

Quantum Physics 1

Class 17/18 Notes

Principles of Quantum Mechanics

Operators and Observables

Chapter 5 in Townsend addresses part of the intellectual core of quantum mechanics (as opposed to quantum physics).

You will address the material in chapter 5 with greater care in Intro to Quantum Mechanics.

Measurement

- A system may be in a superposition of multiple eigenstates of a particular observable.
- When we perform a measurement of an observable, we will only observe one of these eigenvalues.
 - The probability that we observe that one is proportional to the square of the coefficient for that state.
- After we have performed the measurement, the system is now in the eigenstate corresponding to that measured value.
- We say that the superposed quantum state “collapsed” into the eigenstate when we made the measurement.

Operators

- In Quantum Mechanics every observable is represented by an operator that is used to obtain physical information about the system from state functions.

For an observable that in classical physics is represented by $Q(x, p)$, the operator is $\hat{Q}(\hat{x}, \hat{p})$.

Operators

- Operators must act on a function
- Operators act on every function to their right unless their action is constrained by brackets
- The product of operators implies successive operation (starting with the rightmost).
- The sequence of operations does not necessarily commute.
- addition or subtraction of operators means to distribute the operations

Linearity and Superposition

If there exist two distinct state functions of a system with Hamiltonian H , then for arbitrary constants c_1 and c_2 the linear combination $c_1\psi_1 + c_2\psi_2$ also satisfies the TDSE:

$$\begin{aligned} &(\hat{H} - \hat{E})(c_1\psi_1 + c_2\psi_2) \\ &= (c_1(\hat{H} - \hat{E})\psi_1 + c_2(\hat{H} - \hat{E})\psi_2) = 0 \end{aligned}$$

An arbitrary linear combination represents a quantum state of the system.

This property of an operator is known as linearity.

Operators and Eigenvalues

In quantum physics, the form of the eigenvalue equation for an observable \hat{A} with eigenstate ψ_a and eigenvalue a is:

$$\hat{A}\psi_a = a\psi_a.$$

The collection of all eigenvalues is called the spectrum of this operator.

The most familiar eigenstate is the stationary state.

$$\Psi_E = \psi_E e^{-iEt/\hbar} \text{ which satisfies: } \hat{H}\Psi = E\Psi$$

In an eigenstate of an observable, the uncertainty in that observable is zero.

The eigenstate of one observable might not be an eigenstate of another observable (but it can happen).

Example–

An energy eigenstate of the square well is:

$$\Psi(x, t) = A \cos\left(\frac{\pi x}{L}\right) e^{-i\omega_1 t} \quad \text{with} \quad \omega_1 = \frac{E_1}{\hbar} = \frac{\hbar \pi^2}{2mL^2}.$$

Is this an energy eigenstate of momentum $\left(\hat{p} = -i\hbar \frac{\partial}{\partial x}\right)$?

$$\begin{aligned} \hat{p}\Psi &= -i\hbar \frac{\partial}{\partial x} A \cos\left(\frac{\pi x}{L}\right) e^{-i\omega_1 t} = i\hbar A \frac{\pi}{L} \sin\left(\frac{\pi x}{L}\right) e^{-i\omega_1 t} \\ &\neq p\Psi \quad \text{NO!} \end{aligned}$$

Eigenstates of different operators

- Another example:

An energy eigenstate of the free wave is:

$\Psi = Ae^{i(kx-\omega t)}$. Is this an eigenstate of momentum?

$$\hat{p}\Psi = -i\hbar \frac{\partial}{\partial x} Ae^{i(kx-\omega t)} = \hbar k\Psi = p\Psi \quad \text{YES}$$

Hermitian Operators/Hermiticity

\hat{Q} is Hermitian if for any two physically admissible state functions:

$$\int \Psi_1^* \hat{Q} \Psi_2 dx = \int (\hat{Q}^* \Psi_1^*) \Psi_2 dx$$

If an operator is Hermitian, the expectation value of that operator will be real.

All operators for physically measurable quantities are Hermitian.

Plausibility for Hermiticity

- If a quantity is physically observable it must be real, and it's expectation value will be real as well. Thus

$$\langle A \rangle = \langle A \rangle^*$$

- In integral form:

$$\begin{aligned} \int \Psi^* [\hat{A}\Psi] dx &= \left(\int \Psi^* [\hat{A}\Psi] dx \right)^* = \int \Psi [\hat{A}\Psi]^* dx \\ &= \int [\hat{A}\Psi]^* \Psi dx \end{aligned}$$

Hermiticity: Meaning and utility

- All operators representing measurable quantities in quantum mechanics are Hermitian.
 - Expectation values of a Hermitian operator are real.
- Any real function of a Hermitian operator is also Hermitian.
- The product of two Hermitian operators is Hermitian iff the two operators commute.
- A linear combination of two Hermitian operators is Hermitian iff the constants in the linear combinations are real.

Is \hat{p} Hermitian?

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}; \quad \hat{p}^* = i\hbar \frac{\partial}{\partial x}$$

$$\text{Is } \int_{-\infty}^{\infty} \Psi_1^* \left[-i\hbar \frac{\partial}{\partial x} \Psi_2 \right] dx = \int_{-\infty}^{\infty} \left[-i\hbar \frac{\partial}{\partial x} \Psi_1 \right]^* \Psi_2 dx?$$

Start by integrating $\int_{-\infty}^{\infty} \Psi_1^* \left[-i\hbar \frac{\partial}{\partial x} \Psi_2 \right] dx$ by parts.

$$\begin{aligned} \int_{-\infty}^{\infty} \Psi_1^* \left[-i\hbar \frac{\partial}{\partial x} \Psi_2 \right] dx &= -i\hbar \left\{ \Psi_1^* \Psi_2 \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \Psi_2 \left[\frac{\partial}{\partial x} \Psi_1^* \right] dx \right\} \\ &= i\hbar \int_{-\infty}^{\infty} \Psi_2 \left[\frac{\partial}{\partial x} \Psi_1^* \right] dx = \int_{-\infty}^{\infty} \Psi_2 \left[-i\hbar \frac{\partial}{\partial x} \Psi_1 \right]^* dx \end{aligned}$$

Therefore \hat{p} is Hermitian.

Is $\frac{\partial}{\partial x}$ Hermitian?

$$\text{Is } \int_{-\infty}^{\infty} \Psi_1^* \left[\frac{\partial}{\partial x} \Psi_2 \right] dx = \int_{-\infty}^{\infty} \left[\frac{\partial}{\partial x} \Psi_1 \right]^* \Psi_2 dx?$$

- You do the math.

Hermiticity: Real eigenvalues and orthonormal eigenfunctions

- The eigenvalues of a Hermitian operator are real.
- The eigenvalues of a Hermitian operator are the only values that we can observe in a measurement of that observable.

AND

The eigenfunctions of a Hermitian operator are orthogonal, constitute a complete set, and satisfy closure.

Proof of orthogonality of the eigenfunctions of a Hermitian operator

We want to demonstrate that $\int \psi_{q'}^* \psi_q dx = 0$ for two

eigenfunctions of the same observable ($q \neq q'$):

1) $\hat{Q}\psi_q = q\psi_q$ and 2) $\hat{Q}\psi_{q'} = q'\psi_{q'}$

Multiply both sides of 1) by $\psi_{q'}^*$ and integrate:

$$A) \psi_{q'}^* \times 1): \quad \int \psi_{q'}^* \hat{Q}\psi_q dx = q \int \psi_{q'}^* \psi_q dx \quad \text{because } q \text{ is real.}$$

But if \hat{Q} is Hermitian we also have:

$$B) \int \psi_{q'}^* \hat{Q}\psi_q dx = \int (\hat{Q}^* \psi_{q'}^*) \psi_q dx = q' \int \psi_{q'}^* \psi_q dx$$

subtracting A from B we have: $(q' - q) \int \psi_{q'}^* \psi_q dx = 0$,

but we assumed $q \neq q'$ so $\int \psi_{q'}^* \psi_q dx = 0$

The two eigenfunctions are orthogonal.

Hermiticity: Completeness

Completeness of a set of eigenfunctions means that any well-behaved function of the variables on which the eigenfunctions depend can be expanded upon the set.

$$1) \quad f = \sum_q c_q \psi_q$$

We can choose to represent any function in a given range of variables by an expansion in a set of eigenfunctions of any operator.

It's easy to find the coefficients c_q . Multiply both sides of 1) by

$\psi_{q'}^*$,

and integrate

$$\int \psi_{q'}^* f dx = \int \psi_{q'}^* \sum c_q \psi_q dx = \sum c_q \int \psi_{q'}^* \psi_q dx = c_{q'}$$

The coefficient c_q is the "projection" of f onto the eigenfunction ψ_q

A New Operator

The Parity Operator: $\hat{\Pi}$

What are its properties?

Definition

$$\hat{\Pi}f(\vec{r}) = f(-\vec{r})$$

$$\hat{\Pi}f(x, y, z) = f(-x, -y, -z)$$

$\hat{\Pi}$ is linear

$$\begin{aligned} & \hat{\Pi}[c_1f_1(x) + c_2f_2(x)] \\ &= c_1f_1(-x) + c_2f_2(-x) \\ &= [c_1\hat{\Pi}f_1(x) + c_2\hat{\Pi}f_2(x)] \end{aligned}$$

$\hat{\Pi}$ is Hermitian

$$\int \psi_1^*(x) [\hat{\Pi}\psi_2(x)]dx = \int [\hat{\Pi}\psi_1(x)]^* [\psi_2(x)]dx?$$

Working on the LHS:

$$\int \psi_1^*(x) [\hat{\Pi}\psi_2(x)]dx = \int \psi_1^*(x) [\psi_2(-x)]dx$$

change the dummy variable of integration

$$\begin{aligned} \int_{-\infty}^{\infty} \psi_1^*(x) \psi_2(-x)dx &= \int_{\infty}^{-\infty} \psi_1^*(-x) \psi_2(x)d(-x) \\ &= - \int_{\infty}^{-\infty} [\hat{\Pi}\psi_1(x)]^* \psi_2(x)dx = \int_{-\infty}^{\infty} [\hat{\Pi}\psi_1(x)]^* \psi_2(x)dx \end{aligned}$$

And since it is Hermitian it's eigenfunctions must form a complete, orthogonal set. – Let's check.

Eigenfunctions and eigenvalues of the Parity operator

Let's try to find λ 's that solve: $\hat{\Pi}\psi_\lambda(x) = \lambda\psi_\lambda(x)$

$$\psi_\lambda(-x) = \lambda\psi_\lambda(x)$$

Now operate $\hat{\Pi}$ on both sides

$$\hat{\Pi}\psi_\lambda(-x) = \hat{\Pi}\lambda\psi_\lambda(x) \Rightarrow$$

$$\psi_\lambda(x) = \lambda\hat{\Pi}\psi_\lambda(x) = \lambda^2\psi_\lambda(x)$$

from which we deduce $\lambda = \pm 1$

Therefore any function that is an eigenfunction of the parity operator is either even or odd.

Orthogonality of eigenfunctions of the Parity operator

$$\int \phi_{\lambda=-1}^* \psi_{\lambda=1} dx = 0 ?$$

- The product of an even and an odd function is an odd function.
- The integral of an odd function over all space is zero.
- Therefore the overlap of an even and an odd function ϕ_{-1}, ψ_1 is zero.
- Therefore eigenfunctions of different eigenvalues are orthogonal.

Completeness of the Parity Operator

Define the function $\Psi_+(x) = \frac{1}{2} [\psi(x) + \psi(-x)]$.

We can show that $\Psi_+(x)$ is even:

$$\begin{aligned}\hat{\Pi}\Psi_+(x) &= \frac{1}{2} [\hat{\Pi}\psi(x) + \hat{\Pi}\psi(-x)] \\ &= \frac{1}{2} [\psi(-x) + \psi(x)] = \Psi_+(x)\end{aligned}$$

Similarly $\Psi_-(x) = \frac{1}{2} [\psi(x) - \psi(-x)]$ is odd.

So $\Psi_+(x) + \Psi_-(x) = \psi(x)$ shows that any state function can be written as a superposition of an even and an odd function.

Dirac bracket notation

It can be tiresome to write the same integrals repeatedly. Dirac notation saves some ink, and provides conceptual flexibility.

Dirac Notation – "bra"= $\langle \quad |$ "ket"= $|\quad \rangle$

$$\langle Q \rangle = \langle \Psi_1 | \hat{Q} \Psi_1 \rangle = \int_{allspace} \Psi_1^* \hat{Q} \Psi_1 dx = \text{expectation value}$$

$$\langle \Psi_1 | \hat{Q} \Psi_2 \rangle = \int_{allspace} \Psi_1^* \hat{Q} \Psi_2 dx = \text{matrix element}$$

$$\langle \Psi_1 | \Psi_1 \rangle = \int_{allspace} \Psi_1^* \Psi_2 dx = \text{overlap integral}$$

- 1) Take the complex conjugate of the function inside the $\langle \quad |$
- 2) Act with the operator on the function to its right.
- 3) Integrate the integrand over all space.

Useful properties of Dirac notation

$$\langle \psi_1 | c \psi_2 \rangle = c \langle \psi_1 | \psi_2 \rangle$$

where c is a constant

$$\langle c \psi_1 | \psi_2 \rangle = c^* \langle \psi_1 | \psi_2 \rangle$$

$$\langle \psi_1 | \psi_2 \rangle^* = \langle \psi_2 | \psi_1 \rangle$$

$$\langle \psi_1 + \psi_2 | \psi_3 + \psi_4 \rangle$$

$$= \langle \psi_1 | \psi_3 \rangle + \langle \psi_1 | \psi_4 \rangle + \langle \psi_2 | \psi_3 \rangle + \langle \psi_2 | \psi_4 \rangle$$

Eigenvalue Expansions

- This will be a somewhat more formal discussion of composing a wavefunction out of eigenfunctions.
- Note that the wavefunction we wish to represent must obey the same boundary conditions as the eigenfunctions.
- Wavefunctions are normalizable solutions to the wave equation that obey the same boundary conditions as the eigenfunctions.
- Eigenfunctions must additionally obey the relation: $\hat{H}\psi_q = q\psi_q$.

Summarizing Eigenfunction Expansions

TABLE 10.9 PROPERTIES OF THE EIGENFUNCTIONS AND EIGENVALUES OF A HERMITIAN OPERATOR Q .

	Discrete Spectrum	Continuous Spectrum
eigenvalues	q_n real	q real
orthonormality	$\langle \chi_{q'} \chi_q \rangle = \delta_{q',q}$	$\langle \chi_{q'} \chi_q \rangle = \delta(q' - q)$
completeness	$\Psi = \sum_{\text{all } q} c_q \chi_q$	$\Psi = \int_{\text{all } q} c_q \chi_q dq$
projection of Ψ	$c_q = \langle \chi_q \Psi \rangle$	$c_q = \langle \chi_q \Psi \rangle$
closure	$\sum_{\text{all } q} \chi_q(x') \chi_q(x) = \delta(x' - x)$	$\int_{\text{all } q} \chi_q(x') \chi_q(x) dq = \delta(x' - x)$

The meaning and use of expansions

- The collection of coefficients in the expansion of a state function in any complete set is merely an alternate way to represent the state function.
- These coefficients and the eigenfunctions contain the same information as the state function.
- Expressing a state function in terms of eigenfunctions can make apparent some properties of the state function.
- Expressing the state function in terms of eigenfunctions can allow us to get information about other variables. (Expressing the wavefunction (position variable) in terms of momentum eigenfunctions allows us to determine the momentum properties of the state function.)

Using expansions to calculate expectation values

- If we have a wavefunction that is not an eigenfunction of a given operator, the expectation value may be hard to calculate in the old way.
- Expanding the wavefunction in terms of the eigenfunctions of that operator may make things easier.

Example: Calculation of the mean

$$\begin{aligned}\langle Q \rangle(t) &= \int \Psi^* \hat{Q} \Psi dx \\&= \int \left[\sum c_{n'}(t) \psi_{n'}(x) \right]^* \left[\hat{Q} \sum c_n(t) \psi_n(x) \right] dx \\&= \int \left[\sum c_{n'}(t) \psi_{n'}(x) \right]^* \left[\sum c_n(t) q_n \psi_n(x) \right] dx \\&= \sum_{n'} \sum_n c_{n'}^* c_n \langle \psi_{n'} | \psi_n \rangle = \sum_n |c_n|^2 q_n\end{aligned}$$

If we know the projection coefficients,
we know the expectation value (and we know the
probability that we will observe a specific outcome.

Example: Expectation value of energy

Calculate the expectation value of the energy for the following non-stationary state of the SHO.

$$\Psi(x, t) = \frac{1}{\sqrt{50}} [\psi_1 e^{-i\omega_1 t} + 7\psi_2 e^{-i\omega_2 t}]$$

$$c_1(t) = \frac{1}{\sqrt{50}} e^{-i\omega_1 t}; \quad c_2(t) = \frac{7}{\sqrt{50}} e^{-i\omega_2 t} \text{ (all others=0)}$$

$$\langle E \rangle(t) = \sum_{n=0}^{\infty} |c_n|^2 E_n = \frac{1}{50} \frac{3}{2} \hbar \omega_0 + \frac{49}{50} \frac{5}{2} \hbar \omega_0 = \frac{62}{50} \hbar \omega_0$$

Note that any individual measurement of E will yield an eigenenergy.

Physical meaning of expansions

- The collection of expansion coefficients in a state function is merely an alternate way to represent this physical state. They contain the same information as the state function itself.
- The expansion coefficients may be useful.
 - The wave function explicitly shows the dependence of the state function on space and time. If we are interested in another property, such as energy, it may be more informative to represent the state function in terms of energy eigenstates.
 - The coefficients c_q are properly called, the probability amplitudes for the observable Q .
 - Knowledge of the probability of a certain outcome may provide physical insight into the situation.

Commuting Operators

- The commutator is the combination of two operators in which the difference is taken between the operations performed in different order:

$$\text{Commutator} \equiv [A_{op}, B_{op}] = (A_{op}B_{op} - B_{op}A_{op})$$

- Whether two operators commute or not can tell us a lot about the nature of the eigenfunctions of the operators without even solving the Schrodinger equation.

Information from the Commutator

- A complete set of simultaneous eigenfunctions of two Hermitian operators exists iff the operators commute.
- If two operators do not commute and their commutator can be expressed as $[A_{op}, B_{op}] = iC_{op}$ where C_{op} is a Hermitian operator, then an uncertainty relation of the form $\Delta A \Delta B \geq \left| \frac{\langle C \rangle}{2} \right|$ must hold.

Example of Commuting Operators

- Parity Operator: Π
- Hamiltonian for a symmetric potential:

$$- H_{SYM} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \text{ where } V(x) = V(-x)$$

$$\begin{aligned} [H_{SYM}, \Pi] &= \\ & \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Pi \Psi(x) - \Pi \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(x) \\ &= \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(-x) - \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial (-x)^2} + V(-x) \right) \Psi(-x) \\ &= \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \Psi(-x) - \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial (x)^2} + V(x) \right) \Psi(-x) = 0 \end{aligned}$$

When two Hermitian operators commute,
they share a complete set of
eigenfunctions.

- We can then measure both of these quantities simultaneously without uncertainty.
- Argument

Given $[A_{op}, B_{op}] = 0$

Apply B_{op} to the equation $A_{op}\psi_a = a\psi_a$.

$$B_{op}A_{op}\psi_a = aB_{op}\psi_a$$

And because they commute:

$$A_{op}(B_{op}\psi_a) = a(B_{op}\psi_a)$$

This tells us that $(B_{op}\psi_a)$ is an eigenfunction of A_{op}

Uncertainty

- The uncertainty of an arbitrary observable is given by: $\Delta A = \sqrt{\langle (A - \langle A \rangle)^2 \rangle} = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$
- If many measurements are analyzed, then ΔA is the standard deviation of the measurements.
- The variance is defined as $(\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2$
- If we define $U_{op} = A_{op} - \langle A \rangle$, then

$$\int \psi^* U_{op}^2 \psi dx = (\Delta A)^2$$

Uncertainty Relations

- If two Hermitian operators do not commute, their commutator can be expressed as $[A_{op}, B_{op}] = iC_{op}$ where C_{op} is Hermitian so $\int \psi^* C_{op} \psi = \langle C \rangle$.
- It can be shown that $\Delta A \Delta B \geq \frac{|\langle C \rangle|}{2}$.

Momentum-Position Example

- $p_{op} = -i\hbar \frac{\partial}{\partial x}$ and $x_{op} = x$
- $[p_{op}, x]\psi = -i\hbar \frac{\partial}{\partial x} x\psi - x \left(-i\hbar \frac{\partial}{\partial x} \psi \right)$
 $= -i\hbar \left(\frac{\partial}{\partial x} (x\psi) - x \frac{\partial}{\partial x} \psi \right)$
 $= -i\hbar \left\{ \left(\psi + x \frac{\partial \psi}{\partial x} \right) - x \frac{\partial \psi}{\partial x} \right\} = -i\hbar \psi$
- And applying the uncertainty relation from the previous page:
$$\Delta p \Delta x \geq \frac{\hbar}{2} .$$

Commutators of x and p

TABLE 11.3 COMMUTATOR RELATIONS INVOLVING THE POSITION AND MOMENTUM OPERATORS

$$[\hat{x}^2, \hat{p}] = 2i\hbar\hat{x} \quad (\text{I})$$

$$[\hat{x}, \hat{p}^2] = 2i\hbar\hat{p} \quad (\text{II})$$

$$[\hat{x}^2, \hat{p}^2] = 2i\hbar(2\hat{x}\hat{p} - i\hbar\hat{1}) \quad (\text{III})$$

for arbitrary operator functions $\hat{f}(\hat{p})$ and $\hat{g}(\hat{x})$:

$$[\hat{x}, \hat{f}(\hat{p})] = i\hbar \frac{d}{d\hat{p}} \hat{f}(\hat{p}) \quad (\text{IV})$$

$$[\hat{p}, \hat{g}(\hat{x})] = -i\hbar \frac{d}{d\hat{x}} \hat{g}(\hat{x}) \quad (\text{V})$$

for a Hamiltonian $\hat{\mathcal{H}} = \hat{T} + \hat{V}(x)$:

$$[\hat{\mathcal{H}}, \hat{x}] = -\frac{i\hbar}{m}\hat{p} \quad (\text{VI})$$

$$[\hat{\mathcal{H}}, \hat{p}] = i\hbar \frac{\partial V}{\partial x} \hat{1} \quad (\text{VII})$$

- A compendium of what certain symbols represent.
 - https://imgs.xkcd.com/comics/greek_letters.png