

Due Thursday, Feb. 9.

### 1. Commutators

Recall that an *operator* is an instruction to *do something* with the function that follows, in general producing a new function. Here we *define* a new operator  $\hat{\alpha} \equiv \hat{x}\hat{p}_x$ , where  $\hat{x}$  is the position operator and  $\hat{p}_x$  is the operator for momentum along the  $x$  direction. Since we will work in coordinate space in the variable  $x$ , we have the following representations for these two operators:

$$\hat{x} = x$$

$$\hat{p}_x = -i\hbar \frac{d}{dx}.$$

In this problem, we'll first want to evaluate  $\hat{\alpha}\psi(x)$ , where  $\psi(x) = De^{-x^2/w^2}$  ( $D, w$  are constants). So, we'd write

$$\hat{\alpha}\psi(x) = \hat{x}\hat{p}_x De^{-x^2/w^2}.$$

This is evaluated by starting with the operator farthest to the *right*: first,  $\hat{p}_x = -i\hbar \frac{d}{dx}$  operates on  $\psi(x)$ . Then  $\hat{x} = x$  operates on that new result via simple multiplication of the position variable  $x$ .

- (a) Using the above definitions, evaluate  $\hat{\alpha}\psi(x)$ . Is  $\psi(x)$  an eigenfunction of  $\hat{\alpha}$ ?
- (b) Assume another new operator is defined:  $\hat{\beta} \equiv \hat{p}_x\hat{x}$ . Evaluate  $\hat{\beta}\psi(x)$ . Remember that order of operation matters, and you must take the derivative *after* multiplying by  $x$ . Is  $\psi(x)$  an eigenfunction of  $\hat{\beta}$ ?
- (c) We'll now define *yet another* operator:  $\hat{C} \equiv \hat{x}\hat{p}_x - \hat{p}_x\hat{x}$ . Evaluate  $\hat{C}\psi(x)$ , and simplify your answer as much as possible. [Hint:  $(\hat{\alpha} - \hat{\beta})\psi(x) = \hat{\alpha}\psi(x) - \hat{\beta}\psi(x)$ .]
- (d) You should now see that  $\Psi(x)$  is an eigenfunction of  $\hat{C}$ . (If not, you should find your mistakes.) What is the eigenvalue?

There is another way to write  $\hat{C}$ :  $\hat{C} = [\hat{x}, \hat{p}_x] \equiv \hat{x}\hat{p}_x - \hat{p}_x\hat{x}$ . This quantity with the square brackets is called the *commutator of  $\hat{x}$  and  $\hat{p}_x$* , and although it may look a bit funny, it *is* an operator. More generally, for *any* two operators  $\hat{A}$  and  $\hat{B}$ , the *commutator of  $\hat{A}$  and  $\hat{B}$*  is

$$[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}.$$

If  $[\hat{A}, \hat{B}] = 0$  (i.e., for any physical wavefunction  $\Psi$ , if  $\hat{A}\hat{B}\Psi = \hat{B}\hat{A}\Psi$ ) we say that the operators  $\hat{A}$  and  $\hat{B}$  *commute*. Otherwise they do not commute. (Recall the algebraic property of commutation of two variables  $u$  and  $v$ :  $uv = vu$ .)

- (e) Prove that *any* function  $f(x)$  is an eigenfunction of  $[\hat{x}, \hat{p}_x]$ , and thus we can write the equality  $[\hat{x}, \hat{p}_x] = \text{const.}$ , with the constant being the eigenvalue from part (d) above.
- (f) Prove the identity  $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$  for any three operators  $\hat{A}$ ,  $\hat{B}$ , and  $\hat{C}$ .

## 2. Heisenberg's Uncertainty Principle revisited

We have previously encountered the Heisenberg Uncertainty Principle (HUP) in the form  $\sigma_A\sigma_B \geq \hbar/2$ , where  $\sigma_A$  and  $\sigma_B$  are standard deviations for conjugate variables  $A$  and  $B$ . We encountered the specific example of  $x$  and  $p_x$ . Here we restate the HUP in more general terms. The HUP is formally stated as follows:

**For any two physical quantities (observables)  $A$  and  $B$  and their associated linear operators  $\hat{A}$  and  $\hat{B}$ ,**

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

This statement makes use of the commutator defined in the previous problem.

(a) Restate the HUP above for position and momentum observables  $x$  and  $p_x$ . Making use of your answers from the previous problem, evaluate this expression and arrive at the HUP in the form for  $x$  and  $p_x$  that was discussed in class. You should notice that the expectation value of a constant is equal to that same constant, even if that constant is imaginary (and hence not representative of a physical observable such as position or momentum.)

(b) When we're working with the time dependence of a quantum state, we can associate the total energy  $E$  of the state with an operator equivalent  $i\hbar\frac{d}{dt}$ . In other words, we can say  $\hat{E} = i\hbar\frac{d}{dt}$ . (This is not the usual operator equivalent of energy, but we'll use it here.) Here you will evaluate  $[\hat{E}, \hat{t}]$  for any stationary state, using  $\hat{t} = t$  as the operator for time. As mentioned in class, we generally have to be careful when working with time in quantum mechanics, as it's not always straightforward to interpret what we're doing! For the moment though, pretend like you can use  $\hat{t} = t$  as an operator for time without having to worry about it.

To do this problem, you will need to know that any stationary-state wavefunction can be expressed in the form  $\Psi(\vec{x}, t) = \psi(\vec{x})e^{-iE_c t/\hbar}$ . Treat  $E_c$  as a constant. Notice that the probability density  $|\Psi(x, t)|^2$  is time independent, even though  $\Psi(x, t)$  does have time dependence. Now evaluate  $[\hat{E}, \hat{t}]$ , simplify as much as possible, and conclude this part of the problem by stating the HUP for energy and time. While it might not yet make sense to have an uncertainty relationship between  $E$  and  $t$ , for now we will just interpret this relationship as stating that there are limitations on how well the energy difference between two quantum states can be specified, and that those limitations depend on the time available for a measurement (i.e., how long an atom stays in an excited state before it decays). We will return to this concept later in the course when we discuss the natural lifetime of atoms and spontaneous emission of radiation: the natural lifetime of an excited atomic state (a time) is inversely proportional to the natural linewidth (an energy or a frequency) of the atomic transition.

(c) Consider an arbitrary 3-dimensional stationary-state wavefunction of the form  $f(x, y, z)e^{-iEt/\hbar}$ . Evaluate  $[\hat{y}, \hat{p}_x]$  (first try to guess the answer). Notice the subscript on  $p$ , and let  $\hat{y} = y$ . Do  $y$  and  $p_x$  commute? Is there a limitation to simultaneous minimization of uncertainties in  $y$  and  $p_x$ ?

### 3. Dirac notation

This problem is an exercise in using a new type of notation that we will call Dirac ‘bra-ket’ notation. You will encounter some symbols and mathematical statements that you may not recognize or know how to interpret. If this bothers you, don’t worry about interpretation at the moment; this question is more about building familiarity with new symbols. The basic idea is this: we know that for a particular quantum state, there are different ways of providing a written description for the state. For example, a wavefunction might be written as a function of spatial coordinates [say  $\psi(x)$ ], or as a function of momentum coordinates [say  $\phi(p_x)$ ]; they expressions will look different (such as on pages 36 and 37 of the notes), but both represent the same physical state with the same amount of information. Any quantity such as expectation values of  $x$  or  $p_x$  that can be obtained from one can also be obtained from the other. What we want now are more abstract symbols and a new mathematical formalism that allow us to work with the generalized concept of a quantum state, and to not worry about the specific representation as a function over specific variables. Dirac notation gives us this flexibility. It will be extremely useful when we start dealing with quantum states that depend on new concepts that simply can not be represented as functions, or when we have to keep track of many different pieces of information.

To become familiar with Dirac notation formalism, read Appendix F of the class notes. If the concepts still seem vague and you feel totally lost, read Griffiths pp. 118-124 (second edition).

For this problem, fill in the right hand side of the table on the following page (include this page with the rest of your homework, or if you want, recopy the table on your own paper). For each expression given in *wavefunction* notation (either in position space or momentum space), write the more generalized expression in *Dirac* notation. **Note that there is nothing to solve or compute in this problem!** This is just a short exercise in translating between different “languages” of quantum mechanics. Remember that *order matters*, and that Dirac notation does *not* specify  $x$  or  $p$  space. In other words, the variables  $x$  and  $p$  will not appear anywhere on the right-hand column. The labels that do appear in Dirac notation are usually just quantum numbers associated with the quantum state.

Assume the following:

(1)  $\psi$  represents an arbitrary normalized wavefunction, either in momentum coordinates  $\psi(p)$  or spatial coordinates  $\psi(x)$ , in one dimension only. (Don’t worry that we usually might use  $\phi(p)$  as a momentum-space wavefunction.) Remember that  $\psi(x)$  and  $\psi(p)$  are two different ways of expressing information about a particular quantum state. In Dirac notation, the basis (coordinate space or momentum space) does not need to be specified, and we instead use a more generalized notation for a quantum state. In that sense, Dirac notation is kind of like a variable in algebra: it’s a placeholder for some other information that can be inserted later, but we can still work with the symbols in order to represent concepts.

(2)  $\phi_n$  represents the  $n^{\text{th}}$  stationary state (eigenstate) of an arbitrary potential well. As an example, the state on page 18 of the notes is the  $3^{\text{rd}}$  stationary state of the 1D box potential.

(3) Lowercase letters  $a, b, c$  are constants,  $q$  is an eigenvalue, and  $m, n$  label eigenstates.

(4) Integrals span all available values ( $-\infty$  to  $+\infty$ ). A full ‘bra-ket,’ as in the  $4^{\text{th}}$  example on the next page, denotes integration.

A few examples of equivalent expressions are given at the top of the table; you should fill in the blank boxes.

Wavefunction Representation	Dirac notation
Either $\psi(x)$ or $\psi(p)$	$ \psi\rangle$
Either $\psi^*(x)$ or $\psi^*(p)$	$\langle\psi $
$\phi_n(x)$	$ \phi_n\rangle$
$\int \psi^*(x)\psi(x)dx = 1$	$\langle\psi \psi\rangle = 1$
$\hat{H}\phi_n(x) = E_n\phi_n(x)$	$\hat{H} \phi_n\rangle = E_n \phi_n\rangle$
$\hat{Q}\psi(x)$	$ \hat{Q}\psi\rangle$ or $\hat{Q} \psi\rangle$
$\psi(p)$	
$(a + b)\psi(x) = a\psi(x) + b\psi(x)$	
$\psi(x) = \frac{1}{\sqrt{2}}(\psi_1(x) + \psi_2(x))$	
$\int \phi_m^*(x)\phi_n(x)dx = \delta_{mn}$	
$\langle x \rangle = \int \psi^*(x)x\psi(x)dx$	
$\psi(x) = \sum_n \phi_n(x)c_n$	
$\int \phi_m^*(x)\psi(x)dx = \sum_n c_n \int \phi_m^*(x)\phi_n(x)$	
$c_m = \int \phi_m^*(x)\psi(x)dx$	
$\psi(x) = \sum_n \phi_n(x) \int \phi_n^*(x)\psi(x)dx$	(also see eqs. 3.118, 3.119 p. 71)
Proof: the eigenvalues of Hermitian operators are real	Write the same steps of the proof in Dirac notation below
Line A. Definition of an Hermitian operator $\hat{Q}$ : $\int (\hat{Q}\psi_a(x))^*\psi_b(x)dx = \int \psi_a^*(x)(\hat{Q}\psi_b(x))dx$	
Line B. Given: $\hat{Q}\psi_n(x) = q_n\psi_n(x)$	
Line C. $\int \psi_n^*(x)(\hat{Q}\psi_n(x))dx = \int \psi_n^*(x)(q_n\psi_n(x))dx$	
$= q_n \int \psi_n^*(x)\psi_n(x)dx$	
$= q_n$	
Line D. Similarly: $\int (\hat{Q}\psi_n(x))^*\psi_n(x)dx = \int (q_n\psi_n(x))^*\psi_n(x)dx$	
$= q_n^* \int \psi_n^*(x)\psi_n(x)dx$	
$= q_n^*$	
By the property on line A, lines C and D are equal.	Thus $q_n$ and $q_n^*$ are equal and the eigenvalue is real

#### 4. Practice with QM formalism and postulates

In this problem, you're working with an unspecified operator  $\hat{Q}$ , which is linear and Hermitian (see the definition on the Dirac notation worksheet from the previous problem), with eigenvalues  $q_n$  and orthonormal eigenstates  $|\phi_n\rangle$  (so that  $\langle\phi_m|\phi_n\rangle = \delta_{mn}$ ). Or more simply,

$$\hat{Q}|\phi_n\rangle = q_n|\phi_n\rangle,$$

where  $n$  is allowed to be any non-negative integer.  $\hat{Q}$  is an operator that represents an observable  $Q$ .

(a) Suppose a quantum state  $|\psi\rangle$  is written as a superposition of the eigenstates. Specifically, let

$$|\psi\rangle = (i/\sqrt{3})|\phi_0\rangle + (-1/\sqrt{3})|\phi_1\rangle + a_2|\phi_2\rangle,$$

and therefore  $\langle\psi| = (-i/\sqrt{3})\langle\phi_0| + (-1/\sqrt{3})\langle\phi_1| + a_2^*\langle\phi_2|$ ,

where  $a_2$  is a unitless and generally complex number. By evaluating  $\langle\psi|\psi\rangle$  (*which must be equal to what?*), give a **few** possible allowed values for  $a_2$ .

(b) For this particular quantum state  $|\psi\rangle$ , what are the possible results of a measurement of the observable  $Q$ ? (If you're not sure, reread the QM postulates).

(c) What is  $\langle Q \rangle$  in terms of the eigenvalues  $q_n$  for the state  $|\psi\rangle$  given above?

(d) Define a new quantum state to use in the rest of this problem:

$$|\psi\rangle = \sum_{n=0}^{\infty} c_n|\phi_n\rangle,$$

at some instant in time, where the complex expansion coefficients  $c_n$  are unspecified but time-independent. *Any* physically realizable state that can exist in the space spanned by the eigenstates  $|\phi_n\rangle$  can be represented by such a superposition. Give the value for the following summation (*if you're not sure what to do, try to normalize  $|\psi\rangle$* ).

$$\sum_{n=0}^{\infty} |c_n|^2.$$

(e) Evaluate  $\langle Q \rangle$  in terms of the constants  $c_n$  and  $q_n$ , where  $\hat{Q}$  is the operator defined at the beginning of this problem. **Make sure you understand the difference between what  $c_n$  and  $q_n$  represent!**

(f) Suppose we let the unspecified operator  $\hat{Q}$  be replaced with the energy operator  $\hat{H}$ , the Hamiltonian appropriate for our arbitrary system, so that we have the energy eigenvalue equations  $\hat{H}|\phi_n\rangle = E_n|\phi_n\rangle$ , where  $E_n$  are energy eigenvalues. Suppose also that the energy eigenvalues are given by  $E_n = \epsilon(n + 1/2)$ , where  $\epsilon$  is a constant with units of energy and  $n$  is any non-negative integer. With  $|\psi\rangle$  the same state as defined in part (d), evaluate  $\langle H \rangle$ , the expectation value of energy, in terms of  $c_n$  and  $\epsilon$ .

(g) What is the smallest value of energy that can be obtained in any energy measurement on any state  $|\psi\rangle$ ? (This may be a simple question, but it lies at the heart of a powerful technique in quantum mechanics: the “variational principle”, which is used for estimating ground state energy eigenvalues and eigenfunctions when the Time Independent Schrödinger Equation is too hard to solve analytically.)

(h) If the eigenvalue  $E_3$  is obtained in an energy measurement of the state  $|\psi\rangle$ , what is the new “collapsed” quantum state of the system? (If you're not sure, reread the QM postulates.)

## 5. Double square well

(modified from Griffiths, problem 2.44). This is a strictly *qualitative* problem. No calculations allowed! (*Also note: if you have an unsanctioned copy of the Griffiths answer key, the answer to this problem is wrong!*) Consider the time-independent “finite double square well” potential shown in the following figure, and **treat it as a single potential well that just so happens to have a central barrier, rather than as two separate wells**:

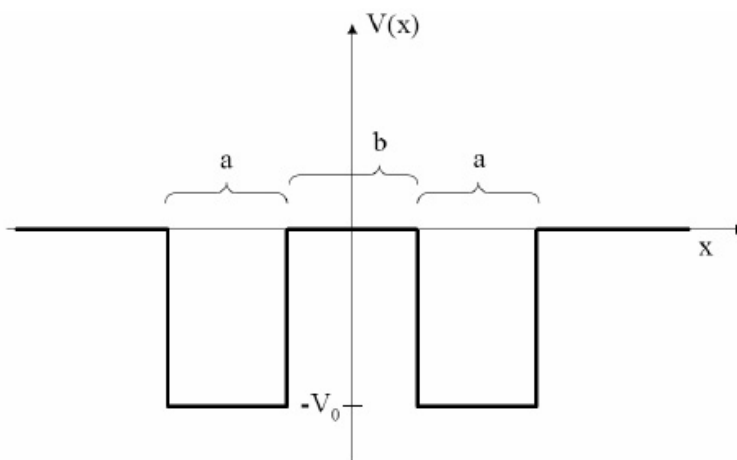


Figure 1: The double square well potential.

(a) Suppose the depth  $V_0$  and the width  $a$  are fixed, and both are large enough that several bound states occur in the overall potential. Sketch the potential  $V(x)$ , the accompanying ground state wave function  $\psi_1$ , and the first excited state wave function  $\psi_2$  for each of the following cases: (i)  $b = 0$  (a single larger square well), (ii)  $0 < b \ll a$ , (iii)  $b \approx a$ , and (iv)  $b \gg a$ . Be sure you label *all* of your axes, and indicate what each sketch refers to. *Important:* Again, you must consider the two smaller wells as merely different spatial regions of a *single potential* that just happens to have two symmetric finite square wells. More specifically, recall how many nodes the ground and first excited state eigenfunctions of an arbitrary potential well should have, and then make sure your sketches reflect this rule, keeping in mind that you’re dealing with one large potential well.

(b) *Qualitatively*, how do the corresponding eigenstate energies ( $E_1$  and  $E_2$ ) vary as  $b$  goes from 0 to  $\infty$ ? Show the dependence by sketching  $E_1(b)$  and  $E_2(b)$  on the same graph. (You can get an idea of the energy trends as  $b$  increases by considering the *wavelength* trends as  $b$  increases. Look in the classically allowed regions — the wavelength is represented by the degree of curvature of the wave function. Sharper curvature means shorter wavelength, thus higher kinetic energy.)

## 6. Harmonic Oscillator

Consider a particle of mass  $m$  in a 1-dimensional time independent quantum harmonic potential of the form  $V(x) = \frac{1}{2}m\omega^2x^2$ . Suppose the wavefunction for the particle is given by:

$$\Psi(x, t) = A \cdot e^{-\frac{m\omega}{2\hbar} [x^2 + \frac{a^2}{2}(1+e^{-i2\omega t}) - 2axe^{-i\omega t}]} \cdot e^{-i\frac{\omega}{2}t}$$

where  $a$  is a real constant and the normalization coefficient  $A = (\frac{m\omega}{\pi\hbar})^{1/4}$ .

- (a) Show that  $\Psi(x, t)$  is a solution to the *time-dependent* Schrodinger equation.
  
- (b) Plot  $\Psi(x, 0)$ . How does this compare to the ground state wavefunction of the simple harmonic oscillator?
  
- (c) Solve for  $|\Psi(x, t)|^2$ .
  
- (d) Compute  $\langle x \rangle(t)$  and describe the motion of the wavepacket.