Ph 12b Recitation Notes

Jaeden Bardati
jbardati@caltech.edu

Week 5
February 10th, 2026

1 The Language of Quantum Mechanics: Linear Algebra

1.1 Quantum States as Vectors (repeated)

As we saw earlier, we can represent functions as vectors in a vector space if we like. We know that the quantum state is represented by the wavefunction and that these wavefunctions must be normalized. It turns out that we can form a vector space of just the square-integrable functions. Practically, this means that the wavefunction Ψ can be represented as a vector where $\langle\Psi|\Psi\rangle = 1$ means it is normalized. Then, if we have some basis of states $|\psi_n\rangle$, then we can represent any wavefunction as $\langle\psi|\psi\rangle = \sum_{n=1}^{\infty} c_n\psi_n$ for an appropriate choice of c_ns. By Fourier transforms, we can also show that these coefficients are $c_n = \langle\psi_n|\psi\rangle$. You may notice that this is very similar to what we have been doing with stationary states.

In fact, in this language, the time-independent Schrödinger equation becomes $\bar{H}|\psi\rangle = E|\psi\rangle$. Indeed, we can now interpret finding the energy of a solution we are simply solving for the *eigenvalues* of the Hamiltonian. We also note that the stationary states are the *eigenvalues* of the Hamiltonian.

In this language, expectation values of an operator $\hat{Q}$ are simply $\left\langle\Psi\middle|\hat{Q}\Psi\right\rangle$.[1] Indeed, observables are represented with **hermitian** operators: operators $\hat{Q}$ that satisfy $\left\langle\psi_1\middle|\hat{Q}\psi_2\right\rangle = \left\langle\hat{Q}\psi_1\middle|\psi_2\right\rangle$, for all ψ_1 and ψ_2. The value of the eigenvalue . We can find, for instance, that the Hamiltonian is Hermitian and since its eigenvalue is the energy, then energy is an observable. We also call the eigenvalues of a Hermitian operator **determinate** states.

We call the eigenbasis (set of eigenvalues) of an operator its **spectrum**. If the spectrum of an operator is *discrete*, then the eigenfunctions are normalizable (and thus are physically realizable states). If the spectrum is *continous*, then they are not normalizable. The best that can happen is instead Dirac orthonormality where $\langle f_p|f_{p'}\rangle = \delta(p-p')$.

One can find a general form of the uncertainty principle between two operators where

$$\sigma_A^2\sigma_B^2 \geq \left(\frac{1}{2i}\left\langle\left[\hat{A},\hat{B}\right]\right\rangle\right)^2 \tag{1}$$

It is clear that operators that commute are mutually observable. Those that do not are called **incompatible** observables (e.g. x and p or E and t).

From this we can find the generalized Ehrenfest theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle Q\rangle = \frac{i}{\hbar}\left\langle\left[\hat{H},\hat{Q}\right]\right\rangle + \left\langle\frac{\partial\hat{Q}}{\partial t}\right\rangle \tag{2}$$

[1] Note that this is sometimes written as $\langle\Psi|\hat{Q}|\Psi\rangle$.

This is particularly useful for finding expectation values just from the operators.

We can change from a basis $\{|e_n\rangle\}$ to a basis $\{|\alpha\rangle, |\beta\rangle, ...\}$ with $|\alpha\rangle = \sum_n \langle e_n|\alpha\rangle |e_n\rangle$, $|\beta\rangle = \sum_n \langle e_n|\beta\rangle |e_n\rangle$, and so on. This can be nicely captured with the **projection operator** $\hat{P} \equiv \sum_n |e_n\rangle \langle e_n|$ (so long as $\{|e_n\rangle\}$ is orthonormal, and turns to an integral if it is a Dirac orthonormal continuous basis).

1.2 Operators as Matrices

The "do-nothing" (identity) operator can be written in terms of the projection operator of a basis $\{|j\rangle\}$ to the same basis. Namely,

$$\hat{I} = \sum_j |k\rangle \langle k|k\rangle = \sum_j |k\rangle \tag{3}$$

This means that we can write any operator $\hat{\Omega}$ as a double sum (in *bilinear form*) as

$$\hat{\Omega} = \hat{I}\hat{\Omega}\hat{I} = \sum_{k,j} |k\rangle \langle k| \hat{\Omega} |j\rangle \langle j| = \sum_{k,j} \Omega_{kj} |k\rangle \langle j| \tag{4}$$

So, operators are very similar to matrix operations. This becomes even more clear if you multiply them with other operators in the above form. In fact, when using a finite basis, it is often useful to represent them with matrices.

Just like with states, we can take the adjoint of an operator (though often we use the dagger symbol instead of the star). That is,

$$\left(\hat{\Omega} |v\rangle\right)^* = \langle v| \hat{\Omega}^\dagger \qquad \left(\langle v| \hat{\Omega}\right)^* = \hat{\Omega}^\dagger |v\rangle \tag{5}$$

Again, this is the same as your usual understanding of the adjoint of a matrix. Similarly, you can also have the inverse of an operator Ω^{-1} where

$$\hat{\Omega} |v\rangle = |w\rangle \iff |v\rangle = \hat{\Omega}^{-1} |w\rangle \tag{6}$$

assuming the inverse exists in the first place. Recall that the commutator of operators A and B is defined as

$$[A, B] = AB - BA \tag{7}$$

And the anti-commutator is

$$\{A, B\} = AB + BA \tag{8}$$

We can also have a *hermitian* operator, just like with matrices. These have the property that $\hat{\Omega}^\dagger = \hat{\Omega}$. You can check that this is consistent with our definition from earlier. Anti-hermitian operators are those that satisfy $\hat{\Omega}^\dagger = -\hat{\Omega}$. You can almost treat hermitian operators as "real" operators, both in the literal sense of being some analog to real numbers in matrix form (real numbers satisfy $x = x^*$) and in that they are guaranteed to have real eigenvalues, which means that they correspond to actually physically measurable quantities. Similarly, anti-hermitian operators are the analogs of purely imaginary numbers.

Now, we can look back at the time-independent Schrödinger equation $\hat{H} |\psi\rangle \equiv \left(\frac{\hat{p}^2}{2m} + V\right) |\psi\rangle = E |\psi\rangle$ and realize that if we want to ensure that we always have real energy eigenvalues E, we will want $\hat{H}$ to be hermitian. This implies that we want V to be real, which is, indeed, always the case.

We can also have unitary operators, which satisfy $\hat{U}^\dagger = \hat{U}^{-1}$. Just like how hermitian operators are the matrix analog of real numbers (or magnitudes), unitary operators are the matrix analog of phase ($e^{i\theta}$ for real θ, which are purely a rotation in the complex plane). These are used to transform the states somehow, such as in time or space. For example, the time translation operator is unitary and equal to $e^{i\hat{H}t\hbar}$. This is because $|\psi(t)\rangle = e^{-i\hat{H}t\hbar} |\psi(0)\rangle$ solves the time-dependent Schrödinger equation (a good exercise to do).

When changing between orthonormal bases $\{|e_n\rangle\}$ and $\{|\alpha\rangle, |\beta\rangle, ...\}$, we simply need to use projection operators as we have seen before. For example, $|v\rangle = \hat{P}|v\rangle = \sum_n \langle e_n|\alpha\rangle |e_n\rangle$. Note that $\langle e_n|\alpha\rangle$ are just numbers (they are in fact the projection of one basis onto the other). But changing between non-orthonormal bases is more complex. It requires you to first convert your non-orthonormal bases to ones that are using Gram–Schmidt orthogonalization. See the lecture notes for an explanation, but generally you have to follow the process

$$|j'\rangle = |v_j\rangle - \sum_{k=1}^{j-1} \frac{|k'\rangle \langle k'|v_k\rangle}{\langle k'|k'\rangle} \tag{9}$$

where $\{|e_n\rangle\}$ is your non-orthogonal basis and $\{|j'\rangle\}$ is your resulting orthogonal basis. Then, just make sure they are also normalized with the transformation $|j'\rangle \to |j\rangle$ via

$$|j\rangle = \frac{|j\rangle}{\sqrt{\langle j'|j'\rangle}} \tag{10}$$

You likely know diagonalization from linear algebra. It turns out that hermitian, anti-hermitian unitary and anti-unitary matrices are diagonalizable since they commute with their adjoints. You should remember how to do diagonalization on matrices from linear algebra classes. It's the same idea here.

2 Recitation Problems

2.1 Custom problem

The time translation operator is defined as

$$\hat{U}(t) = \exp\left(-\frac{it}{\hbar}\hat{H}\right) \tag{11}$$

(a) Show that $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$ satisfies the time-dependent Schrödinger equation. *Hint:* Use a Taylor series expansion of the exponential if you are not familiar with using operators in the exponent. Assume that the Hamiltonian does not depend on time.

Solution: Time-dependent Schrödinger equation is

$$\hat{H}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle$$

but $i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\left(e^{-it\hat{H}/\hbar}\right)|\psi(0)\rangle = i\hbar\frac{\partial}{\partial t}\left(-\frac{i}{\hbar}\hat{H}e^{-it\hat{H}/\hbar}\right)|\psi(0)\rangle = \hat{H}\left(e^{-it\hat{H}/\hbar}\right)|\psi(0)\rangle = \hat{H}|\psi(t)\rangle$. QED.

(b) Show that the time translation operator is unitary. *Hint:* Remember that $\hat{H}$ is hermitian (that is $\hat{H}^\dagger = \hat{H}$). You can use the small $\hat{H}$ approximation and Taylor expand to first-order if you prefer.

Solution: We have

$$\begin{aligned}
\hat{U}(t)^\dagger &= \left(e^{-it\hat{H}/\hbar}\right)^\dagger \\
&= \left[\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{i}{\hbar}\hat{H}t\right)^n\right]^\dagger \\
&= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i}{\hbar}\hat{H}^\dagger t\right)^n
\end{aligned}$$

$$= e^{it\hat{H}^\dagger/\hbar}$$
$$= e^{it\hat{H}/\hbar}$$

But also the inverse of U is

$$\hat{U}(t)^{-1} = \left(e^{-it\hat{H}/\hbar}\right)^{-1} = e^{it\hat{H}/\hbar}$$

Thus, $\hat{U}(t)^\dagger = \hat{U}(t)^{-1}$ so the time translation operator is indeed unitary.

(c) So far, we have been using the so-called "Schrödinger picture," where the states (wave functions) evolve with time, but operators are generally time-independent (with the recent exception of this time-translation operator). In the "Heisenberg picture," operators are generally time-dependent and states are not. We write operators in such a picture as $\hat{Q}_H(t) \equiv \hat{U}(t)^\dagger \hat{Q} \hat{U}(t)$. Show that both pictures are completely consistent with each other by differentiating this equation to get the Heisenburg equations of motion

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \hat{Q}_H(t) = \left[\hat{Q}_H(t), \hat{H}\right] \tag{12}$$

and then plugging in the time translation operator above to get the usual time-dependent Schrödinger equation.

2.2 Sakurai 1.6 and 1.8 (modified)

Using the rules of bra-ket algebra, prove or evaluate the following.

(a) $\mathrm{tr}(\hat{X}\hat{Y}) = \mathrm{tr}(\hat{Y}\hat{X})$, where $\hat{X}$ and $\hat{Y}$ are general operators. *Hint:* Expand in an orthonormal basis and use the trace definition $tr(\hat{X}) \equiv \sum_n \langle n| \hat{X} |n\rangle$.

(b) $\left(\hat{X}\hat{Y}\right)^\dagger = \hat{Y}^\dagger \hat{X}^\dagger$, where $\hat{X}$ and $\hat{Y}$ are general operators.

(c) Suppose $|i\rangle$ and $|j\rangle$ are eigenvectors of some Hermitian operator $\hat{A}$. Under what conditions can we conclude that $|i\rangle + |j\rangle$ is also an eigenvalue of $\hat{A}$? Justify.