

Ph 1b Recitation Notes

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Week 1
January 14, 2026
(updated 01/21)

1 Intro to Non-Relativistic Quantum Mechanics

1.1 The 1D Schrödinger Equation

Everything in non-relativistic quantum mechanics (QM) revolves around the Schrödinger equation. In 1 spatial dimension, it is

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V(x)\Psi(x, t) \quad (1)$$

where $\hbar \equiv \frac{h}{2\pi} = 1.054573 \times 10^{-34}$ J s is the reduced Planck's constant.

The basic concept revolves around treating particles as “probability waves”. The probability of a given particle being at location x at time t is determined from a complex function called the *wavefunction* $\Psi(x, t)$. This wavefunction (and thus particle probability) evolves in space and time according to equation 1.1. It's not until you “observe” the particle that it “picks” a location at random, weighted by it's probability distribution. This is called the “Copenhagen” interpretation of QM. For the majority of your time in this course, the act of observing will remain vague, and it is often one of the hardest parts to wrap your head around when first learning QM. There are other “interpretations” of QM, such as many-worlds, but historically, the Copenhagen is the one people usually first learn.

1.2 Properties of the Wavefunction

The probability of finding the particle at time t between locations $x = a$ and $x = b$ is

$$P(a \leq x \leq b, t) = \int_a^b |\Psi(x, t)|^2 dx \quad (2)$$

Note that $\Psi(x, t)$ is complex (can have both real and imaginary parts), and $|\Psi(x, t)|^2 \equiv \Psi^* \Psi$ is real¹. Of course, it must be real because it's a probability.

Since the total probability must be one, the wave function is normalized

$$1 = \int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx \equiv \langle \Psi | \Psi \rangle \quad (3)$$

The second part is just some fancy notation (“bra-ket notation”) that makes this whole thing easier later on in the course, but I show it here so you can get used to it. If you are familiar with linear algebra, it just

¹Note that I use the upper index star symbol to denote the complex conjugate. If you are fussy with complex numbers, please review them (or ask me to summarize). They will be quite important to this course.

denotes an inner product on a Hilbert space (don't worry, we'll get there).

Okay, so we can set the probability to be normalized at some time t . But how do we know that it *stays* normalized? In some sense we require the probability to be conserved. To do this, we need to show that $\frac{\partial \langle \Psi | \Psi \rangle}{\partial t} = 0$. See the lecture notes for a derivation.

1.3 Using the Wavefunction

We now know that $|\Psi(x, t)|^2$ is a probability density of the particle. This means that if we want to compute the expected value of some quantity $Q(x)$, then it is

$$\langle Q \rangle = \int_{-\infty}^{\infty} |\Psi(x, t)|^2 Q(x) dx \quad (4)$$

In some sense, this is the "average" of Q . So, for example you could find the average expected position with $\langle x \rangle$ above. You can also get some estimate of the uncertainty or variance in your measurements with

$$\sigma^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \quad (5)$$

1.4 Operators

We can now find the position of the particle, but what about momentum? In classical mechanics, you might recall that the momentum is $p = m \frac{dx}{dt}$. If we want this to be true at large scales, we need this to hold for the expectation values of the quantities². Namely, we need $\langle p \rangle = m \frac{d\langle x \rangle}{dt}$.

If you input equation 1.3 in for $\langle x \rangle$, and then manipulate the integral a bit, you can find that

$$\langle p \rangle = \int_{-\infty}^{\infty} \Psi^* (-i\hbar \frac{\partial}{\partial x}) \Psi dx \quad (6)$$

which suggests the idea that we could define $p = -i\hbar \frac{\partial}{\partial x}$. This is called the momentum "operator." Operators aren't really functions, since they can include derivatives and instead "act" on functions. In this case the momentum operator "acts" on the wavefunction. Often we like to add little "hats" to denote operators and clean the notation up with some bracket notation like $\langle p \rangle = \langle \Psi | \hat{p} | \Psi \rangle$.

Sometimes it is useful to define the "commutator" of two operators \hat{Q}_1 and \hat{Q}_2 as $[\hat{Q}_1, \hat{Q}_2] \equiv \hat{Q}_1 \hat{Q}_2 - \hat{Q}_2 \hat{Q}_1$. Note that this is not identically zero because the order of "action" can affect the outcome. For example, multiplying a function by x and then taking a derivative is different than taking a derivative of a function and then multiplying by x . This is why one can find that the commutator of the position and momentum operators is $[\hat{x}, \hat{p}] = i\hbar$. In general, it is useful to know that $[\hat{Q}_1, \hat{Q}_2] = -[\hat{Q}_2, \hat{Q}_1]$.

1.5 Heisenberg Uncertainty Principle

One can show that the standard deviation of position multiplied by the standard deviation of momentum for any wavefunction is

$$\sigma_x \sigma_p \geq \frac{\hbar}{2} \quad (7)$$

This means that you can never know both the position and momentum of a particle with infinite precision. This is not true of macroscopic objects. Wave packets have a similar property, where you cannot perfectly know both its wavelength/frequency and its position. Since we treat particles as wave packets in QM,

²Generally, this is called Ehrenfest theorem, some versions of which you will prove in the homework

this is fundamentally where the uncertainty principle gets its origin. Indeed, De Broglie³ postulated this relationship between the momentum and wavelength of a particle with the famous

$$p = \frac{h}{\lambda} = h\nu = \hbar\omega \quad (8)$$

In fact, there are actually many uncertainty relations and they arise between any two operators that do not commute. The principle generalizes to

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \langle [\hat{A}, \hat{B}] \rangle \right)^2 \quad (9)$$

You can find that this, for instance, also leads to an energy-time uncertainty principle, where

$$\Delta t \Delta E \geq \frac{\hbar}{2} \quad (10)$$

1.6 Generally Solving the Schrödinger Equation

The Schrödinger equation is a partial differential equation (PDE). The easiest way to solve PDEs is with separation of variables. In this case, we just have two variables x and t , so we can take the ansatz of the wavefunction breaking into the multiplication of two independent functions $\Psi(x, t) = \psi(x)\phi(t)$. This allows us to split equation 1.1 into two independent ordinary differential equations. Namely,

$$i\hbar \frac{d\phi}{dt} = E\phi(t) \implies \phi(t) = \exp(-iEt/\hbar) \quad (11)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x) = E\psi(x) \quad (12)$$

for some constant E . Equation 1.6 is thus the equation that we need to solve to get the 1d wavefunction, given a certain potential function $V(x)$. It is called the “time-independent” Schrödinger Equation, and can generally be used for potential functions that only depend on position. Time-varying potential functions are more annoying, but we will start with the simpler cases. Note that the solutions of the time-independent equation are called *stationary* states, since they do not depend on time, and they have definite energies E_n (see lecture notes for proofs). Non-stationary states do not have definite energy and are thus more annoying to deal with.

Once you have a solution (say, $\psi_n(x)$) to the time-independent equation, you can construct time-dependent solutions with $\Psi_n(x, t) = \psi_n(x)\phi_n(t)$. Note that you generally get a different $\phi_n(t)$ for each $\psi_n(x)$ because you will have a different energy E_n . However, it is not always the case that you will get a unique solution for each energy, but when it is, it’s called a “non-degenerate” solution⁴.

However, that only gets us one particular solution, but we want all solutions, or solutions specific to a given set of initial conditions. So to do this, we can note that our time-independent ODE is linear, meaning that we can construct general solutions from linear combinations of the solutions we get. Namely, a general solution to the time-dependent Schrödinger equation in 1d, with time-dependent solutions $\psi_n(x)$ and corresponding energies E_n , is

$$\Psi(x, t) = \sum_n c_n \psi_n(x) e^{-iE_n t/\hbar} \quad (13)$$

The initial conditions of the wavefunction $\Psi(x, t)$ give us the coefficients c_n . To keep the wavefunction normalized, we require

³Pronounced “de broy.”

⁴“Degenerate” solutions are those where multiple wavefunctions have the same energy level. This will become more clear to you as the course progresses.

$$\sum_n |c_n|^2 = 1 \tag{14}$$

To set the initial conditions (say to $|\Psi(x, t) = \sum_n c_n(t) f_n(x)$), we can simply use the Fourier transform (assuming that the solutions are orthonormal) to get

$$c_n(t) = \langle f_n | \Psi \rangle = \int f_n(x)^* \Psi(x, t) dx \tag{15}$$

Again, this will make more sense when we get to the full mathematical formalism.

2 Recitation Problems

2.1 Griffiths Problem 1.11

2.2 Griffiths Problem 1.12

2.3 Griffiths Problem 1.15

2.4 Griffiths Problem 1.16