T_{m \cdot a}$ for some fixed choice of a_1, \dots, a_n . Then there exists an orthonormal basis of vectors, where each is an eigenvector of H as well as $T_{m \cdot a}$ for all m . Additionally, each eigenvector can be written in the following form:

$$\psi(x) = e^{ik \cdot x} u(x)$$

Where $T_{m \cdot a}u(x) = u(x)$ (i.e. $u(x)$ is periodic under the lattice defined by a_1, \dots, a_n).

⁴Note that our system need not have an eigenvectors for every possible k .

Proof:

From the previous section, we know that all $T_{m \cdot a}$ are normal and they commute with each other. By assumption they commute with the Hamiltonian. By the last theorem in the mathematical preliminaries section, it is clear that there exists an orthonormal basis of vectors that are all eigenvectors of $T_{m \cdot a}$ and of H . We just need to show they have the form as above. This form is in fact just the form of a vector that is an eigenvector of all of $T_{m \cdot a}$.

Let $\psi(x)$ be an eigenvector of all $T_{m \cdot a}$. We then know from the previous section that:

$$T_{m \cdot a} \psi(x) = \exp \left(ik \cdot \left(\sum_i m_i a_i \right) \right) \psi(x)$$

For some k , depending on what the eigenvalues of $\psi(x)$ under $T_{m \cdot a}$ are. Lets define $u(x) = e^{-ik \cdot x} \psi(x)$
It is clear that:

$$\psi(x) = e^{ik \cdot x} u(x)$$

Now, we just need to show that $T_{m \cdot a} u(x) = u(x)$

$$\begin{aligned} T_{m \cdot a} u(x) &= T_{m \cdot a} (e^{-ik \cdot x} \psi(x)) \\ &= \exp(-ik \cdot (x + \sum_i m_i a_i)) \psi(x + \sum_i m_i a_i) \\ &= \exp(-ik \cdot x) \exp(-ik \cdot (\sum_i m_i a_i)) T_{m \cdot a} \psi(x) \\ &= \exp(-ik \cdot x) \exp(-ik \cdot (\sum_i m_i a_i)) \exp(ik \cdot (\sum_i m_i a_i)) \psi(x) \\ &= \exp(-ik \cdot x) \psi(x) \\ &= u(x) \end{aligned}$$

We therefore conclude the proof.

Some Remarks

From Bloch's theorem, we see that if we have a system that is translationally invariant (i.e. the potential of the Hamiltonian has some periodicity), then its eigenstates must be eigenvectors of translations. More over, we know how these eigenstates have to look like! It is some plane wave, multiplied by a periodic function. This is indeed a lot of information. This says, if you go to a plane wave ("momentum" space) basis then you will only need to diagonalize the Hamiltonian over the intersection of these subspaces: $\bigcap_{i=1}^n \text{Eig}_{a_i}(e^{ik \cdot a_i})$ (as it would restrict on these subspaces). This in principle could be a huge reduction in the size of space over which you are diagonalizing your matrix. In some cases, the Hamiltonian will just immediately be diagonal in the plane wave basis.

Following this idea with quantum numbers, we would want to label our basis using the eigenvalues of $T_{m \cdot a}$. In this case, we see that if something is an eigenvector of all $T_{m \cdot a}$ (as is the case with elements of our basis), then the eigenvalue is determined by some vector k . We could then chose k to label my eigenvalues instead. In the suggested exercises, you will see that this choice of k is not unique (i.e. there is more than one k that corresponds to the same eigenvalues for translation operators $T_{m \cdot a}$). This interesting choice of labelling will be of consequence later (somewhat inviting topology into the picture).

Note that if we were able to successfully label our states using k in this way, we could think of eigenvalues of H , as some functions of k . If there are multiple eigenvectors labeled by k , that have different energies, then we get multiple such functions. This is often referred to as "bands". We will discuss/define this more carefully later.

Suggested Exercises

- I) Suppose we are working in two dimensions. Let $a_1 = (a, 0)$ and $a_2 = (0, a)$, for some positive constant a .
- i) Prove lemma (3) for this case.
 - ii) As mentioned before, the choice of k in this lemma is not unique. Find vectors G_1 , and G_2 , such that $k + G_i$ labels the same eigenvector.
- II) Repeat the exercise above but for lattice vectors $a_1 = a(\cos(\frac{\pi}{3}), \sin(\frac{\pi}{3}))$ and $a_2 = a(\cos(\frac{2\pi}{3}), \sin(\frac{2\pi}{3}))$
- III) Now repeat the exercises above for a 3 dimensional case where $a_i = ae_i$
- IV) A manifold appears:
- i) Argue why the following is a useful definition
- Definition 6** *Given some lattice in \mathbb{R}^n defined by vectors a_1, \dots, a_n , we define its reciprocal lattice vectors G_i by requiring that $G_i \cdot a_j = 0$ for all $i \neq j$ and $G_i \cdot a_i = 2\pi$*
- ii) Suppose we work in \mathbb{R}^2 and we are able to label our states with these vectors k . We have a natural identification defined by $k \sim k'$ if $k - k' = b_1 G_1 + b_2 G_2$ where b_1, b_2 are integers. Show that \mathbb{R}^2 quotiented by this equivalence relation is the torus. (I.e. our states in some sense live on the torus)
- V) Sign up to rinse Ivan's teapot next week.