Quantum Mechanics Homework

The 'daily' work is material we will use as exercises in class; you should have a go at them before the associated class day, but you needn't have completed them. The 'weekly' work should be turned in and will be graded. "Ready to start weekly" problems are not due at that time, but you may want to look at them.

Homework Week 1

Daily 1.W Wed 9/7 Physical Background: Zettili 1.1-1.8.0 (Q2-5):

Conceptual: The Zettili reading gives an overview of the 'modern' physics that lead up to the development of Quantum Mechanics.

- 1. In plain English (just a sentence or two per item), what was the new fundamental physics that each of these demonstrated and lead to Quantum Mechanics:
 - a. Blackbody Radiation
 - b. Photoelectric Effect
 - c. Compton Effect
 - d. De Broglie's Hypothesis
 - e. Wave-Particle Duality
 - f. Heisenberg's Uncertainty Principle
 - g. The Probabilistic Interpretation
 - h. Atomic Spectroscopy
- 2. In plain English, prior to Plank, what were the two approaches to modeling the energy density of blackbody radiation for what energy ranges did they do well, and for what ranges did they do poorly?
- 3. For the photoelectric effect, how did the photon theory address the four key observations (p. 10)?
- 4. How does a double-slit experiment differentiate between particle-like and wave-like behavior?
- 5. What do we mean by "deterministic" and "indeterministic" and how do those relate to "predictable" and "unpredictable" or "causal" and "uncausal"?
- 6. What kind of atom could Bohr's model get quantitatively right, and what kind of atom *couldn't* it?

- **1.** *Conceptual*: Many of Moore's Quantum "rules" (Q6) are applications of the more general mathematical rules that Mandl's discusses in his Chapter I. Make those connections.
- **2.** *Math:* Consider the ordinary vectors in 3 dimensions $(a_x \hat{i} + a_y \hat{j} + a_z \hat{k})$, with complex components.
 - **a.** Does the subset of all vectors with $a_z=0$ constitute a vector space? If so, what is its dimension; if not, why not?
 - **b.** What about the subset of all vectors whose *z* component is 1? *Hint:* Would the sum of two such vectors be in the subset: How about the null vector?
 - c. What about the subset of vectors whose components are all equal?
- 3. Math: Find the angle (in the sense of Equation A.28) between the vectors

$$|\alpha\rangle = (2+i)\hat{i} + (2)\hat{j} + (i)\hat{k}$$
 and $|\beta\rangle = (4-i)\hat{i} + (0)\hat{j} + (2-2i)\hat{k}$.

4. *Math* (I.1): Show that for the fundamental domain $-L \le x \le L$, the set of functions

$$\psi_0 = \frac{1}{\sqrt{2L}}, \ \psi_n = \frac{1}{\sqrt{L}} \cos\left(\frac{n\pi}{L}x\right), \ \varphi_n = \frac{1}{\sqrt{L}} \sin\left(\frac{n\pi}{L}x\right), \ (n = 1, 2, 3, ..)$$

Form a normed orthogonal set.

Ready to start Weekly HW: Read Griffiths' problem A.2, and then consider the following. Instead of a collection of all polynomials (with complex coefficients) of degree less than N in x, what about a linear combination of sine waves of the form $\sin(n\pi \frac{x}{t})$ for n < N.

a. Does this set constitute a vector space (with the sines as "vectors")? If so, suggest a convenient basis, and give the dimension of the space. If not, which of the defining properties does it lack?

- b. What if we only include even values of *n*?
- c. What if we require that the coefficient for the highest-order term, $\sin((N-1)\pi \frac{x}{L})$ be 1?

- d. What if we require that the coefficient for the n=1 term is 0?
- e. What if we require that the coefficient for the n =1 term is 1?

Daily 2.M Mon 9/12 Mandl II 4-5, 1 (Q10) The Wavefunction (Q6):

- Conceptual: Suppose you have a particle with wavefunction Ψ, whereΨ(t=0) is graphed at right. What is the probability of measuring x>0 at t=0?
- 2. *Math*: Let *s* be the number of spots shown by a die thrown at random. Calculate $\langle s \rangle$ and σ_s .
- 3. *Math:* Consider the Gaussian distribution $\rho(x) = Ae^{-\lambda(x-a)^2}$, where A, a, and λ are positive real constants. (note: while *I* enjoyed actually doing the integrals, *you* may choose to avail yourself of the inside back cover of the text.)
 - a. Find the normalization constant *A*.
 - b. Find $\langle x \rangle$, $\langle x^2 \rangle$, and σ .
 - c. Sketch the graph of $\rho(x)$.
- 4. To practice the mathematical manipulations of sections 1.4 and 1.5, derive an expression for d /dt in terms of V(x).

Starting Weekly: Do not turn in, but try all weekly problems.

55pts Weekly: 2 Tues 9/13 Griffiths Ch 1 The Wavefunction (Q6 & Q10):

- 10pts 1. Read Griffiths' problem A.2, and then consider the following. Instead of a collection of all polynomials(with complex coefficients) of degree less than N in x, what about a linear combination of sine waves of the form $sin(n\pi \frac{x}{L})$ for n < N.
 - f. Does this set constitute a vector space (with the sines as "vectors")? If so, suggest a convenient basis, and give the dimension of the space. If not, which of the defining properties does it lack?
 - g. What if we only include even values of *n*?
 - h. What if we require that the coefficient for the highest-order term, $\sin((N-1)\pi \frac{x}{L})$ be 1?
 - i. What if we require that the coefficient for the n=0 term is 0?
 - j. What if we require that the coefficient for the n =0 term is 1?
- 5pts 2. Computational: Exercises 1 & 2 of Setting Up Discrete Schrodinger Eq'n handout
- 5pts 3. The size of an atom is approximately 10^{-8} cm. To locate an electron within the atom, one should use electromagnetic radiation of wavelength not longer than, say, 10^{-9} cm.
 - a. What is the energy of a photon with such a wavelength (in eV)?
 - b. What is the uncertainty in the electron's momentum if we are uncertain about its position by 10^{-9} cm?

$$\frac{-(x-x_o)^2}{4a^2} \quad \frac{ip_o x}{b} \quad -i\omega$$

4. Consider the wave function
$$\Psi(x,t) = Ae^{-4a^2}e^{-\hbar}e^{-i}$$

- 5pts a. What is the normailization constant A?
- 20pts b. Calculate the expectation of x, x^2 , p and p^2 . Note: the given wavefunction is a popular approximation, but not strictly correct; a result of that is that the two ways of getting give different answers; try both (one is trivial).
- 5pts c. For what potential energy function V(x) would Ψ satisfy the Schrodinger equation if

p_o=0? To make it even cleaner, let's say
$$a^2 = \frac{\hbar}{2m\omega_o}$$
.

5pts d. Calculate σ_x and σ_p . Are they consistent with the uncertainty principle?

5pts 5. For $\psi(x) = \sqrt{\frac{2}{\pi a}} \frac{1}{1 + (\frac{x}{a})^2}$, if a = 4.0 nm, what is the probability that the object is found between

x = 0 an 8.0nm?

Daily 2.W Wed 9/14 2.1-.2 Stationary States & Infinite Square Well (Q7.1-3):

1. Math: A particle in the infinite square well has the initial wave function

$$\Psi(x,0) = \begin{cases} A, & 0 \le x \le a/2 \\ -A, & a/2 < x \le a \end{cases}$$

- a. Sketch $\Psi(x,0)$ and determine the constant A.
- b. Find $\Psi(x,t)$
- c. What is the probability that a measurement of the energy would yield the value $E_{1;}$ how about E_2 (by these subscripts, I mean the corresponding energies according to eq'n 2.27, regardless of how *you* happened to number your wave functions)?
- d. Find the expectation value of the energy. So, is this square-wave state physically achievable?
- 2. Conceptual: What did Unit Q call a stationary state?
- 3. Conceptual: Equation 2.15 is related most closely to which of the "rules" from Unit Q?
- 4. *Math*: Calculate <*x*>, <*x*²>, <*p*>, <*p*²>, σ_x , and σ_p , for the *n*th stationary state of the infinite square well. Check that the uncertainty principle is satisfied. Which state comes closest to the uncertainty limit?

Ready to Start Weekly HW: Exercises 1 & 2 of Implementing Discrete Schrodinger Eq'n handout

Ready to Start Weekly HW: A particle in the infinite square well has as its initial wave function: $\Psi(x,0) = A[\psi_1(x) + \psi_4(x)]$

- a. Normalize $\Psi(x,0)$.
- b. Find $\Psi(x,t)$ and $|\Psi(x,t)|^2$. Express the latter as a sinusoidal function of time, as in example 2.1. So simplify the result, use $\omega \equiv \pi^2 \hbar / 2ma^2$
- c. Compute <*x*>. Notice that it oscillates with time? What is the angular frequency of the oscillation? What is the amplitude?
- d. Compute <*p*>. Hint: There is an easy way.
- e. If you measured the energy of this particle, what values might you get, and what is the probability of getting each of them?
- f. Find the expectation value of *H*. How does it compare with the answer to e?

Daily 2.F Friday 9/16 2.3.0-.1 (to Ex 2.4) Harmonic Oscillator-algebraic part1 (Q7.4):

1. *Computational:* Recall from last time's computational work that you can approximate the Schrodinger Equation by the matrix relation

$$\begin{pmatrix} 2+\widetilde{v}(x_1) & -1 & & \\ -1 & 2+\widetilde{v}(x_2) & -1 & & \\ & & \ddots & & \\ & & -1 & 2+\widetilde{v}(x_j) & -1 & & \\ & & & & \ddots & \\ & & & & -1 & 2+\widetilde{v}(x_N) \end{pmatrix} \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_j) \\ \vdots \\ \psi(x_N) \end{pmatrix} = \varepsilon \begin{pmatrix} \psi(x_1) \\ \psi(x_2) \\ \vdots \\ \psi(x_j) \\ \vdots \\ \psi(x_N) \end{pmatrix}.$$

So, for example, you could create an infinite square well with a sloped bottom by having the diagonal terms be $2 + \text{slope}^* x_j$. With an eye on future modifications to your code, modify your Python code as follows. Soon after the constants section, define a potential function: def v(j): #sloped potential

V = 0.1*j/N #vary the 0.1 to vary the slope Return V

Then where you currently have the line H[j,j] = 2, change it to H[j,j] = 2 + v(j).

So you can visually relate the wavefunctions to the potential energy well, you can add to the wavefunction plot a plot of the potential well with the following lines:

```
Vvalues = []
for j in arange(1,N+1):
Vvalues.append(v(j))
plot(xs,Vvalues)
```

For that matter, you can also see how the wavefunction's energies relate to each other and the well by offsetting each wavefunction's plot by its energy. That can be done by change your code to plot Wavefunctions[:,j-1]+Energies[j] rather than just Wavefunctions[:,j-1].

Then run it and see what the low-*n* eigenfunctions look like (don't bother looking at the ones for values of n > N/4 since you learned that the program does a poor job with those anyway.) You can vary the "0.1" to vary the slope and see its effect.

Note: To get smooth and understandable plots, crank N up to about 100.

- 2. *Math:* Which integral from the back of the book does he use to evaluate the integral before equation 2.59?
- 3. *Math:* For the equation just after eq'n [2.64]: write out each term separately. Which term should use integration by parts? Show explicitly and mark which term goes to 0 and why.
- 4. *Math:* Find the second excited state of the harmonic oscillator.
 - a. Sketch ψ_0 , ψ_1 , and ψ_2 .
 - b. Check the orthogonality of ψ_0 , ψ_1 , and ψ_2 , by explicit integration. Hint: If you exploit the even-ness and odd-ness of the functions, there is only one integral left to do.

Ready to Start Weekly HW: For ψ_2 for the harmonic oscillator:

- c. Compute <x>, , <x²>, and <p²> by explicit integration. Use the variable $\xi \equiv \sqrt{m\omega/\hbar x}$ and the constant $\alpha \equiv (m\omega/\pi\hbar)^{1/4}$.
- d. Check the uncertainty principle for this state.
- e. Compute <T> and <V> for these states without integration. Is their sum what you would expect?

Ready to Start Weekly HW: Find <*x*>, <*p*>, <*x*²>, <*p*²>, and <*T*>, for the *n*th stationary state of the harmonic oscillator, using the method of example 2.5. Check that the uncertainty principle is satisfied.

Homework Week 3

Daily 3.M Monday 9/19 2.3.1 (rest of) Harmonic Oscillator – algebraic part2 :

- 1. *Conceptual*: In words, explain the concept and usefulness of ladder operators.
- 2. Conceptual: What is a hermitian conjugate?
- 3. *Math:* If you haven't already, finish off numbers 2 and 3 from last Friday.
- 4. *Math:* In number 4 for last Friday, you got started on one of the weekly problems due tomorrow. You may not yet have worked out part (c) which asks you to find <T> and <V>, but you should be able to answer this question: what do you expect <T> + <V> to be and why?

Ready to Start Weekly HW: By now, you should have made a good attempt at all of the weekly HW problems; keep that rolling.

Weekly: 3	3 Tues 9/20 Griffiths Ch 2.1-2.3.1:
<i>1.</i> A	particle in the infinite square well has as its initial wave function: $\Psi(x,0) = A[\psi_1(x) + \psi_4(x)]$
5pts	a. Normalize $\Psi(x,0)$.
5pts	b. Find $\Psi(x,t)$ and $ \Psi(x,t) ^2$. Express the latter as a sinusoidal function of time, as in example 2.1. To simplify the result, use $\omega \equiv \pi^2 \hbar / 2ma^2$
5pts	c. Compute <x>. Notice that it oscillates with time? What is the angular frequency of the oscillation? What is the amplitude?</x>
2pts	d. Compute . Hint: There is an easy way.
2pts	e. If you measured the energy of this particle, what values might you get, and what is the probability of getting each of them?
2pts	f. Find the expectation value of <i>H</i> . How does it compare with the answer to e?
2. Fo 17pts 5 pts 5pts	 a. Compute <x>, , <x<sup>2>, and <p<sup>2> by explicit integration. Use the variable ξ = √mω/ħx and the constant α = (mω/πħ)^{1/4}.</p<sup></x<sup></x> b. Check the uncertainty principle for this state. c. Compute <t> and <v> for these states without integration. Is their sum what you would expect?</v></t>
<i>3.</i> Ex	ercises 1 & 2 of Implementing Discrete Schrodinger Eq'n handout
ts <i>4.</i> Fir th	nd < <i>x</i> >, < <i>p</i> >, < <i>x</i> ² >, < <i>p</i> ² >, and < <i>T</i> >, for the <i>n</i> th stationary state of the harmonic oscillator, using e method of example 2.5. Check that the uncertainty principle is satisfied.
	Weekly: 3 1. A 5pts 5pts 2pts 2pts 2pts 2pts 2pts 2pts 5pts 5pts 5pts 2pts 2pts 3. Ex ts 4. Fin

Daily 3.W Wednesday 9/21 Griffiths 2.3.2 Harmonic Oscillator – analytic (Q10.6)

- 1. *Math*: Construct the third through fifth excited states of the harmonic oscillator using Hermite polynomials.
- 2. *Math*: Show explicitly that equation 2.75 satisfies 2.74.

Ready to Start Weekly HW, Computational: To approximate the simple harmonic oscillator's parabolic well, of the form $V(x) = \frac{1}{2m} \left(\frac{\hbar}{\Delta x}\right)^2 \left(\frac{1}{2} - \frac{x}{L}\right)^2$, you can add to your DiscretePIB.py program the following definition def v(j): #Simple Harmonic Oscillator $v = 1.0^*(0.5 - j/(N-1))^{**2}$ #vary the 1.0 to vary the well's concavity return v Then rename your previously defined potential from v(j) to vslope(j) (so you can easily switch back to using it if you want.) For the states of n<N/4, you should see that the energies vary linearly with n, and the wavefunctions behave as expected. Ready to Start Weekly HW: Based on Equation 2.85 (and Table 2.1), compute <x²> for ψ_5 and compare your result with what you'd get for that according to problem 5 of the previous week's weekly homework if n=5. *Ready to Start Weekly HW*: A particle in the harmonic oscillator has the initial wave function:

$$\Psi(x,0) = \frac{1}{\sqrt{2}} [\psi_0 + \psi_2] \; .$$

a. Compute $\langle x^2(t) \rangle$.

b. If you measured the energy of this particle, what values might you get, and what is the probability of getting each of them?

Daily 3.F Friday 9/23 Griffiths 2.4 Free Particle (Q11)



Daily 4.M Monday 9/26 2.4 Free Particle, Gaussian Wave Packet (problem 2.22 in class)

1. *Math*: Let $y = \sqrt{a}[x + (b/2a)]$. Write out the equivalent for $(ax^2 + bx)$ in terms of y instead of x. What is the advantage of this change of variables?

Ready to Start Weekly HW: The Gaussian wave packet. A free particle has the initial wave function $\Psi(x,0) = Ae^{-ax^2}$, where A and a are constants (a is real and positive). e. Normalize $\Psi(x,0)$. f. Find $\Psi(x,t)$. g. Find $|\Psi(x,t)|^2$. Express your answer in terms of the quantity $w \equiv \sqrt{\frac{a}{1+(2\hbar at/m)^2}}$. Sketch $|\Psi|^2$ (as a function of x) at t=0, and again for some very large t. Qualitatively, what happens to $|\Psi|^2$ as time goes on? h. Find <x>, , <x²>, <p²>, σ_x , and σ_p . i. Does the uncertainty principle hold? At what time t does the system come closest to the uncertainty limit?

Ready to Start Weekly HW, Computation. Use VPython to visualize the Gaussian wavefunction's (featured in the preceding problem) time evolution. Whether you've completed the preceding problem or not, you can do this one. Expressed in terms that Python can understand, the wavefunction is

Wave = (2*a/pi)**0.25 *exp(-a*x**2 / (1+2j*hbar*a*t/m))/(1+2j*hbar*a*t/m)**0.5

That's right, it *can* handle complex numbers (using the engineer's convention that $j \equiv \sqrt{-1}$)! Note that the lack of a "*" between the 2 and the j is no mistake: when Python sees a number immediately followed by j, it interprets that as being imaginary. To ask for just the real or imaginary part of Wave or its amplitude, in Python you simply ask for

Wave.real, Wave.imag, or abs(Wave)

Here's what I'd suggest for visualizing. Python itself isn't great with time evolution, but VPython has no problem, so we'll use VPython objects to help visualize the wavefunction. First off, create "curves" along the x axis, from some –L to L and spaced some deltaX. That can be done with

g = curve(x=arange(-L,L,deltaX), color=color.green) #represents the wave's amplitude

r = curve(x=arange(-L,L,deltaX), color=color.red) #represents the wave -real and imaginary

x_axis = curve(x=arange(-L,L,deltaX), color=color.blue) #represents the x-axis

You'll then adjust the y component s of their positions to represent the amplitude of the wavefunction at each x position. This can be achieved as follows:

Wave = (2*a/pi)**0.25 *exp(-a*g.x**2 / (1+2j*hbar*a*t/m))/(1+2j*hbar*a*t/m)**0.5

g.y = abs(Wave)*scalefactor

r.y = Wave.real*scalefactor

r.z = Wave.imag*scalefactor

Since you've not written something quite like this before, a word of explanation: "g" is a curve that's defined by a long list of positions; "g.y" calls up its y components. You'll notice that the definition of Wave involves g.x, but g is a list of points along a curve, thus it has several x values. What does Phython do when you ask it to use g.x in an equation? It figures you want to use each value in turn, thus it returns a whole list of corresponding values for Wave. Then g.y, r.y, and r.z, which are calculated using Wave, are also lists of the corresponding values.

Write this much of the program and make sure you can get a reasonable looking Gaussian before modifying the code to make it time evolve. A unit system such that hbar = 1, a = 1, m = 1, L = 20, t = 0, and deltaX = 0.01, should work, though you'll want to multiply abs(Wave) by a scale factor of about 10 to make the plot more pronounced.

Once you've got this much of your code working, nest the above loop inside a while t < tmax: loop (tmax = 100 and deltat = 0.001 work well; don't forget to add a t = t + deltat line in the loop). Now the amplitude of your wavefunction should time evolve. Play around with the parameter *a* to see how it effects the packet's initial sharpness and the time scale over which it evolves.

Now run your program. For the page of text it took me to describe writing this program, the program itself should be impressively short – Vpython's just that good.

Note: You'll want to rotate the Vpython movie while it's running so you can see the imaginary component of the wavefunction, which is plotted in the z direction.

p.s. Don't forget that it's advisable to start all python programs with from __future__ import division. That makes it so if you ever find yourself diving an integer by an integer, you get the appropriate fraction (as in $\frac{1}{4} = 0.25$) rather than having the result truncated to the nearest integer (0). You're also going to need to include inside your loop a "rate" statement, like "rate(100)" to slow down the execution. Also, *don't* import pylab.

Weekly: 4 Tues 9/27 Griffiths Ch 2.3.2-2.4:

- 5pts 1. Based on Equation 2.85 (and Table 2.1), compute $\langle x^2 \rangle$ for ψ_5 and compare your result with what you'd get for that according to problem 5 of the previous week's weekly homework if n=5.
- 5pts 2. Computational: To approximate a parabolic well, you can modify you DiscretePIB.py program so that $H[j,j] = 2 + 1.0^{*}(0.5 - j/(N-1))^{**2}$. The additional term is equivalent to

saying that $V(x) = \frac{1}{2m} \left(\frac{\hbar}{\Lambda x}\right)^2 \left(\frac{1}{2} - \frac{x}{L}\right)^2$ Replacing the 1.0 with larger or smaller values

will adjust the potential well's concavity (how wide or narrow the parabola is.). For the lower-n states, you should see that the energies vary linearly with n, and the wavefunctions behave as expected. On the same graph, produce a plot of the scaled eigenvalues (Eivenvalues/Eigenvalues[0]) and the corresponding expected energies ((n+0.5)/0.5). Note: unlike with the particle in a box, n should start at 0.

3. A particle in the harmonic oscillator has the initial wave function: $\Psi(x,0) = \frac{1}{\sqrt{2}} [\psi_0 + \psi_2]$.

6pts a. Compute $\langle x^2(t) \rangle$.

2pts b. If you measured the energy of this particle, what values might you get, and what is the probability of getting each of them?

4. A free particle has the initial wave function
$$\Psi(x,0) = \begin{cases} Ae^{-ax} & \text{for } x \ge 0 \\ 0 & \text{for } x < 0 \end{cases}$$
, where *A* and *a* are

positive real constants.

- 3pts a. Normalize $\Psi(x,0)$.
- 3pts b. Find $\phi(k)$.
- 1pt c. Construct $\Psi(x,t)$ in the form of an integral.
- 5. The Gaussian wave packet. A free particle has the initial wave function $\Psi(x,0) = Ae^{-ax^2}$ where A and a are constants (a is real and positive).

```
5pts a. Normalize \Psi(x,0).
2pts b. Find \Psi(x,t).
```

7pts c. Find $|\Psi(x,t)|^2$. Express your answer in terms of the quantity $w \equiv \sqrt{\frac{a}{1+(2\hbar at/m)^2}}$

Sketch $|\Psi|^2$ (as a function of x) at t=0, and again for some very large t. Qualitatively, what happens to $|\Psi|^2$ as time goes on?

23pts d. Find $\langle x \rangle$, $\langle p \rangle$, $\langle x^2 \rangle$, $\langle p^2 \rangle$, σ_x , and σ_p .

2pts e. Does the uncertainty principle hold? At what time t does the system come closest to the uncertainty limit?

69pts

⁵pts 5. Computational: write a program that visualizes the Gaussian wavefunction's time evolution (see problem 3 for daily 4.M)

Daily 4.W Wednesday 9/28 Griffiths 2.5 Scattering from the Delta Potential (Q7.1, Q11)

- 1. *Conceptual*: Compare Griffith's definition of a bound state with Q7.1.
- 2. *Conceptual*: Compare Griffith's definition of tunneling with Q11.3.
- 3. *Conceptual*: Possible energy levels are quantized for what kind of states (bound, and/or unbound)? Why / why not?
- 4. *Conceptual*: State the rules from Q11.4 in terms of mathematical equations. Can you match the rules to equations in Griffiths? If you can, give equation numbers.

Ready to Start Weekly HW: Evaluate the following integrals:

a.
$$\int_{-3}^{+1} (x^3 - 4x^2 + 3x - 2)\delta(x+1)dx$$

a.
$$\int_{0}^{-3} [\cos(2x) + 5]\delta(x - \pi)dx$$

b.
$$\int_{0}^{+1} e^{(|x|+6)}\delta(x-4)dx$$

c.
$$-3$$

Ready to Starting Weekly HW: Consider the double delta-function potential

 $V(x) = -\alpha[\delta(x+a) + \delta(x-a)]$, where α and a are positive constants.

- d. Sketch this potential.
- e. Write the schrodinger equation in each of the three regions.
- f. What is the solution to each of these differential equations?
- g. What are the boundary conditions?
- h. Does problem 2.1(c) apply here? Does it help?
- a. Write the possible solutions for $\psi(x)$.
- b. How many bound states are there?

Ready to Start Weekly HW, Computational: Follow the instruction in the handout "Discrete Time-Dependent Schrodinger" to simulate a Gaussian packet's interacting with a delta-well.

Daily 4.F Friday 9/30 Griffiths 2.6 The Finite Square Well (Q 11.1-.4) beginning

- 1. Conceptual: What physical properties determine the number of bound states in a finite well?
- 2. *Conceptual*: How do we determine the number of *scattering* states?
- 3. *Math*: Derive equations 2.167 and 2.168. Show all steps. Hints:
 - j. First use 2.165 and 2.166 to write C and D in term of F (without A or B).
 - k. Solve for $Ae^{-ika} + Be^{ika}$ and $Ae^{-ika} Be^{ika}$ in terms of $\sin(2la)$ and $\cos(2la)$ using the double angle formulas in trig.
 - I. Add the equations you get in the previous section to get rid of B and then solve for F in terms of A (eq. 2.168).

m. Now subtract the equations to get rid of A and solve for B in terms of F (eq. 2.167).

Ready to Start Weekly HW: Consider the "step" potentials:

$$V(x) = \begin{cases} 0, & \text{if } x \le 0 \\ V_0, & \text{if } x > 0 \end{cases} \text{ and } V(x) = \begin{cases} V_o, & \text{if } x \le 0 \\ 0, & \text{if } x > 0 \end{cases}$$

a. Conceptual/Computational: In your DiscretePIB.py program, define a step potential (though it will be convenient to move the border to j = N/2 rather than 0). I suggest a height of V_o around 0.05 so you can easily get some wave functions with energies below and some with energies above. So, define

#step potential well

def V(j):

V = 0

if j> N/2: #flipping inequality will flip which half of the space has the barrier

V = 0.05 #barrier height

return V

Run this for the first few wavefunctions so you can see the qualitative behavior. (This is due with conceptual questions.)

- b. Analytical: Show that the reflection coefficients for the two cases are equal when $E > V_0$.
 - i. Start by doing the first case. How many regions are you using? What are your boundary conditions?
 - ii. Write the Schrödinger equation in each region and solve. Solutions should be exponentials, not sines and cosines. You should be using k from equation 2.130 and I similar to (but not exactly) equation 2.148. Careful when defining these in terms of E and V_0 .
 - iii. Label your diagrams in part (h) with coefficients like in figure 2.15. Assume wave enters from left. What goes to zero?
 - iv. Apply boundary conditions and calculate the reflection coefficient
 - v. Repeat above for other case.
- c. Analytical: What happens when $E < V_0$? Show calculation and comment on solution. Do only for the first case.

Daily 5.M Monday 10/3 Griffiths 2.6 The Finite Square Well (Q 11.1-.4) continuing

- 1. *Conceptual*: Can you come up with a "recipe" like the Q11 rules that will help with solving ANY 1D Schrödinger equation problem mathematically?
- 2. *Conceptual*: Are the following functions odd, even, or neither? Write a formula for each and plot to check yourself after you've given an answer.
 - a. The fifth Hermite polynomial.
 - b. The fourth excited state of the harmonic oscillator.
 - c. $e^{x/b}$
 - d. $(x^5 + x^2)e^{-ax^2}$
- 3. Conceptual: A particle is in a finite square well (V(x) given by eq. 2.145) with V_0 and a such that there are 11 bound states. The initial wave function of the particle is given by

$$\Psi(x,0) = A\left[\frac{3}{7}\psi_1 + \frac{2}{11}\psi_3 + \frac{1}{3}\psi_4\right] \text{ where } \psi_1, \psi_3 \text{ and } \psi_4 \text{ are stationary states.}$$

- a. Find A.
- b. What are the approximate energies that would be measured (given these are deep in the well) and, given that the stationary states are orthonormal (to be proven in Ch. 3), what are the probabilities of measuring each one?

Ready to Start Weekly HW, Computational: Modify your DiscretePIB.py program to handle the finite well instead. Here's how: near the beginning add the lines

#finite square well

def V(j):

V = 0

if j< N/3 or j > 2*N/3: #well is central $1/3^{rd}$ of simulated range

V = 0.15 #barrier height

return V

You can vary the width of the well and the height of the barriers on either side. This is

essentially a finite well inside an infinite well (boundaries at j = 0 and j = N), which should work

well as long as the wave functions die off well before reaching the simulations outer edges.

0, $x \leq 0$ *Ready to Start Weekly HW*: Consider the following potential: V(x) = $V_{0,}$ 0 < x < a $-\alpha V_0$, $x \ge a$ c. Sketch this potential and comment on what you think will happen for $E < V_0$. d. Calculate the reflection coefficient. e. For fun (not assigned) you can make your particle-in-a-box program do this one too: def v(j): #tunneling through barrier V = 0if j>=24*N/50 and j<=26*N/50: V = 0.5 + 0.5*(4/10 - j/N)if j > 26*N/50: V = -0.1return V You'll notice that I actually gave the potential a little bit of a slope - that's to match the situation in scanning tunneling microscopy. You have a metal tip of one type on the left, a conducting sample of another type on the right (as different metal have different work functions for removing electrons, the potential energies in the two will be different), and a vacuum region in between. With the tip and sample at two different voltages, and imagining it's a (negatively charged) electron who's wavefunction we're finding, it would experience a fairly uniform electric field / linearly changing potential across the gap / barrier.

Weekly: 5 Tues 10/4 Griffiths Ch 2.5-2.6: 55 pts

1. Evaluate the following integrals:

1 pt
$$\int_{-3}^{+1} (x^3 - 4x^2 + 3x - 2)\delta(x+1)dx$$

a.
$$\int_{-3}^{-3} [\cos(2x) + 5]\delta(x-\pi)dx$$

b.
$$\int_{0}^{+1} e^{(|x|+6)}\delta(x-4)dx$$

- 2. Consider the double delta-function potential $V(x) = -\alpha[\delta(x+a) + \delta(x-a)]$, where α and a are positive constants.
- 1 pt a. Sketch this potential.

c. ⁻³

- 1 pt b. Write the Schrödinger equation in each of the three regions.
- 5 pts c. What is the solution to each of these differential equations?
- 3 pts d. What are the boundary conditions? Note: consider the point made in problem 2.1 (c).
- 5 pts e. Write the possible normalized and bound solutions for $\psi(x)$
- 1 pt f. How many bound states are there?
- 3 pts g. Write the transidental relation that E must satisfy for each bound state and reason the ordering of the different states' energies which is higher and which is lower energy

- 6 pts *3.* Computational: Follow the instruction in the handout "Discrete Time-Dependent Schrodinger" to simulate a Gaussian packet's interacting with a delta-well.
 - 4. Consider the "step" potentials: $V(x) = \begin{cases} 0, & \text{if } x \le 0 \\ V_0, & \text{if } x > 0 \end{cases}$ and $V(x) = \begin{cases} V_o, & \text{if } x \le 0 \\ 0, & \text{if } x > 0 \end{cases}$
 - a. Conceptual/Computational: In your DiscretePIB.py program, define a step potential (see HW 4.F problem 4 for details)
 - b. Analytical: Show that the reflection coefficients for the two cases are equal when $E > V_0$.
 - 2 pts i. Start by doing the first case. How many regions are you using? What are your boundary conditions?
 - 2 pts
 ii. Write the Schrödinger equation in each region and solve. Solutions should be exponentials, not sines and cosines. You should be using k from equation 2.130 and I similar to (but not exactly) equation 2.148. Careful when defining these in terms of E and V₀.
 - 2 pts iii. Label your diagrams in part (h) with coefficients like in figure 2.15. Assume wave enters from left. What goes to zero?
 - 2 pts iv. Apply boundary conditions and calculate the reflection coefficient. (Hint: write as something over $(k^2-l^2)^2$.) Finally, plug back in for k and l to get reflection in terms of E and V₀ and simplify.
 - 4 pts v. Repeat above for other case.
 - 3 pts c. Analytical: What happens when $E < V_0$? Show calculation and comment on solution. Do only for the first case.

5. Consider the following potential:
$$V(x) = \begin{cases} 0, & x \le 0 \\ V_{0,} & 0 < x < a \\ -\alpha V_{0}, & x \ge a \end{cases}$$

1 pt a. Sketch this potential and comment on what you think will happen for $E < V_0$.

7 pts b. Calculate the reflection coefficient.

6. Computational: Modify your Discrete SHO program to handle the finite well instead. See
 2 pts Monday's number 5.

Daily 5.W Wednesday 10/5 Griffiths 1-2

2 pts

come to class with a written list of equations you'd like on Friday's exam.

Daily 6.W Wednesday 10/12 Griffiths Appendix A.3-.6 Linear Algebra

1. Math: (like A.8) Given the following two matricies:

	1	i	-1]		- i	0	2	
A =	3	0	2	and ${f B}=$	0	1	0	,
	2i	2	-2i		2	3	i	

Compute (a) $\mathbf{A} + \mathbf{B}$, (b) \mathbf{AB} , (c) $[\mathbf{A},\mathbf{B}]$, (d) $\widetilde{\mathbf{A}}$, (e) \mathbf{A}^* , (f) \mathbf{A}^+ , (g) det(**B**), and (h) \mathbf{B}^{-1} . Also, (i) check that $\mathbf{BB}^{-1} = 1$. (j) Does **A** have an inverse?

- 2. Math: A.14
- 3. Math A.19

Ready to Start Weekly HW: Using the square matrices in the previous problem and the column matrices (vectors) $\mathbf{a} = \begin{pmatrix} 2i \\ i \\ 2 \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} 2 \\ (1-i) \\ 0 \end{pmatrix}$, find (a) Aa, (b) $\mathbf{a}^{\dagger}\mathbf{b}$, (c) $\mathbf{\widetilde{a}Bb}$, (d) $\mathbf{a}\mathbf{\widetilde{b}}^{\dagger}$ Ready to Start Weekly HW: Let $\mathbf{T} = \begin{bmatrix} 2 & 2+i \\ 2-i & 0 \end{bmatrix}$. a. Verify that T is Hermitian. b. Find its eigenvalues (note that they are real). c. Find and normalize the eigenvectors and show that they are orthogonal. d. Construct the unitary diagonalizing matrix S, and check explicitly that it diagonalizes T. e. Check that det(T) and Tr(T) are the same for T as they are for its diagonalized form.

Daily 6.F Friday 10/14 Griffiths 3.1-.2 Formalism: Hilbert Space & Observables (Q5.6, 6.2-3)

- 1. *Conceptual*: Explain all the steps in the derivation in eq. 3.19.
- 2. *Math*: Consider the spin eigenvectors (Table Q6.1).
 - a. Show that the two eigenvectors for a given s component (x, y, or z) are orthonormal.
 - b. Do they live in Hilbert Space? Explain.
- 3. *Math:* Consider the operator $\hat{Q} = \frac{d^2}{d\phi^2}$, where ϕ is the azimuthal angle in polar coordinates,

and the functions are subject to the same boundary condition shown in eq. 3.26. Is this operator hermition? Find its eigenfunctions and eigenvalues.

Daily 7.M Monday 10/17 Griffiths 3.3-3.4 Formal: Hermitian Operator's Eigenstates & Statistical Interp (Q11)

- 1. *Conceptual*: Discuss the relationship between continuous, discrete, quantization, normalization, stationary states, bound states, and scattering states. Which of these correspond to each other?
- 2. *Math*: Is the ground state of the infinite square well an eigenfunction of momentum? If so, what is its momentum? If not, *why* not?
- 3. Math: A particle of mass m is bound in the delta function well. What is the probability that a

measurement of its momentum would yield a value between 0 and $p_0 = \frac{m\alpha}{t}$?

Ready to Start Weekly HW: A particle in the infinite square well has the initial wave function $\Psi(x,0) = Ax(a-x)$

- a. What is $\Psi(x,t)$ (feel free to quote the example in Ch. 2)?
- b. What is the probability a measurement of the energy would yield the value $\frac{4\pi^2\hbar^2}{2ma^2}$?
- c. What is the probability a measurement of the energy would yield the value $\frac{9\pi^2\hbar^2}{2mr^2}$?
- d. What is the probability of measuring the location of the particle at t = 0 to be between 3a/4 and a?
- e. If, at time *t*, you measure the energy to be $\frac{9\pi^2\hbar^2}{2ma^2}$, what is the probability of measuring the location of the particle to be between 3a/4 and a?

Ready to Start Weekly HW: Find the momentum-space wave function, $\Phi(p,t)$, for a particle in the first excited state of the harmonic oscillator (the real-space wave function is given in example 2.4.) What is the probability (to 2 significant digits) that a measurement of p on a particle in this state would yield a value outside the classical range (for the same energy)? (remember the trick from Daily 4.M pr. 1; classically expect $\frac{p^2}{2m} = K \leq E$) To get a numerical value, you'll need to look in a math table under the first derivative of the "normal distribution" or "error function"; equivalently, Wolfram Alpha might do it for you.

Daily 7.W Wednesday 10/19 Griffiths 3.5 Uncertainty Principle

- 1. Any questions about the mathematical derivations in this section. Are there steps that didn't make sense?
- 2. *Math*: Construct the uncertainty relation for Energy and position.
- 3. *Math:* Write $\begin{vmatrix} a \\ b \end{vmatrix}$ in terms of |+x> and |-x>.
- 4. *Math* Griffiths Problem 3.15

Ready to Start Weekly HW: Consider three observables, A, B, and C. We know that [B, C] = A and [A, C] = B. Show that $\sigma_{AB}\sigma_C \ge \frac{1}{2i} \langle A^2 + B^2 \rangle$. Note: if you use Eq'n 3.64 (I didn't), you've got to *prove* it first.

Ready to Start Weekly HW: Show that the expectation value of any observable in a stationary state does not change with time, provided the time rate of change of the operator for the observable is zero.

37 pts Weekly: 7 Thurs 10/20 Griffiths A.3-6, ch 3.1-5
5 pts 1. Using the square matrices
$$\mathbf{A} = \begin{bmatrix} 1 & i & -1 \\ 3 & 0 & 2 \\ 2i & 2 & -2i \end{bmatrix}$$
 and $\mathbf{B} = \begin{bmatrix} -i & 0 & 2 \\ 0 & 1 & 0 \\ 2 & 3 & i \end{bmatrix}$ and the column matrices
(vectors) $\mathbf{a} = \begin{pmatrix} 2i \\ 2 \\ 2 \end{pmatrix}$ and $\mathbf{b} = \begin{pmatrix} 2 \\ (1-i) \\ 0 \end{pmatrix}$, find (a) Aa, (b) $\mathbf{a}^{\dagger}\mathbf{b}$, (c) $\mathbf{\tilde{a}}\mathbf{B}\mathbf{b}$, (d) $\mathbf{a}\mathbf{\tilde{b}}^{\dagger}$
10 pts2. Let $\mathbf{T} = \begin{bmatrix} 2 & 2+i \\ 2-i & 0 \end{bmatrix}$.
a. Verify that **T** is Hermitian.
b. Find its eigenvalues (note that they are real).
c. Find and normalize the eigenvectors and show that they are orthogonal.
d. Construct the unitary diagonalizing matrix **S**, and check explicitly that it diagonalized form.
9 pts 3. A particle in the infinite square well has the initial wave function $\Psi(x,0) = Ax(a-x)$
1 pt a. What is $\Psi(x,t)$ (feel free to quote the example in Ch 2)?
1 pt b. What is the probability a measurement of the energy would yield the value $\frac{4\pi^2 \hbar^2}{2ma^2}$?
3 pts d. What is the probability of measuring the location of the particle at $t = 0$ to be between $3a/4$ and a ?
3 pt e. If, at time t, you measure the energy to be $\frac{9\pi^2 \hbar^2}{2ma^2}$, what is the probability of measuring the location of the particle at $dat a$?
3 pt 4. Consider three observables, A, B, and C. We know that [B, C] = A and [A, C] = B. Show that $\sigma_{AB}\sigma_C \ge \frac{1}{2i}(A^2 + B^2)$.
3 pts 4. Show that the expectation value of any observable in a stationary state does not change with time, provided the time rate of change of the operator for the observable is zero.

8 pts 5. Find the momentum-space wave function, $\Phi(p,t)$, for a particle in the first excited state of the harmonic oscillator (the real-space wave function is given in example 2.4.) What is the probability (to 2 significant digits) that a measurement of p on a particle in this state would yield a value outside the classical range (for the same energy)? (remember the trick from Daily 4.M pr. 1; classically expect $\frac{p^2}{2m} = K \le E$) To get a numerical value, you'll need to look in a math table under the first derivative of the "normal distribution" or "error function"; equivalently, Wolfram Alpha might do it for you.

Daily 7.F Friday 10/21 Griffiths 3.6 Dirac Notation(Q5.6)

- 1. *Math*: Compute $\langle u | w \rangle$, $\langle w | u \rangle$, and $|\langle w | u \rangle|^2$ for the following vectors:
 - a. $|u\rangle = [1,-i], |w\rangle = [2i,3]$ b. $|u\rangle = [1,-2], |w\rangle = [i,-5]$ c. $|u\rangle = [1+i,-2+i], |w\rangle = [i,2-i]$
- 2. Conceptual/Math: Let operator \hat{A} , representing observable A, have 2 normalized eigenstates ψ_1 and ψ_2 , with eigenvalues a_1 and a_2 . Operator \hat{B} , representing observable B, has 3 normalized eigenstates ϕ_1 , ϕ_2 , and ϕ_3 , with eigenvalues b_1 , b_2 , and b_3 . The eigenstates are related by $\psi_1 = C(2\phi_1 + \phi_2 + 3\phi_3)$ and $\psi_2 = D(3\phi_1 + 2\phi_2 + \phi_3)$.
 - a. Can we always write eigenstates of one operator as linear combinations of another eigenstate? Explain.
 - b. If observable A is measured to be a₁, what is the state of the system (immediately) after the measurement?
 - c. If B is now measured, what are the possible results and what are their probabilities?
 - d. Do A and B commute? Explain.

Ready to Start Weekly HW: Consider the infinite well, for which $\Psi_n(x,t) = \sqrt{\frac{2}{a} \sin(\frac{n\pi}{a}x)} e^{-n^2 \omega_o t}$

where
$$\omega_o \equiv \frac{\hbar}{2m} \left(\frac{\pi}{a}\right)^2$$
.

a. Using equation 3.81, solve for an expression for $p_{n,m}^2$, that is, the n,mth element of the \hat{p}^2

matrix that corresponds to applying the operator $\hat{p}^2 = -\hbar^2 \frac{d^2}{dx^2}$. Start populating the

matrix with its first 16 elements, 1,1 through 4,4. Aside from being hermitian, there's a name for a matrix that looks like this, what is it? That's a signature of the basis set you're using being eigen states of the operators since it obeys $\hat{A} | \alpha_n \rangle = a_n | \alpha_n \rangle$

b. Do the same but to find the elements of the $\,\hat{p}\,$ matrix which corresponds to the operator

 $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$. Show that the matrix is hermitian by demonstrating that $p_{n,m} = p_{m,n}^*$. Notice

that the "trace" of this matrix, i.e., the sum of its diagonal terms, is 0. That's a signature of a measurable whose average is 0.

Ready to Start Weekly HW: One cans associate each one of the spin observables S_x , S_y , and S_z with a 2×2 matrix $S_x \leftrightarrow \begin{bmatrix} 0 & s \\ s & 0 \end{bmatrix}$, $S_y \leftrightarrow \begin{bmatrix} 0 & -is \\ is & 0 \end{bmatrix}$, and $S_z \leftrightarrow \begin{bmatrix} s & 0 \\ 0 & -s \end{bmatrix}$ where *s* is a real number related to

the intrinsic magnitude of the quanton's spin.

- c. Determine the eigenvalues and the corresponding eigenvectors (up to a possibly complex multiplicative constant) for each of these matrices. (The eigenvalues of one of these matrices represents the possible values that can result from an experiment to determine the observable corresponding to the matrix, and the corresponding eigenvector the eigenvector for that value.)
- d. Show that the following eigenvectors are consistent with the constraints on the eigenvectors imposed by part (a) and the requirement that the vectors be normalized:

$$|+x\rangle = \begin{bmatrix} \sqrt{1/2} \\ \sqrt{1/2} \end{bmatrix} + y\rangle = \begin{bmatrix} \sqrt{1/2} \\ i\sqrt{1/2} \end{bmatrix} + z\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
$$|-x\rangle = \begin{bmatrix} \sqrt{1/2} \\ -\sqrt{1/2} \end{bmatrix} + y\rangle = \begin{bmatrix} i\sqrt{1/2} \\ \sqrt{1/2} \end{bmatrix} + z\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

Homework Week 8

Daily 8.M Monday 10/24 Griffiths 5.4 Schrodinger's Cat, Scholosauer 7 & 3 Measurment & Interpretation

- 1. *Conceptual* : Summarize Scholosauer's 17 participant's main points about the Measurement Problem what are the main perspectives? What do you find most or least compelling?
- 2. *Conceptual* : Summarize Scholosauer's 17 participant's main points about the Interpretations organized per interpretation (rather than per participant) and see what interpretation you find most or least compelling.

Daily 8.W Wednesday 10/26 Griffiths 4.1.1-4.1.2 Schrödinger in Spherical: Separation & Angular (Q9.1)

- 1. *Conceptual*: What the limits of integration when you integrate over all space in spherical coordinates? Why?
- 2. *Conceptual*: Write the momentum operator in 3 dimensions in terms of unit vectors xhat, yhat, and zhat.
- 3. *Conceptual*: What variables can the potential energy in the Schrödinger equation depend on (in other words, V in eq. 4.8 is generally a function of what)? Is equation 4.8 valid if V is a function of time? Why? Is equation 4.4 valid if V is a function of time? Why? In the derivation of equations 4.16 and 4.17 what is V a function of? What can't it be a function of?
- 4. Math: Fill in any missing steps in the derivation of equations 4.16 and 4.17. Any questions?
- 5. *Prep for in class:* Read problem 4.2; we will do this problem in class.
 - a. Conceptual: Set up the problem. Where do you start?
 - b. *Math*: How would the solution change if the box is not cubical? Say the particle is confined to: 0 < x < a and 0 < y < b and 0 < z < c.
- 7. *Conceptual*: What are the possible values of *m*? Why?
- 8. Conceptual: This time griffith's simply gives you the solution to a differential equation (4.26 solves 4.25). List some of the properties of these solutions.
- 9. Conceptual: the figure accompanying Table 4.2 is a little misleading since distance from the origin represents the magnitude of P, |P|; so you lose sign and what looks like r is really |P|. You can do a bit better in Python. Plot each of the 10 functions listed in table 4.2 using (change your definition of P for each) the following code (or something similar that you like better).

```
from __future__ import division
```

```
from visual import *
n = 50
dtheta = 2*pi/n

def P(theta):
    return 1/2 * (3*(cos(theta)**2) -1)

pen = sphere(pos=(1,0,P(0)),radius = 0.1, color = color.red, make_trail = true)
unitring = sphere(pos=(1,0,0),radius = 0.1, color = color.blue, make_trail = true)
theta = 0
while theta < 2*pi + dtheta:
    pen.pos = vector(cos(theta),sin(theta),P(theta))
    unitring.pos = vector(cos(theta),sin(theta),0)
    theta = theta + dtheta
    rate(50)</pre>
```

Daily 8.F Friday 10/28 Griffiths 4.1.2-4.1.3 Schrödinger in Spherical: Angular & Radial (Q9.1):

- 1. *Conceptual*: Is equation 4.32 valid if V is a function of θ ? Explain.
- 2. *Math*: Where does equation 4.30 come from? Explain.
- 3. *Conceptual*: Mathematically, why doesn't the energy depend on *m*?
- Conceptual: The solution to the infinite spherical well potential consists of Bessel functions (eq. 4.47). What happened to the Neumann functions?
- 5. *Conceptual*: What is meant by β_{nl} ? Realistically, how would you solve for it?

Ready to Start Weekly HW: Use equations 4.27, 4.28, and 4.32 to construct Y_1^0, Y_2^0 , and Y_2^{-2} . Show that they are normalized and orthogonal. Show that they satisfy the differential equation 4.18.

Ready to Start Weekly HW: Consider $u(r) = Arj_2(kr)$.

- a. Show that it satisfies the differential equation 4.41 with *I*=2.
- b. Make a plot of this function. Note: for a simple example of plotting in python, see <u>http://bulldog2.redlands.edu/facultyfolder/deweerd/tutorials/Plotting.html</u>.
- c. Where is the first place the function goes to zero where *x*>0?
- d. What is *n*? What does this mean for *k*? What is the energy in terms of \hbar , *m*, and *a*?

Ready to Start Weekly HW: Computational: Create a version of your Discrete, time-independent program to find the Angular components of the wave function in spherical coordinates and modify it to find the Radial components of the wave function for an infinite spherical well. See Handout.

Homework Week 9

Daily 9.M Monday 10/31 Griffiths 4. 2 Hydrogen Atom (Q9.1)

- 1. Conceptual: What do ρ and ρ_0 stand for? Don't just give an equation. What are they, physically? What units do they have?
- 2. Math: Show that $u(\rho) = C \rho^{l+1} + D \rho^{-l}$ satisfies $\frac{d^2 u}{d \rho^2} = \frac{l(l+1)}{\rho^2} u$.
- 3. *Math*: Explicitly plug in constants to derive numbers in equations 4.72 and 4.77. Show explicitly that the units work.
- 4. *Math*: Calculate the Rydberg constant. Be explicit, especially with units.
- 5. *Conceptual*: What is the wavelength of Hydrogen-alpha? What is the transition that produces this wavelength?

Ready to Start Weekly HW: Normalize R_{32} : $R_{32} = A(\frac{r}{a})^2 e^{-\frac{r}{3a}}$. With it, construct ψ_{32-1} .

Ready to Start Weekly HW:

- a. Find<r> and <r²> for an electron in hydrogen's ψ_{200} state.
- b. Find <x> and <x²> for the same state. *Hint:* This requires no new integration note that $r^2 = x^2 + y^2 + z^2$, and exploit the rotational symmetry of the state.
- c. Find <x²> for an electron in hydrogen's ψ_{211} state. *Warning:* This state is *not* symmetrical in *x*, *y*, *z*. Use $x = r \sin \theta \cos \phi$.

57 pts Weekly: 9 Tues 11/1 Griffiths 3.6, 4.1

7 pts 1. One cans associate each one of the spin observables S_x , S_y , and S_z with a 2×2 matrix

$$S_x \leftrightarrow \begin{bmatrix} 0 & s \\ s & 0 \end{bmatrix}$$
, $S_y \leftrightarrow \begin{bmatrix} 0 & -is \\ is & 0 \end{bmatrix}$, and $S_z \leftrightarrow \begin{bmatrix} s & 0 \\ 0 & -s \end{bmatrix}$ where *s* is a real number related

to the intrinsic magnitude of the quanton's spin.

- a. Determine the eigenvalues and the corresponding eigenvectors (up to a possibly complex multiplicative constant) for each of these matrices. (The eigenvalues of one of these matrices represents the possible values that can result from an experiment to determine the observable corresponding to the matrix, and the corresponding eigenvector the eigenvector for that value.)
- b. Show that the following eigenvectors are consistent with the constraints on the eigenvectors imposed by part (a) and the requirement that the vectors be

normalized:
$$|+x\rangle = \begin{bmatrix} \sqrt{1/2} \\ \sqrt{1/2} \end{bmatrix} |+y\rangle = \begin{bmatrix} \sqrt{1/2} \\ i\sqrt{1/2} \end{bmatrix} |+z\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

 $|-x\rangle = \begin{bmatrix} \sqrt{1/2} \\ -\sqrt{1/2} \end{bmatrix} |-y\rangle = \begin{bmatrix} i\sqrt{1/2} \\ \sqrt{1/2} \end{bmatrix} |-z\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

10 pts 2. Consider the infinite well, for which $\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi}{a}x) e^{-n^2 \omega_o t}$ where $\omega_o \equiv \frac{\hbar}{2m} (\frac{\pi}{a})^2$.

5 pts

a. Using equation 3.81, solve for an expression for $p_{n,m}^2$, that is, the n,mth element of

the \hat{p}^2 matrix that corresponds to applying the operator $\hat{p}^2 = -\hbar^2 \frac{d^2}{dx^2}$. Start

populating the matrix with its first 16 elements, 1,1 through 4,4. Aside from being hermitian, there's a name for a matrix that looks like this, what is it? That's a signature of the basis set you're using being eigen states of the operators since it obeys $\hat{A} | \alpha_n \rangle = a_n | \alpha_n \rangle$

5 pts b. Do the same but to find the elements of the \hat{p} matrix which corresponds to the operator $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$. Show that the matrix is hermitian by demonstrating that $p_{n,m} = p_{m,n}^*$. Notice that the "trace" of this matrix, i.e., the sum of its diagonal

terms, is 0. That's a signature of a measurable who's average is 0.

15 pts 3. Use equations 4.27, 4.28, and 4.32 to construct Y_1^0, Y_2^0 , and Y_2^{-2} . Show that they are normalized and orthogonal. Show that they satisfy the differential equation 4.18.

9 pts 4. Consider
$$u(r) = Arj_2(kr)$$
.

5 pts a. Show that it satisfies the differential equation 4.41 with *I*=2.

2 pts b. Make a plot of this function.

1 pt c. Where is the first place the function goes to zero where *x*>0?

1 pt d. What is *n*? What does this mean for *k*? What is the energy in terms of \hbar , *m*, and *a*?

 6 pts
 5. Computational: Create a version of your Discrete, time-independent program to find the Angular components of the wave function in spherical coordinates and modify it to find the Radial components of the wave function for an infinite spherical well. See Handout. 5 pts 6. Normalize R_{32} : $R_{32} = A(\frac{r}{a})^2 e^{-\frac{r}{3a}}$. With it, construct ψ_{32-1} .

- a. Find<r> and <r²> for an electron in hydrogen's ψ_{200} state.
- b. Find $\langle x \rangle$ and $\langle x^2 \rangle$ for the same state. *Hint:* This requires no new integration note that $r^2 = x^2 + y^2 + z^2$, and exploit the rotational symmetry of the state.
- c. Find $\langle x^2 \rangle$ for an electron in hydrogen's ψ_{211} state. *Warning:* This state is *not* symmetrical in *x*, *y*, *z*. Use $x = r \sin \theta \cos \phi$.

Daily 9.W Wednesday 11/2 Griffiths 4. 3 Angular Momentum

- 1. *Conceptual*: Work out the canonical commutation relations for the components of r and p (eq 4.10). Actually, you can explain instead of doing the math, if you want.
- 2. Conceptual: Prove the following commutator identity: [AB,C]=A[B,C]+[A,C]B.
- 3. *Conceptual*: Why does $[yp_z, x_p_z]=0$? Explain. Why does $[yp_z, zp_x]=yp_x[p_z, z]$? Why can y and p_x come out of the commutator?
- 4. Conceptual: For each equation from 4.103 through 4.118, write down whether that equation is: A result of something earlier (if so, state what), or an assumption, or a guess he's trying to prove. Which of these equations proves that L_{\pm} are ladder operators? Example: 4.103 is a

direct result of the definition of the *r* and *p* operators.

- 5. *Math*: Griffiths 4.21
- 6. *Conceptual*: Griffiths 4.22 (a) only

Ready to Start Weekly HW: Griffiths problem 4.19

Hints: if you keep L_z intact in part c (rather than substituting $xp_y - yp_x$) you can quickly get your relations in terms of the commutators you'd found in part a, and so just plug those results in. For part d, you'll need to argue that the results you'd found for L_z generalize to L_x and L_y .

Ready to Start Weekly HW: Apply the raising operator to the expression for Y_3^0 (given in table 4.3) to derive the expression for Y_3^1 . Use equation 4.121 to find the normalization constant.

Daily 9.F Friday 11/4 Griffiths 4. 4.1-.4.2 Spin ½ and Magnetic Fields (Q5.5, 6.1-.2, 8.5)

- 1. *Conceptual*: Find the eigenvectors in Table Q6.1 in Griffiths. Give equation numbers.
- 2. *Conceptual*: Q5S.3 AND Q5R.1 of Moore's Unit Q (note: SG(- θ) means SG(ϕ) where ϕ =- θ , rather than simply switching which output is + and which is -)
- 3. *Math*: Using the eigenvectors in Table Q6.1,
 - a. Calculate the probability of measuring up and down in an SGy device if the particles entering the device are in |+x>.
 - b. Calculate the probability of measuring up and down in an SG θ device if the particles entering the device are in |+y>.

Ready to Start Weekly HW: An electron is in the spin state

$$\chi = A \begin{pmatrix} 2i \\ 5 \end{pmatrix}.$$

- c. Determine the normalization constant A.
- d. Find the expectation values of S_{x} , S_{y} , and S_{z} .
- e. Find the "uncertainties" σ_{s_x} , σ_{s_y} , and σ_{s_z} . (Note: These sigmas are standard deviations, not Pauli matrices!)
- f. Confirm that your results are consistent with all three uncertainty principles (Equation 4.100 and its cyclic permutations only with *S* in place of *L*, of course).

Ready to Start Weekly HW: Construct the spin matrices (S_x , S_y , and S_z) for a particle of spin 3/2. *Hint:* How many eigenstates of S_z are there? Determine the action of S_z , S_+ and S_- on each of these states. Follow the procedure used in the txt for spin $\frac{1}{2}$.

Homework Week 10

Daily 10.M Monday 11/7 Griffiths 4.4.3 Addition of Angular Momenta

- 1. *Conceptual*: With 2 spin-1/2 particles, what are the possible results of a measurement of spin for the entire system?
- 2. *Conceptual*: If we take 2 spin-1/2 particles in combined state |1 1> and measure the spin of ONE of the particles, only, what are the possible results of a measurement and what are the probabilities? What if the combined system was |1 0>?
- 3. *Conceptual*: Say you have 2 particles, one with spin 1 and the other with spin ½. You measure the total spin of the system to be 3/2 and the z-component to be -1/2. What are the possible results of measuring each individual particle's z-component of spin and what are the probabilities?
- 4. *Conceptual*: Say we have 2 particles, one is in state |3/2 -3/2> and the other in state |½ ½>. What are the possible states of the combined system of these 2 particles and what is the probability of measuring each?
- 5. *Math*:
 - a. Apply $S_{\rm to} \ket{10}$ (Equation 4.177), and confirm that you get $\sqrt{2}\hbar |1\!-\!1
 angle$.
 - b. Apply S_{\pm} to $|00\rangle$ (Equation 4.178), and confirm that you get zero.

Ready to S	tart Weekly HW:
	Show that $ig 11ig angle$ and $ig 1\!-\!1ig angle$ (Equation 4.177) are eigenstates of S^{2} with the appropriate
	eigenvalues
Ready to S	tart Weekly HW:
a.	A particle of spin 1 and a particle of spin 3/2 are at rest in a configuration such that the
i i	total spin is 3/2 and its z component is $rac{1}{2}\hbar$. If you measured the z component of the
	angular momentum of the spin-3/2 particle, what values might you get, and what is the probability of each one?
b.	An electron with spin up is in the state ${\psi}_{\scriptscriptstyle 511}$ of the hydrogen atom. If you could
	measure the total angular momentum squared of the electron alone (<i>not</i> including the proton spin), what values might you get, and what is the probability of each?

60 pts Weekly: 10 Tuesday 11/8 Griffiths 4.3-.4

- 18 pts1. Griffiths problem 4.19; see hint in Daily 9.W.
- ⁵ pts 2. Apply the raising operator to the expression for Y_3^0 (given in table 4.3) to derive the expression

for Y_3^1 . Use equation 4.121 to find the normalization constant.

16 pts4. An electron is in the spin state

$$\chi = A \begin{pmatrix} 2i \\ 5 \end{pmatrix}$$

4 pts a. Determine the normalization constant A.

- 4 pts b. Find the expectation values of S_{xy} S_{yy} and S_{z} .
- 4 pts c. Find the "uncertainties" σ_{s_x} , σ_{s_y} , and σ_{s_z} . (Note: These sigmas are standard deviations, not Pauli matrices!)
- 4 pts d. Confirm that your results are consistent with all three uncertainty principles (Equation 4.100 and its cyclic permutations only with S in place of L, of course).
- 7 pts 3. Construct the spin matrices $(S_x, S_y, \text{ and } S_z)$ for a particle of spin 3/2. *Hint:* How many eigenstates of S_z are there? Determine the action of S_z , S_+ and S_- on each of these states. Follow the procedure used in the txt for spin $\frac{1}{2}$.
- ⁵ pts₄. Show that $|11\rangle$ and $|1-1\rangle$ (Equation 4.177) are eigenstates of S^2 with the appropriate eigenvalues.

5 pts 5.

- a. A particle of spin 1 and a particle of spin 3/2 are at rest in a configuration such that the total spin is 3/2 and its z component is $\frac{1}{2}\hbar$. If you measured the z component of the angular momentum of the spin-3/2 particle, what values might you get, and what is the probability of each one?
- b. An electron with spin up is in the state ψ_{511} of the hydrogen atom. If you could measure the total angular momentum squared of the electron alone (*not* including the proton spin), what values might you get, and what is the probability of each?

Daily 11.M Monday 11/14 Griffiths 5.1 Identical Particles: 2-Particle Systems (Q8.6, 11.5)

- 1. *Conceptual*: List several properties of bosons vs. fermions.
- 2. *Conceptual*: Explain, using Quantum Mechanics, the source of the covalent bond.

Ready to S	tart Weekly HW:
a.	If ψ_a and ψ_b are orthogonal, and both normalized, what is the constant A in Equation
	5.10 such that ψ_+ are normalized? Note: you can probably guess it, but actually set up
	the inner products to solve for it. Hint: though you're really solving for two cases, + or - you can do the math just once using \pm , and you'll see that the term with \pm vanishes regardless.
b.	If $\psi_a = \psi_b$ and is normalized, what is A? (This case, of course, occurs only for bosons.)
Ready to S in state n t	<i>tart Weekly HW</i> : Say you had two particles in a simple harmonic oscillator potential, one he other in state <i>m</i> . What would be their average separation if
<i>Ready to S</i> in state <i>n</i> t c.	<i>tart Weekly HW</i> : Say you had two particles in a simple harmonic oscillator potential, one he other in state <i>m</i> . What would be their average separation if They were distinguishable particles
<i>Ready to S</i> in state <i>n</i> t c. d.	tart Weekly HW: Say you had two particles in a simple harmonic oscillator potential, one he other in state <i>m</i> . What would be their average separation if They were distinguishable particles They were Fermions (neglecting the spin degree of freedom)
Ready to S in state n t c. d. e.	tart Weekly HW: Say you had two particles in a simple harmonic oscillator potential, one he other in state <i>m</i> . What would be their average separation if They were distinguishable particles They were Fermions (neglecting the spin degree of freedom) They were Bosons (again, neglecting the spin degree of freedom)
Ready to S in state n t c. d. e. Hin	tart Weekly HW: Say you had two particles in a simple harmonic oscillator potential, one he other in state <i>m</i> . What would be their average separation if They were distinguishable particles They were Fermions (neglecting the spin degree of freedom) They were Bosons (again, neglecting the spin degree of freedom) nt: You shouldn't have to actually <i>do</i> any integrals if you recall that $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_+ + \hat{a})$

Daily 11.W Wednesday 11/16 Griffiths 5.2 Atoms (Q9.2)

- 1. Conceptual: Why must the Helium ground state include antisymmetric spin?
- 2. Conceptual: Explain parahelium and orthohelium. Which is the ground state?
- 3. Conceptual: Griffiths 5.12

Ready to Start Weekly HW: Say you have a helium atom in which one electron, call it *a*, has been excited to the n = 2 level and the other, call it *b*, has been excited to the n=3 level. This clearly isn't a stable situation. Say electron *b* falls to the n = 1 level; if all that energy went into kicking electron *a*, it would be ejected – what would electron *a*'s kinetic energy be after it leaves the atom?

Ready to Start Weekly HW: For the lone electron left in a doubly-ionized lithium atom, the available energy levels would be the same as in the hydrogen atom, with the key difference that Z = 3. What would be the equivalent of the Bohr radius, a_{Li} for this ion? How would the spectrum of this ion differ from that of Hydrogen; specifically, how would equation 4.93 be changed?

21 pts Weekly: 11 Thursday 11/17 Griffiths 5.1-.2

5 pts 1.

- a. If ψ_a and ψ_b are orthogonal, and both normalized, what is the constant A in Equation 5.10 such that ψ_{\pm} are normalized? Note: you can probably guess it, but actually set up the inner products to solve for it. Hint: though you're really solving for two cases, + or -, you can do the math just once using \pm , and you'll see that the term with \pm vanishes regardless.
- b. If $\psi_a = \psi_b$ and is normalized, what is A? (This case, of course, occurs only for bosons.)

10 pts 2. Say you had two particles in a simple harmonic oscillator potential, one in state *n* the other in state *m*. What would be their average separation if

- f. They were distinguishable particles
- g. They were Fermions (neglecting the spin degree of freedom)
- h. They were Bosons (again, neglecting the spin degree of freedom)

Hint: You shouldn't have to actually *do* any integrals if you recall that $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_+ + \hat{a}_-)$ and equations 2.66 tell you the result of the raising and lowering operators operating on a wavefunction. In fact, you should find that, in some old, chapter 2 homework you've already solved most of the key integrals.

- 3 pts 3. Say you have a helium atom in which one electron, call it *a*, has been excited to the n = 2 level and the other, call it *b*, has been excited to the n=3 level. This clearly isn't a stable situation. Say electron *b* falls to the n = 1 level; if all that energy went into kicking electron *a*, it would be ejected what would electron *a*'s kinetic energy be after it leaves the atom?
- 3 pts 4. For the lone electron left in a doubly-ionized lithium atom, the available energy levels would be the same as in the hydrogen atom, with the key difference that Z = 3. What would be the equivalent of the Bohr radius, a_{Li} for this ion? How would the spectrum of this ion differ from that of Hydrogen; specifically, how would equation 4.93 be changed?

Daily 11.F Friday 11/18 Griffiths 5.3 Solids

1. Math: Griffiths 5.15

Ready to Start Weekly HW, Computational: To see how the strength of the potential effects the width of allowed bands and forbidden gaps, use Python or another language (but *don't* just draw it by hand) to plot equation 5.66 for $\beta = 01., 1, 10, 100$. Remember, the allowed states only exist for $-1 \le f(z) \le 1$. For sample plotting code, see the "computational" page on Dr. DeWeerd's website.

Ready to Start Weekly HW: The density of gold is 91.3 gm/cm³, and its atomic mass is 197 gm/mole.

- a. Calculate the Fermi energy for gold (Equation 5.43). Assume q = 1, and give your answer in electron volts.
- b. What is the corresponding electron velocity? *Hint:* Set $E_F = \frac{1}{2} mv^2$. Is it safe to assume that electrons in gold are nonrelativistic?
- c. At what temperature would the characteristic thermal energy (k_BT , where k_B is the Boltzmann constant and T is the Kelvin temperature) equal the Fermi energy, for gold?
- d. Calculate the degeneracy pressure (Equation 5.46) of gold, in the electron gas model.

Ready to Start Weekly HW:

i. Using Equations 5.59 and 5.63, show that the wave function for a particle in the periodic delta function potential can be written in the form

 $\psi(x) = C\left[\sin(kx) + e^{-iKa}\sin(k(a-x))\right], \quad \text{for} \quad 0 \le x \le a \,.$

Express the constant C in terms of B of equations 5.59 and 5.63. Hint: You'll need to use a trig identity.

j. There is an exception: At the top of a band, where z (that is, ka, as defined in Equation 5.65) is an integer multiple of π (Figure 5.6), the approach of (a) erroneously yields $\psi(x) = 0$. Find the correct wave function for this case and note what happens to it at the location of each delta function. Hint: If you apply the condition that $z = ka = n\pi$ to Equation 5.61, you'll learn something about what e^{-iKa} must be at the top of a band. Then applying this condition to Equation 5.62 tells you what B must be, so then you can see what becomes of Equation 5.59 for the top-of-the-gap state.

Homework Week 12

Daily 12.M Monday 11/21 Griffiths 8.1-.2 WKB Approximation & Tunneling

- 1. Conceptual: Compare the following equations and comment on the similarities and differences:
 - c. 8.13 and 2.149
 - d. 8.15 and 2.26
 - e. 8.17, 8.10 and 2.150
 - f. Based on this, how would you describe the WKB approximation and how it differs from the exact solutions in chapter 2.
- 2. *Math*: Write equation 8.16 in terms of Energy by using equation 8.2. Explain how this is used to calculate the Energy.

Ready to Start Weekly HW: Use the WKB approximation to find the allowed energies (E_n) of an infinite square well with a "shelf", of height V₀ extending a third of the way across (like figure 6.3, but the shelf is only $1/3^{rd}$ the well's width):

$$V(x) = \begin{cases} V_0, & \text{if } 0 < x < a/3\\ 0, & \text{if } a/3 < x < a\\ \infty, & \text{otherwise} \end{cases}$$

Express your answer in terms of V₀ and $E_n^0 \equiv (n\pi\hbar)^2 / 2ma^2$ (the *n*th allowed energy for the infinite square well with *no* shelf). Assume that $E_1^0 > V_0$, but do *not* assume that $E_n >> V_0$.

Ready to Start Weekly HW: Consider an electron tunneling between two charged capacitor plates. The energy situation is illustrated below.



You may recall from the photo-electric effect, that the energy it would take to free an electron from a metal plate is known as the plate's "work function", W_f . Thanks to the uniform electric field between the two charged plate, the potential energy varies linearly across the gap, as illustrated (sorry about the confusing notation but while V(x) means 'energy', ΔV means voltage.)

- a. Formulate an approximate expression (according to eq'n 8.22) for the transmission coefficient for an electron to tunnel from one plat to the other.
- b. If you imagine replacing one of the plates of the capacitor with a sharp metal tip and bringing it *very* close to the other plate, you've got the basic setup of a Scanning Tunneling Microscope (STM) which relies on the transmission coefficient's extreme sensitivity to the separation, *a*. To get an idea of how sensitive it is, here are some typical values: W = 4 eV, $\Delta V = 1.5$ Volts, and $a = 8 \times 10^{-10}$ m. By what factor does the transmission coefficient change if the separation changes from $a = 8 \times 10^{-10}$ m to $a = 8 \times 10^{-10}$ m to

8.5×10⁻¹⁰m, that is, what's
$$\frac{T_{a=8\times10^{-10}m}}{T_{a=8.5\times10^{-10}m}}$$
 ?

45 pts Weekly 12 Tuesday 11/22 Griffiths 5.3, 8.1-2

10 pts 1. The density of gold is 91.3 gm/cm³, and its atomic mass is 197 gm/mole.

- a. Calculate the Fermi energy for gold (Equation 5.43). Assume q = 1, and give your answer in electron volts.
- b. What is the corresponding electron velocity? *Hint:* Set $E_F = \frac{1}{2} mv^2$. Is it safe to assume that electrons in gold are nonrelativistic?
- c. At what temperature would the characteristic thermal energy (k_BT , where k_B is the Boltzmann constant and T is the Kelvin temperature) equal the Fermi energy, for gold?
- d. Calculate the degeneracy pressure (Equation 5.46) of gold, in the electron gas model.
- 10 pts 2. To see how the strength of the potential effects the width of allowed bands and forbidden gaps, use Python or another language (but *don't* just draw it by hand) to plot equation 5.66 for $\beta = 0.1, 1, 10, 100$. Remember, the allowed states only exist for $-1 \le f(z) \le 1$. For sample plotting code, see the "computational" page on Dr. DeWeerd's website.

10 pts 3.

a. Using Equations 5.59 and 5.63, show that the wave function for a particle in the periodic delta function potential can be written in the form

 $\psi(x) = C\left[\sin(kx) + e^{-iKa}\sin(k(a-x))\right], \quad \text{for} \quad 0 \le x \le a \,.$

Express the constant C in terms of B of equations 5.59 and 5.63. Hint: You'll need to use a trig identity.

- b. There is an exception: At the top of a band, where z (that is, ka, as defined in Equation 5.65) is an integer multiple of π (Figure 5.6), the approach of (a) erroneously yields $\psi(x) = 0$. Find the correct wave function for this case and note what happens to it at the location of each delta function. Hint: If you apply the condition that $z = ka = n\pi$ to Equation 5.61, you'll learn something about what e^{-iKa} must be at the top of a band. Then applying this condition to Equation 5.62 tells you what B must be, so then you can see what becomes of Equation 5.59 for the top-of-the-gap state.
- 5 pts 3. Use the WKB approximation to find the allowed energies (E_n) of an infinite square well with a "shelf", of height V₀ extending a third of the way across (like figure 6.3, but the shelf is only $1/3^{rd}$ the well's width):

$$V(x) = \begin{cases} V_0, & \text{if } 0 < x < a/3 \\ 0, & \text{if } a/3 < x < a \\ \infty, & \text{otherwise} \end{cases}$$

Express your answer in terms of V₀ and $E_n^0 \equiv (n\pi\hbar)^2 / 2ma^2$ (the *n*th allowed energy for the infinite square well with *no* shelf). Assume that $E_1^0 > V_0$, but do *not* assume that $E_n >> V_0$.





You may recall from the photo-electric effect, that the energy it would take to free an electron from a metal plate is known as the plate's "work function", W_f . Thanks to the uniform electric field between the two charged plate, the potential energy varies linearly across the gap, as illustrated (sorry about the confusing notation but while V(x) means 'energy', ΔV means voltage.)

- a. Formulate an approximate expression (according to eq'n 8.22) for the transmission coefficient for an electron to tunnel from one plat to the other.
- b. If you imagine replacing one of the plates of the capacitor with a sharp metal tip and bringing it *very* close to the other plate, you've got the basic setup of a Scanning Tunneling Microscope (STM) which relies on the transmission coefficient's extreme sensitivity to the separation, *a*. To get an idea of how sensitive it is, here are some typical values: W = 4 eV, $\Delta V = 1.5$ Volts, and $a = 8 \times 10^{-10}$ m. By what factor does the transmission coefficient change if the separation changes from $a = 8 \times 10^{-10}$ m to $a = 8 \times 10^{-10}$ m to

8.5×10⁻¹⁰m, that is, what's
$$\frac{T_{a=8\times10^{-10}m}}{T_{a=8\times10^{-10}m}}$$
?

Daily 13.M Monday 11/28 Griffiths 6.1 Time-independent Perturbations, non-degenerate

- 1. *Conceptual*: What is the point of λ in equation 6.8?
- 2. *Conceptual*: Can we use equation 6.13 to determine wavefunctions for the Helium atom based on a perturbation to a Hydrogen atom? Why or why not?

Ready to Start Weekly HW: Suppose we perturbed the bottom of an infinite square well with $H' = \lambda V_a \sin(\pi x / a)$, where λ is a constant.

- a. Find the first-order correction to the allowed energies.
- b. Find the first three nonzero terms in the expansion (Equation 6.13) of the correction to the ground state, ψ_1^1 .

Ready to Start Weekly HW:

- a. Find the expression for the second-order correction to the energies (E2n) for the potential in Griffiths' problem 6.1. No need to explicitly sum the series.
- b. Consider the scenario of Griffiths' problem 6.2 except if, rather than changing the spring constant, there were slight anharmicity, that is, a κx^3 term in the potential as well as the usual kx^2 term. Calculate the second-order correction to the ground state energy (E_0^2) .

For part b) Hint: You shouldn't have to actually *do* any integrals if you recall that $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a}_+ + \hat{a}_-)$ and equations 2.66 tell you the result of the raising and lowering operators operating on a wavefunction. In fact, you should find that, in some old, chapter 2 homework you've already solved most of the key integrals.

Daily 13.W Wednesday 11/30 Griffiths 6.2 Time-independent Perturbations, degenerate

- 1. Conceptual: In a two-fold degenerate system, generally the perturbation will break the degeneracy. One state will go to a higher energy and an orthogonal state will go to a lower energy. But, these states may not be the same states used in the unperturbed case. Note that there are an infinite number of wavefunctions with the same energy: $\psi = \alpha \psi_a + \beta \psi_b$, where a and b are the 2 wavefunctions in the unperturbed case. If these happed to be the states with the most extreme new energies, what are α and β ?
- 2. *Conceptual*: If the states in the unperturbed case are not the good states, what are their energies in the perturbed system? How do they relate to the energies of the "good" states?

Ready to Start Weekly HW: Griffiths problem 6.7 parts b and c only. Hint: for part c, use equation 6.22.

Ready to Start Weekly HW: Consider a quantum system with just *three* linearly independent states. Suppose the Hamiltonina, in matrix form, is

$$\mathbf{H} = V_o \begin{pmatrix} 1 & 0 & 0 \\ 0 & (2 - \varepsilon) & \varepsilon \\ \varepsilon & 0 & 1 \end{pmatrix}$$

Where V_{o} is a constant and ε is some small number (ε <<1).

- a. Write down the eigenvectors and eigensvalues of the *unperturbed* Hamiltonian ($\varepsilon = 0$).
- b. Solve for the *exact* eigenvalues of **H**. Expand each of them as a power series in ε , up to second order.
- c. Use first- and second-order *non*degenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the nondegenerate eigenvector of H^o.
 Compare with the exact result, from (a).
- d. Use *degenerate* perturbation theory to find the first-order correction to the two initially degenerate eigenvalues. Compare with the exact results.

17 pts Weekly 13 Tue	sday 12/1 Griffiths 6.12
7 pts 1. Suppos	e we perturbed the bottom of an infinite square well with $H' = \lambda V_o \sin(\pi x / a)$, where
λ is a c	onstant.
3 pts	a. Find the first-order correction to the allowed energies.
4 pts	b. Find the first three nonzero terms in the expansion (Equation 6.13) of the
	correction to the ground state, ψ_1^1 .
10 pts2.	
5 pts	c. Find the expression for the second-order correction to the energies (E2n) for the potential in Griffiths' problem 6.1. No need to explicitly sum the series.
5 pts	d. Consider the scenario of Griffiths' problem 6.2 except if, rather than changing
	the spring constant, there were slight anharmicity, that is, a ϵkx^3 term in the potential as well as the usual kx^2 term. Calculate the second-order correction to the ground state energy (F_{α}^2).
10 pts 3 Griffith	s problem 6.7 parts b and c only. Hint: for part c, use equation 6.22
20 pts 4. Consid	er a quantum system with just <i>three</i> linearly independent states. Suppose the
Hamilt	onina, in matrix form, is
	$(1 \ 0 \ 0)$
п	$-V \left[\begin{array}{c} 0 & (2 - c) \\ 0 & (2 - c) \\ \end{array} \right]$
п	$= v_o \begin{bmatrix} 0 & (2-\varepsilon) & \varepsilon \end{bmatrix}$
	$\begin{pmatrix} \varepsilon & 0 & 1 \end{pmatrix}$
Wł	ere V_{o} is a constant and ε is some small number (ε <<1).
5 pts a.	Write down the eigenvectors and eigensvalues of the <i>unperturbed</i> Hamiltonian (ϵ = 0).
5 pts b.	Solve for the <i>exact</i> eigenvalues of H . Expand each of them as a power series in ε , up to second order.
5 pts c.	Use first- and second-order <i>non</i> degenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the nondegenerate eigenvector of H° . Compare with the exact result, from (a).
5 pts d.	Use <i>degenerate</i> perturbation theory to find the first-order correction to the two initially degenerate eigenvalues. Compare with the exact results.

Daily 13.F Friday 12/2 Griffiths 6.3 Fine Structure of Hydrogen

- 1. Math: 6.11 a
- 2. *Math:* 6.16

.

Ready to Start Weekly HW: 6.12

a. In the context of the derivation in which this result is used, you can approximate

$$\langle E \rangle \approx \langle E^o \rangle$$

Ready to Start Weekly HW: 6.17

Daily 14.M Monday 12/5 Griffiths 6.4-.5 Hyper-Fine Structure of Hydrogen & Zeeman Effect

1. Math: 6.22

Ready to Start Weekly: Computational / Conceptual: Talking about the Zeeman effect, Griffiths -notes that there are three regimes: when it's far weaker than the relativistic & spin-orbit effects, - - - when it's far greater, and when they're comparable. To get a feel for how perturbations mix, return to the program you'd written and modified for simulating the particle in an infinite square well with a variety of different well bottoms. Two of the bottoms you'd used were sloped and stepped. Define a new potential function which is simply the sum of the sloped and stepped potentials. For example, if you'd defined those as Vslope(j) and Vstep(j), then you'd add the lines

def v(j):

return: a*Vslope(j) +b*Vstep(j)

To get a sense of how these 'perturbations' interact with each other, plot the 15th wavefunction and print out its energy when you have

- a. just the sloped potential: a = 1, b = 0
- b. just the stepped potential: a = 0, b = 1
- c. mostly the sloped potential with a step perturbation: a = 1, b = 0.1
- d. mostly the stepped potential with a sloped perturbation: a = 0.1, b = 1
- e. and equal stepped and sloped potentials: a = b = 1

you should observe that the wavefunction and energy in case c) are only a little different from case a) and for case d) they're only a little different from case b) – suggesting that we could indeed treat the lesser of the potentials as a mere perturbation. However, the wavefunction and energy in case e) should look like an equal mix of the two.

Ready to Start Weekly: Griffiths 6.21

Ready to Start Weekly: Griffiths 6.25

For $\langle \hat{H}'_z \rangle$, using the 2nd term in 6.79 is much less tedious than using 6.75. Similarly, 6.66 is less tedious than 6.82, but you'll need to rephrase the pre-factor yourself (replacing $(E_n)^2$ with $(E_o)^2 / n^4$. The matrix elements are $W_{ij} = -\langle \psi_i | \hat{H}^1 \psi_j \rangle$ for the wavefunctions as enumerated just above the matrix. Ready to Start Weekly: Griffiths 6.28 (for next week)

a. Be careful: eq'n 6.89 gives the correct dependence on m_e an a; equation 6.92's only valid in under the approximation that the reduced mass that should be featured in a, $m_e m_p$ as m_e which is protty good for regular bydrogon, but not so good when you

 $\frac{m_e m_p}{m_e + m_p} \approx m_e$, which is pretty good for regular hydrogen, but not so good when you

start replacing electrons or protons with muons as in this problem.

Daily 14.W Wednesday 12/7 Griffiths 7.1-.2 The Variation Principle: Theory & Helium

1. Math: Griffiths 7.4

Ready to Start Weekly: Griffiths 7.1

Ready to Start Weekly: Griffiths 7.7

```
63 ptsWeekly 14 Tuesday 11/25 Griffiths 6.3-.5, 7.1-.2
   3 pts 1. Griffiths problem 6.12
   5 pts 2. Griffiths problem 6.17
  10 pts 3. Computational / Conceptual: Talking about the Zeeman effect, Griffiths notes that there are
              three regimes: when it's far weaker than the relativistic & spin-orbit effects, when it's far
              greater, and when they're comparable. To get a feel for how perturbations mix, return to the
              program you'd written and modified for simulating the particle in an infinite square well with a
              variety of different well bottoms. Two of the bottoms you'd used were sloped and stepped.
              Define a new potential function which is simply the sum of the sloped and stepped potentials.
              For example, if you'd defined those as Vslope(j) and Vstep(j), then you'd add the lines
                      def v(j):
                              return: a*Vslope(j) +b*Vstep(j)
              To get a sense of how these 'perturbations' interact with each other, plot the 15<sup>th</sup> wavefunction
              and print out its energy when you have
                          f. just the sloped potential: a = 1, b = 0
                          g. just the stepped potential: a = 0, b = 1
                          h. mostly the sloped potential with a step perturbation: a = 1, b = 0.1
                              mostly the stepped potential with a sloped perturbation: a = 0.1, b = 1
                          i.
                              and equal stepped and sloped potentials: a = b = 1
                          j.
              you should observe that the wavefunction and energy in case c) are only a little different from
              case a) and for case d) they're only a little different from case b) – suggesting that we could
              indeed treat the lesser of the potentials as a mere perturbation. However, the wavefunction
              and energy in case e) should look like an equal mix of the two.
  10 pts 4. Griffiths problem 6.21
  10 pts 5. Griffiths problem 6.25
   5 pts 6. Griffiths problem 6.28
  10 pts 7. Griffiths problem 7.1
  10 pts 8. Griffiths problem 7.7
      Daily 14.F Friday 12/9 Griffiths 12.1-.2, Scholosauer 8 EPR and Bell's Theorem
```

- 1. Griffiths 12.1
- Demonstrate that Quantum Mechanics' predictions violate Bell's inequality for the three axes being a = z-axis, b = 30° off the y-axis toward the z-axis, and c = 60° off the y-axis toward the zaxis.
- 3. *Conceptual* : Summarize Scholosauer's 17 participant's main points about Bell's Theorem. What do you find most or least compelling?