PHY293 Lecture #18

December 5, 2017

1. Linear Superposition of Solutions to the Schrodinger Equation

   - Yesterday saw solutions to the TDSE, that have definite energy and momentum
   - These are specific, or special solutions to the Schrodinger Equation
   - As with waves on a string, any linear combination of these special solutions will also be a solution
   - Suppose Ψ_1 and Ψ_2 are both solutions of the Schrodinger equation for some $U(x)$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_1(x,t)}{\partial x^2}+U(x)\Psi_1(x,t)=i\hbar\frac{\partial\Psi_1(x,t)}{\partial t}\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_1(x,t)}{\partial x^2}+U(x)\Psi_1(x,t)-i\hbar\frac{\partial\Psi_1(x,t)}{\partial t}=0$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_2(x,t)}{\partial x^2}+U(x)\Psi_2(x,t)=i\hbar\frac{\partial\Psi_2(x,t)}{\partial t}\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_2(x,t)}{\partial x^2}+U(x)\Psi_2(x,t)-i\hbar\frac{\partial\Psi_2(x,t)}{\partial t}=0$$

   - Show that a linear combination: $c_1\Psi_1+c_2\Psi_2$ is also a solution:

$$-\frac{\hbar^2}{2m}\frac{\partial^2[c_1\Psi_1+c_2\Psi_2]}{\partial x^2}+U(x)[c_1\Psi_1+c_2\Psi_2]-i\hbar\frac{\partial[c_1\Psi_1+c_2\Psi_2]}{\partial t}=0$$

$$c_1\Big[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_1}{\partial x^2}+U(x)\Psi_1-i\hbar\frac{\partial\Psi_1}{\partial t}\Big]+c_2\Big[-\frac{\hbar^2}{2m}\frac{\partial^2\Psi_2}{\partial x^2}+U(x)\Psi_2-i\hbar\frac{\partial\Psi_2}{\partial t}\Big]=0$$

   - But both the terms in $[\quad]$ are separately 0 (since Ψ_1 and Ψ_2 are solutions to the TDSE for this potential).
   - So independent of c_1 or c_2 the entire sum is 0, as required: A linear combination of solutions is also a solution.

2. Non Stationary States

   - Last time saw that any single energy level state was 'stationary'

$$\Psi^*\Psi=\psi^*e^{iEt/\hbar}\psi e^{-iEt/\hbar}=\psi^*\psi$$

   - General solutions to a bound particle made up of linear superpositions of different energy level states
   - Such a linear combination, however, is not a stationary state
   - Consider a set of solutions $\Psi_n(x,t)=\psi_n(x)e^{-iE_nt/\hbar}$ with different n (need not be infinite well states... but could be)
   - Consider a state which is the sum of two such solutions: $\Psi(x,t)=\frac{1}{\sqrt{2}}\big[\psi_n(x)e^{-iE_nt/\hbar}+\psi_m(x)e^{-iE_mt/\hbar}\big]$
   - Convince yourself that each state is individually is a solution to the Schrodinger equation, but the combined state does not have well defined energy (ie. not equally E_m+E_n for all time)
   - It also does not have a probability density that is time independent

$$\frac{1}{2}\big[\psi_n(x)e^{iE_nt/\hbar}+\psi_m(x)e^{iE_mt/\hbar}\big]\big[\psi_n(x)e^{-iE_nt/\hbar}+\psi_m(x)e^{-iE_mt/\hbar}\big]=\frac{1}{2}\big[\psi_n^2(x)+\psi_m^2(x)+\psi_m(x)\psi_n(x)(e^{-i(E_m-E_n)t/\hbar}+e^{i(E_m-$$

   - This last term is just the cos of the argument ($e^{i\theta}+e^{-i\theta}=2\cos\theta$) so finally get:

$$\frac{1}{2}\big[\psi_n^2(x)+\psi_m^2(x)+2\psi_m(x)\psi_n(x)\cos(E_m-E_n)t/\hbar)\big]$$

   - So the probability density becomes a function of time, with a frequency of $|E_m-E_n|/\hbar$
   - See for example `https://phet.colorado.edu/en/simulation/bound-states`

3. Interpreting the Probabilities

   - Interpret $\Psi^*(x,t)\Psi(x,t)$ as the probability density to find the particle at a particular point in space (x) at a particular time (t), if we make a measurement
   - In the sketch: A is most probable location, B is rather unlikely, the shaded region allows us to sum up the probability to find the particle over a range of x – which is all we can actually do

- ◦ Can never measure a particle to be at 'exactly' x, but only between x and $x + dx$ where dx is consistent with the precision of the momentum and the Heisenberg Uncertainty principle
  - ◦ Most widely used interpretation of quantum mechanics: Particle represented by $\Psi(x,t)$ has no specific location prior to measurement
  - ◦ Electron in H-atom doesn't radiate – not travelling around in circles – 'shows up' with the predicted probability when measured
  - ◦ If measured at C, then it becomes a $\delta(x - C)$ distribution
  - ◦ If we measure it a second time 'right afterwards' it will still be at C
  - ◦ After a measurement, previous wavefunction no longer valid – particle's position is disturbed by measurement.
  - ◦ If we measure it some time later, since δ-function wavefunction is not a stationary state, it will 'spread out' again, evolving according to solution of time dependent Schrodinger equation ... this need not be the original shape of $|\Psi|^2$
  - ◦ This is referred to as the statistical or Copenhagen interpretation of QM.
- When we make a sum, like this, must constrain A_n so that total wavefunction is normalised (probability to find particle anywhere = 100%)

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x.t)dx = 1 \qquad [1]$$

4. How does the wavefunction evolve with time?

- Consider an infinite square well that suddenly doubles in size
- If the particle was in the initial (narrow well) ground state, what happens to the wave-function after the well doubles?
- New solution is no longer a stationary state (not of the shape $\sin[n\pi x/(2L)]$)
- Instead must expand this as a combination possible solutions (basis states)

$$\Psi(x,t) = \Sigma_{n=1}^{\infty} A_n \psi(x) e^{-iE_n t/\hbar} \qquad \text{with} \quad \psi_n(x) = \sin[n\pi x/(2L)]$$

- This is not just true for square well, but any bound state will be a sum of eigenstates like this.
- Then the $e^{-iE_n t/\hbar}$ terms determine how each part of the spatial wavefunction evolves.
- What about the normalisation?
- Have already seen that the individual bound states have normalisation $\sqrt{2/L}$
- When we make a sum, like this, must constrain A_n so that total wavefunction is normalised (probability to find particle anywhere = 100%)

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x.t)dx = 1 \qquad [1]$$

5. Measurements (Expectation Values) in Quantum Mechanics

- Brief primer on statistics:
  - ◦ Given a distribution of ages (like the one in the figure)
  - ◦ Could ask a number of questions
    - (a) What is the total number of people (14) (N=14)
    - (b) What is probability to find a 14-year old? (1/14): $P(j) = N(j)/N$ and $\Sigma P(j) = \Sigma N(j)/N = 1$
    - (c) What is the most probable age? 25, largest $P(j)$
    - (d) What is the median age? 23 (7 people are younger than 23 and 7 people are older than 23)
    - (e) What is the average (mean) age? $< \text{age} >= \Sigma \frac{j \cdot N(j)}{N} = \Sigma j \cdot P(j) = 21$
  - ◦ Note that (as in this case) no one has median, or mean age
  - ◦ In quantum mechanics refer to mean as "expectation value"... if you measured system N times this is the average result you'd expect. It is not (necessarily) the most probable outcome of a measurement (here that would be 25).
- Could also ask: What is the average value of the square of all the ages? $< j^2 >= \Sigma \frac{j^2 \cdot N(j)}{N} = \Sigma j^2 \cdot P(j)$
- Or, in general, the average value of any function of these ages $< f(j) >= \Sigma \frac{f(j) \cdot N(j)}{N} = \Sigma f(j) \cdot P(j)$
- Note that average of the squares is not the same as square of averages...
- Consider the two distributions in figure. They have same mean, median, most probable value and number of entries

- Left distribution is sharply peaked and right is very spread out, characterised by the "width" of the distribution
- Consider $\Delta j = j- < j >$, the average of which is zero by definition
- But $\sigma_j^2 =< (\Delta j)^2 >$ is not zero and referred to as the Standard deviation of a distribution (often in lab this will be taken as a one-sigma uncertainty on a measurement)
- Can also be written as: $\sigma_j^2 =< (j- < j >)^2 >=< j^2 > -2 < j >< j > - < j >^2 =< j^2 > - < j >^2$
- Quantum mechanics is "built" to make predictions like these $P(j) \equiv |\Psi|^2$
- Only difference is this is now a continuous distributions (so sums are replaced by integrals)
- We can determine the average position – expectation value of position – or a particle from:

$$< x >= \int_{-\infty}^{\infty} x|\Psi(x,t)|^2 dx$$

- Could also determine the expectation value for x^2:

$$< x^2 >= \int_{-\infty}^{\infty} x^2|\Psi(x,t)|^2 dx$$

- But the standard deviation of x is $\sqrt{< x^2 > - < x >^2}$
- Example 5.5 in text computes $< x >, < x^2 >$ and σ_x for a particle in the ground state of an infinite square well
- Can do the same for momentum. One additional ingredient: The function for "momentum"
  - It turns out the 'function' for momentum is $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ [comes from identifying $p^2/2m$ with $(-\hbar^2/2m)\frac{\partial \Psi}{\partial x}$
  - When the momentum "operator" $\hat{p}_x$ operates on the wavefunction it produces the momentum $\hbar k$
  - You will see more examples of quantum mechanical 'operators' in PHY294 (angular momentum, Energy, etc.)
  - But using just this one for now we can get:

$$< p >= \int_{-\infty}^{\infty} \Psi^*(x,t)\hat{p}\Psi(x,t)dx = -i\hbar \int_{infty}^{\infty} \Psi^*(x,t)\frac{\partial \Psi(x,t)}{\partial x}dx$$

  - And

$$< p^2 >= \int_{-\infty}^{\infty} \Psi^*(x,t)\hat{p}^2\Psi(x,t)dx = -\hbar^2 \int_{-\infty}^{\infty} \Psi^*(x,t)\frac{\partial^2 \Psi(x,t)}{\partial x^2}dx$$

  - This allows them to compute, for the ground state in an infinite square well of width L

$$\Delta x \equiv \sigma_x = 0.18L \qquad \Delta p \equiv \sigma_p = \pi\hbar/L$$

  - Which in turn gives $\Delta x \Delta p = 0.59\hbar > \hbar/2$
  - These definitions, in the case of an infinite square well are consistent with the Heisenberg Uncertainty Principle
  - They are true more generally, and in PHY294 you will see some additional examples.

6. Extra Proof of Normalisation being Time Independent (not discussed in class)

- When we make a sum, like this, must constrain A_n so that total wavefunction is normalised (probability to find particle anywhere = 100%)

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x.t)dx = 1 \qquad [1]$$

- This must remain 100% at all times so require time variation of normalisation condition must vanish

$$\frac{d}{dt}\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x.t)dx = \int_{-\infty}^{\infty} \frac{d}{dt}[\Psi^*(x,t)\Psi(x.t)]dx = 0$$

- Use the product rule to get

$$\int_{-\infty}^{\infty} [\frac{\partial}{\partial t}\Psi^*(x,t)]\Psi(x.t)] + \Psi^*(x,t)[\frac{\partial}{\partial t}\psi(x,t)]dx = 0$$

- But the Schrodinger equation gives us $\frac{\partial}{\partial t}\Psi(x,t) = \frac{i\hbar}{2m}\frac{\partial^2}{\partial x^2}\Psi - i/\hbar U(x)\Psi$ and $\frac{\partial}{\partial t}\Psi^*(x,t) = \frac{-i\hbar}{2m}\frac{\partial^2}{\partial x^2}\Psi^* + i/\hbar U(x)\Psi^*$ [NB: changes of sign for i terms in equation]

- We can substitute this in to the expression above (note that $U(x)$ terms cancel – assuming $U(x)$ is real) to get

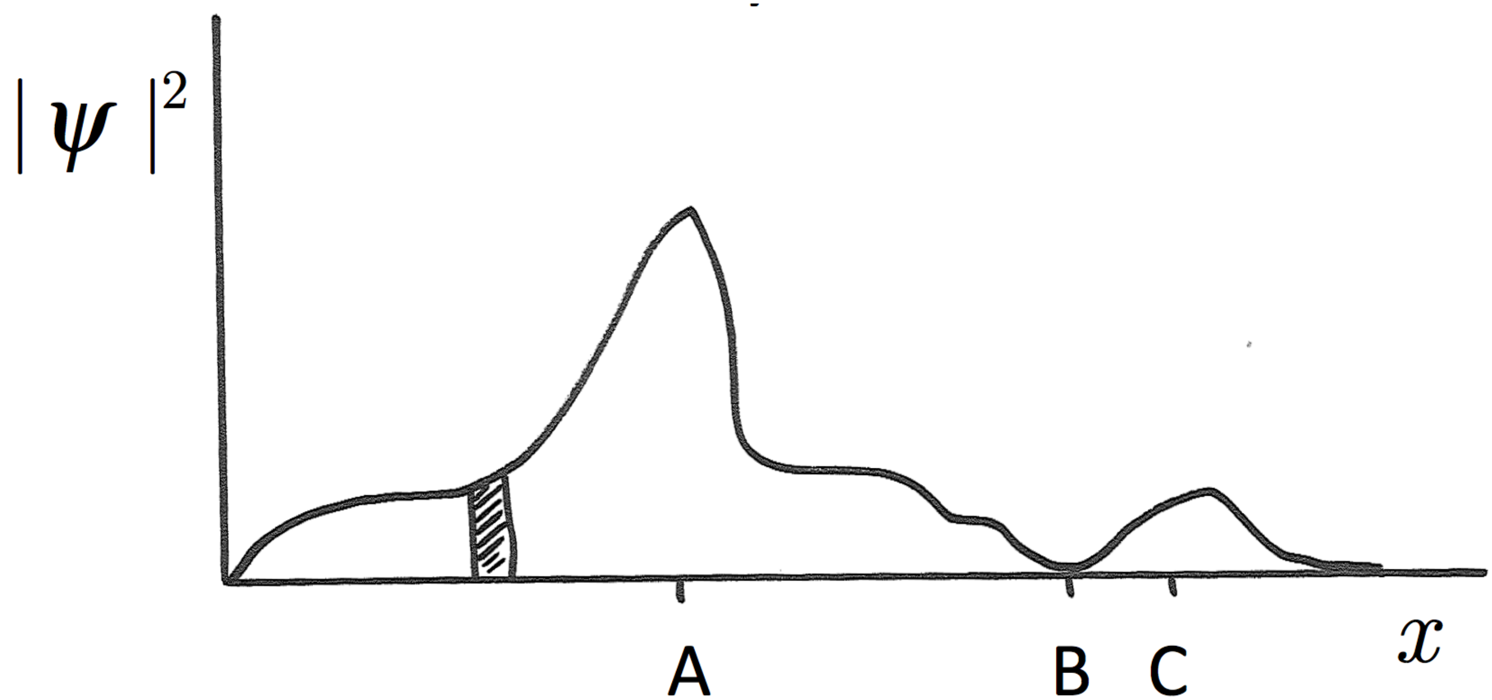
$$\frac{\partial}{\partial t}\Psi^*(x,t)]\Psi(x.t) = \frac{i\hbar}{2m}\big[\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{\partial^2\Psi^*}{\partial x^2}\Psi\big] = \frac{\partial}{\partial x}\big[\frac{i\hbar}{2m}\big(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\big)\big]$$

- But we can plug this back into the spatial (normalisation integral – eqn [1] above) and that just 'wipes out' the spatial derivative:

$$\frac{d}{dt}\int_{-\infty}^{\infty}\Psi^*(x,t)\Psi(x.t)dx = \frac{i\hbar}{2m}\big(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\big)\big|_{-\infty}^{\infty}$$

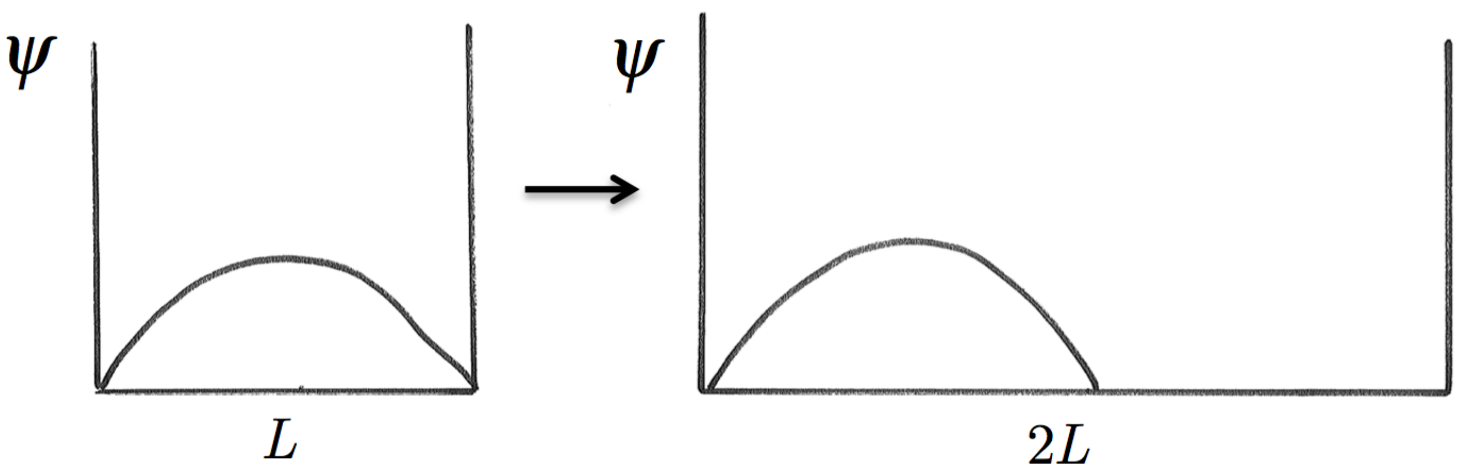
- But if the wave function is going to be normalisable $\Psi(x,t) \to 0$ as $x \to \pm\infty$ so this vanishes
- The normalisation of the wavefunction (because it is a solution to the Schrodinger equation) is preserved for all time – even if the solution is not a stationary (time independent) state.
- Even if full solution is a random combination of states, if normalised initially, it will evolve according to sum of states, and stay normalised

Probability from Wavefunction



Probability after Measurement

Square-well Solution: Doubling Well size



Age Distribution

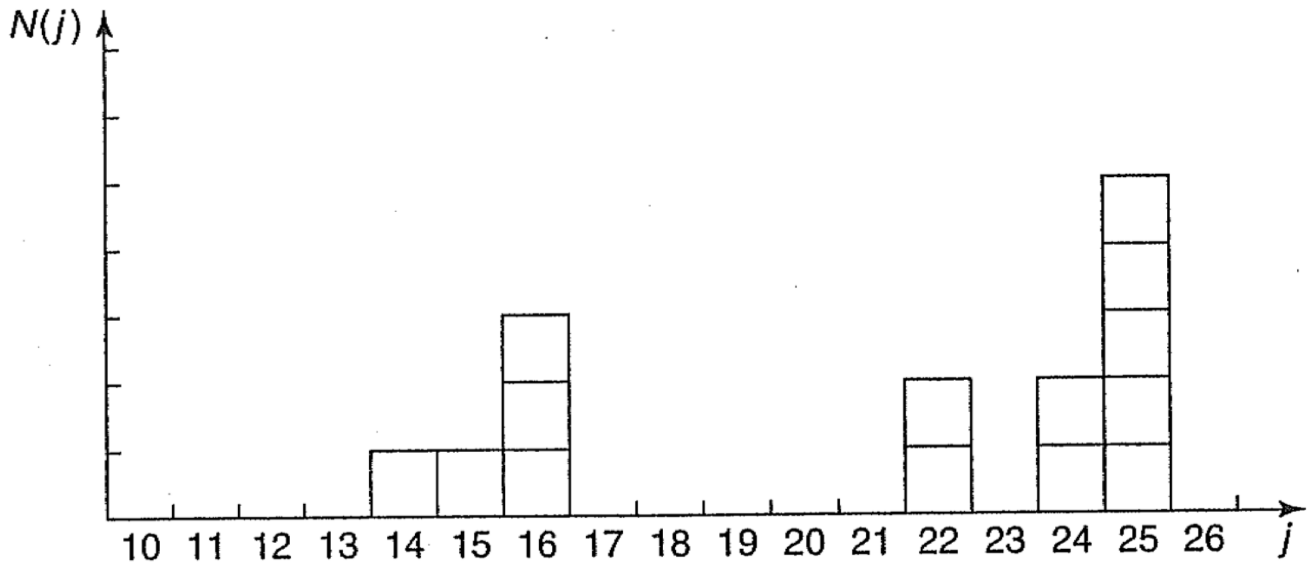


FIGURE 1.4: Histogram showing the number of people, $N(j)$, with age j, for the distribution in Section 1.3.1. [Griffiths: Introduction to Quantum Mechanics]

Peaked Distribution

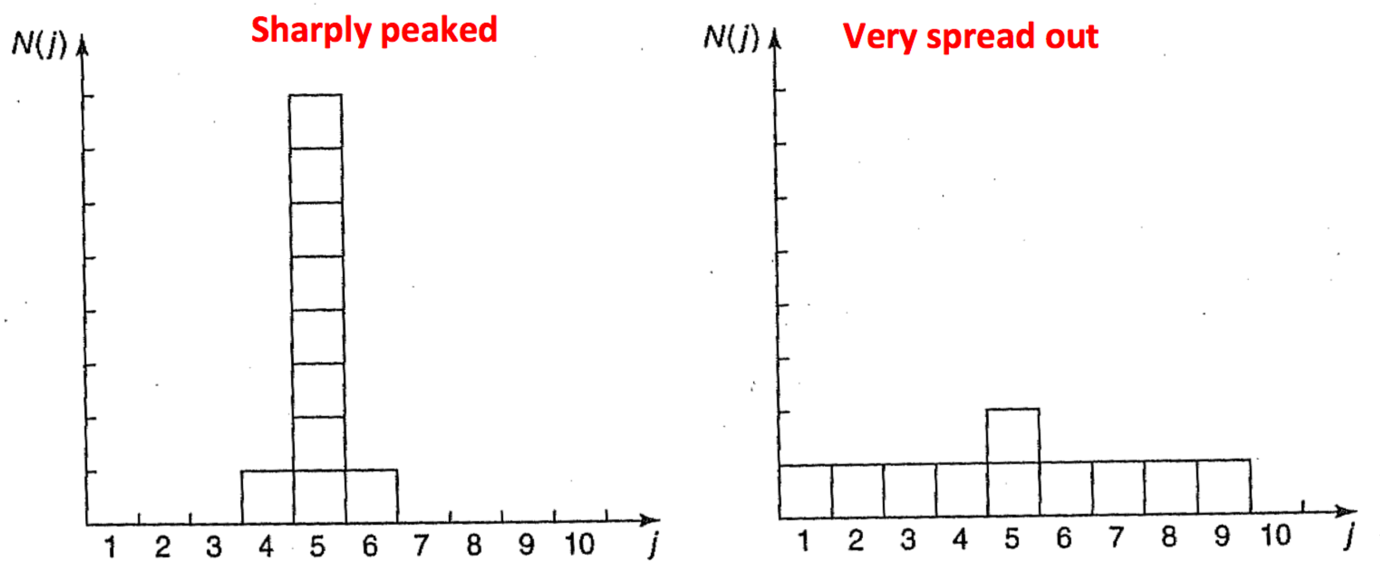


FIGURE 1.5: Two histograms with the same median, same average, and same most probable value, but different standard deviations. [Griffiths: Introduction to Quantum Mechanics]