PHYS 3317 Fall 2012
Homework 1 Quantum States and Operators

It is important to have a good handle on states and operators. Use lecture notes or your favorite QM textbook to brush up on basics of the Dirac notation. I'll try to mention additional reading material each week for those interested in more details.

For the first week's overview of QM formalism refer to Chapter 3 of *Griffiths*. Chapter 4 of Miller's "Quantum Mechanics for Scientists and Engineers" (hereafter simply referred to as *Miller*) has a review dealing with states and operators using powerful linear algebra formalism (nothing other than Dirac notation but with the emphasis on space representation). In particular, brush up on the notions of Hermitian and unitary matrices and operators. Also, note the definition of *outer product*, which, as opposed to inner product, generates a matrix (= operator) from ket and bra vectors in some representation:

$$|g\rangle\langle f| = \begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ \vdots \end{bmatrix} \begin{bmatrix} f_1^* \ f_2^* \ f_3^* \ \cdots \end{bmatrix} = \begin{bmatrix} g_1 f_1^* & g_1 f_2^* & g_1 f_3^* & \cdots \\ g_2 f_1^* & g_2 f_2^* & g_2 f_3^* & \cdots \\ g_3 f_1^* & g_3 f_2^* & g_3 f_3^* & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Another succinct and to the point review can be found in Tannor's "Introduction to Quantum Mechanics: A Time-Dependent Perspective" Chapter 8 (hereafter dubbed *Tannor*).

We begin using MATLAB (or Octave, its open source counterpart – though it is better to avoid it when doing large projects) starting from this homework. If you are new to MATLAB, a short intro can be found under *Simulations* on the course web-site. There will also be a several hour tutorial session detailing MATLAB for quantum mechanics during the second week of classes. For more details on solving 1D Schrödinger equation in MATLAB refer to Chapter 3 of Levi's "Applied Quantum Mechanics" (referred to as *Levi* in future) or Chapter 2 of Datta's "Quantum Transport: Atom to Transistor" (simply *Datta* in future).

1. Matrix representation of operator

The ability to represent linear operator as a matrix is the foundation for most numerical work in this course. Note that an abstract operator is not one and the same as its particular matrix representation, so this result is significant. The relationship here is similar to that of vector coordinates to the vector itself, e.g. one operator can have many different representations in different bases.

Prove the formula from lecture (also known as a *bilinear expansion* of the operator)

$$A_{ij} = \langle\psi_i|\hat{A}|\psi_j\rangle.$$

Here $|\psi_i\rangle$ represent an orthonormal basis (which don't have to be eigenstates for $\hat{A}$). In other words, the operator $\hat{A}$ turning state $|f\rangle$ into $|g\rangle$, $|g\rangle = \hat{A}|f\rangle$, can be identically represented in any complete orthonormal basis as a matrix $\mathbf{A}$ relating two vectors in the same basis:

$$
\begin{bmatrix} g_1 \\ g_2 \\ g_3 \\ \vdots \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{bmatrix},
$$

where $g_i = \langle \psi_i | g \rangle$ and $f_i = \langle \psi_i | f \rangle$ are themselves representations of states $|g\rangle$ and $|f\rangle$ in the basis $|\psi_i\rangle$. You will find the following form of the identity operator useful $\hat{I} = \sum_i |\psi_i\rangle\langle\psi_i|$ (to see that this is true simply write $|f\rangle = \sum_i \langle\psi_i|f\rangle |\psi_i\rangle = \sum_i |\psi_i\rangle\langle\psi_i|f\rangle$, from which it follows that $\sum_i |\psi_i\rangle\langle\psi_i|$ must be the identity operator). This rather obvious expression is so important in quantum mechanics that it enjoys a special name: a *closure relationship*.

2. Dirac notation and probability amplitude

In quantum mechanics we deal with probability amplitudes. These are *essentially* complex numbers and as such are not directly observable. The probability (or its density) is given by modulus squared of the probability amplitude. In statistics we add or multiply probabilities. In quantum mechanics we add and multiply probability amplitudes, then compute modulus squared to find the probability of an event. Complex probability amplitudes allow for interference of probabilities similar to superposition of waves. That's pretty much the whole idea behind quantum mechanics.

Probability amplitude in Dirac notation is written as bra-kets or inner products. For example, consider a probability amplitude $\langle\psi|\phi\rangle$. We read Dirac brackets from right to left. In this case we would say: "the probability amplitude for a particle in state ϕ to end up in state ψ". (Note: it is "probability amplitude", **not** just probability). Of course, we can put a more descriptive language inside Dirac brackets (anything goes here), e.g. $\langle v = 10\,\text{m/s} | x = 5\,\text{m} \rangle$ or $\langle n = 2 | n = 3 \rangle$, which we would read: "the probability amplitude for a particle with x-position of $5\,\text{m}$ to have velocity of $10\,\text{m/s}$" or "the probability amplitude of the system with quantum number $n = 3$ to go to $n = 2$". Just like in statistics, we add probability amplitudes of mutually exclusive events when either of them leads to the desired outcome (A or B) and multiply probability amplitudes of independent events when happening together (A and B). For example, the famous double-slit experiment can be written in Dirac notation as following

$$\langle x|S\rangle = \langle x|1\rangle\langle 1|S\rangle + \langle x|2\rangle\langle 2|S\rangle.$$

S represents the source, x represents the position in the detector plane, 1 and 2 are the two slits. Thus, $\langle x|S\rangle$ is the probability amplitude of an electron (for example) emitted

from the source to be detected with position x. $\langle x|1\rangle\langle 1|S\rangle$ says "the probability amplitude of an electron from the source S to end up at slit 1 times the probability amplitude of the electron to go from slit 1 to the detector position x". As one moves along x-coordinate in the detector plane, the probability amplitudes $\langle x|1\rangle$ and $\langle x|2\rangle$ acquire complex phase factors leading to interference pattern in the detector plane described by $|\langle x|S\rangle|^2$.

To form the inner product we require a bra and a ket. For a given state ψ these are related to each other as conjugate transpose. In a given basis, the convention for $|\psi\rangle$ is to be a column vector and for $\langle\psi|$ to be a row vector will all elements being complex conjugate. (Incidentally, in MATLAB the inner product $\langle\psi|\phi\rangle$ for two states represented by column vectors (or kets) `psi` and `phi` can be neatly written as `psi'*phi`, where operator `'` performs conjugate transpose. If you want a simple transpose without complex conjugate, you have to use `.'` instead (dot apostrophe). Invoking `psi'*phi` will return a scalar, a single generally complex number, – the probability amplitude). The inner product does not depend on the representation basis much the same way as a scalar product of two vectors does not depend on the choice of the coordinate system. This, among other things, means that we are free to choose the most convenient basis to represent states and operators and don't have to worry about computed probabilities depending on our choice.

Turning a ket into a bra or vice versa ($|\psi\rangle \to \langle\psi|$ or $\langle\psi| \to |\psi\rangle$) is easy if you follow the following simple rules:

a) $c \to c^*$ (c is a complex number)

b) $\hat{A} \to \hat{A}^\dagger$

c) reverse order of operators.

The same rules apply for finding adjoint of operators.

(a) Using these rules, find the bra that corresponds to the ket

$$c^* \langle f|\hat{A}\hat{B}|g\rangle \, \hat{C}\hat{D} \, |p\rangle \, .$$

(b) Find the adjoint of the operator

$$c \, \langle f|\hat{A}|g\rangle \, |p\rangle\langle q| \, .$$

3. Position and momentum representation

When learning quantum mechanics, one is usually first introduced to the wavefunction $\psi(x)$. It's easy to recognize that we are dealing with the probability amplitude: $\psi(x)$ is generally complex and not directly observable whereas $|\psi(x)|^2$ is the probability density. Following the discussion of the previous problem we conclude that $\psi(x)$ is

"the probability (density) amplitude of a particle in the state ψ to have coordinate x", or in the Dirac notation

$$\psi(x) \equiv \langle x|\psi \rangle .$$

$\psi(x)$ can be viewed as an element of $|\psi\rangle$ in the position representation. This is not the only possible representation. As a matter of fact, we can have an arbitrary number of representations of both states and operators (all we need is a complete orthonormal basis then essentially follow the recipes discussed in Problem 2).

There are two particular bases, however, that provide most physical meaning when it comes to representing a quantum state ψ. These are given by eigenstates of the position and the momentum operators: $\hat{x}$ or $\hat{p}$. Just like in classical mechanics where position and momentum play a central role for describing motion (mainly due to the beautiful symmetry of motion as it is viewed in position-momentum space, also known as *phase space*), a quantum system with all its peculiarities is also best viewed in position-momentum or phase space. (I will mention in passing here that such representation of states and operators is known as Wigner or Wigner-Weyl formulation, and its importance extends beyond quantum mechanics to optics, signal processing, and statistical mechanics). Short of describing quantum mechanics in phase space we proceed below stating several important facts about momentum representation, which can be viewed as complementing (and fully equivalent) view to the position representation. For example: whereas well-localized states are best represented by position space wavefunction, other scenarios with well-defined momentum can be more naturally described by momentum space wavefunction. This is often the preferred representation in solid state physics among others (usually using k-space, $k = p/\hbar$, to reduce clutter from $\hbar$'s).

The probability (density) amplitude of a particle in the state ψ to have momentum p is an element of $|\psi\rangle$ in the momentum representation

$$\tilde{\psi}(p) \equiv \langle p|\psi \rangle .$$

(We use a tilde to underline the fact that the functional dependence $\tilde{\psi}(p)$ can be completely different from $\psi(x)$ even though both represent the same state ψ). To better understand the relationship between momentum and position representations, we need to invoke some basic properties of operators $\hat{x}$ and $\hat{p}$ and their eigenkets $|x\rangle$ and $|p\rangle$:

$$\hat{x}|x\rangle = x|x\rangle , \quad \hat{p}|p\rangle = p|p\rangle ,$$

or, equivalently for eigenbras:

$$\langle x|\hat{x} = x\langle x| , \quad \langle p|\hat{p} = p\langle p| .$$

Very generally, since $\hat{x}$ and $\hat{p}$ are Hermitian operators, their eigenstates form complete orthonormal sets:

$$\langle x'|x\rangle = \delta(x - x'), \quad \langle p'|p\rangle = \delta(p - p').$$

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Here Dirac's delta function is essentially Kronecker's delta in the limit of infinite basis size: it is nonzero for $x = x'$ and zero outside, and its sum (integral) across x elements is 1. The physical meaning of these expressions is rather obvious (by reading the Dirac notation out loud): a particle with (perfectly) defined position (and *separately* momentum) is guaranteed to be found at exactly that position (momentum) and not be found anywhere else. Another obvious but very useful fact is the closure relationship (the only difference from the previously introduced expression in Problem 1 is that the sum is now replaced with an integral):

$$\int_{-\infty}^{+\infty} |x\rangle\langle x|\, dx = \hat{I}, \quad \int_{-\infty}^{+\infty} |p\rangle\langle p|\, dp = \hat{I}.$$

(a) Show that $\tilde{\psi}(p)$ is the Fourier transform of $\psi(x)$. Obviously the reciprocal statement must hold: the wavefunction in position space is the inverse Fourier transform of the wavefunction in momentum space. Hint: start by writing $\tilde{\psi}(p) = \langle p|\psi\rangle$ and acting with the identity operator (closure relationship) on $|\psi\rangle$. Afterwards, you will need $\langle p|x\rangle = \langle x|p\rangle^*$. Because the inner product does not depend on the choice of basis, you can use position representation of the eigenfunction $\phi_p(x) \equiv \langle x|p\rangle$ of $\hat{p} = -i\hbar(d/dx)$: $\hat{p}\phi_p(x) = p\phi_p(x)$. Of course, eigenstates with perfectly defined momentum correspond to a plane wave. Additionally, you should perform normalization of $\phi_p(x)$ to Dirac's delta function:

$$\int_{-\infty}^{+\infty} \phi_{p'}^*(x)\phi_p(x)dx = \delta(p - p').$$

To do so you can use the following definition of the Dirac delta function:

$$\delta(a) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{iab}db.$$

(b) Show that the momentum operator in momentum representation is simply $\hat{p} = p$. Hint: to see that simply explore the wavefunction in momentum space after acting with $\hat{p}$ on some arbitrary ψ: $\langle p|\hat{p}|\psi\rangle$.

(c) Show that the position operator in the momentum representation is $\hat{x} = i\hbar(d/dp)$. Hint: to do that express $\langle p|\hat{x}|\psi\rangle$ in terms of $\tilde{\psi}(p)$. You will need to use the closure relationship once, $\int_{-\infty}^{+\infty} |x\rangle\langle x|\, dx = \hat{I}$, then recognize the Fourier transform which will give you $\tilde{\psi}(p)$. There comes a point when a factor of x will prevent you from treating the integral as the Fourier transform. It can be replaced, however, by $i\hbar(d/dp)$ which, acting on the exponent just pulls down x. As the differential operator doesn't itself contain x, it can be taken outside the integral.

Note the suggestive symmetry for operators $\hat{x}$ and $\hat{p}$ in position vs. momentum representations.

	position space	momentum space
wavefunction	$\psi(x)$	$\tilde{\psi}(p)$
$\hat{x}$	x	$i\hbar(d/dp)$
$\hat{p}$	$-i\hbar(d/dx)$	p

4. Numerical solution of 1D Schrödinger equation

(In this problem you don't need to submit the printouts of your code. You do, however, need to provide printouts of plots as indicated. Remember to label all the axes and include legends in all the plots.)

We have talked in lecture about representing 1D Schrödinger equation in matrix form for an arbitrary potential $V(x)$ defined on interval $0 < x < L$ with boundary conditions $V(x) \to +\infty$ for $x < 0$ and $x > L$ (so that the wavefunctions vanish at those points). Consider wavefunction $\psi(x)$, which is sampled on a grid of $x_j = h_0$ with $j = 0, 1 \ldots N$ and step h_0 in the interval $x_0 = 0$ to $x_N = Nh_0 = L$. We can then construct a matrix for the Hamiltonian if we find a way to represent (an approximate) second derivative for $\hat{p}^2 \propto d^2/dx^2$. In technical terms, we chose (finite) position basis to represent all our states and operators. Note that the actual problem requires an infinite basis, therefore we expect that there will be some artifacts arising from our treatment of the problem. Still, with a proper linear algebra simulation package we can investigate quantum behavior in an arbitrary potential. The goal of this exercise is both to "feel" the power of numerical approach to solving QM problems as well as to recognize limitations arising from the necessary approximations.

(a) To construct matrix for Hamiltonian, we need a way to represent (an approximate) second derivative for $\hat{p}^2 \propto d^2/dx^2$ acting on a wavefunction $\psi(x_j)$. One approach is to construct the matrix $\hat{p} \propto d/dx$ then multiply it by itself to obtain the second derivative. E.g. $d\psi(x_j)/dx \approx (\psi(x_{j+1}) - \psi(x_{j-1}))/2h_0$. This differential operator can be written as a square matrix acting on a column vector:

$$
\begin{bmatrix}
d\psi(x_1)/dx \\
d\psi(x_2)/dx \\
d\psi(x_3)/dx \\
\vdots \\
d\psi(x_{N-2})/dx \\
d\psi(x_{N-1})/dx
\end{bmatrix}
=
\frac{1}{2h_0}
\begin{bmatrix}
0 & 1 & 0 & \cdots & 0 & 0 \\
-1 & 0 & 1 & \cdots & 0 & 0 \\
0 & -1 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & -1 & 0 & 1 \\
0 & 0 & \cdots & 0 & -1 & 0
\end{bmatrix}
\begin{bmatrix}
\psi(x_1) \\
\psi(x_2) \\
\psi(x_3) \\
\vdots \\
\psi(x_{N-2}) \\
\psi(x_{N-1})
\end{bmatrix}.
$$

Forming higher derivatives by recursively applying this formula (or, equivalently by raising to power the derivative matrix) is not most optimal. This is because

this method quickly increases the span of adjacent values around $\psi(x_j)$ required to compute higher derivatives. For example, the second derivative now requires the knowledge of $\psi(x_{j-2})$ and $\psi(x_{j+2})$ elements which are 2 elements away from $\psi(x_j)$ so that $d^2\psi(x_1)/dx^2$ and $d^2\psi(x_{N-1})/dx^2$ can no longer be evaluated this way. Instead, we are better off using a more compact form:

$$\frac{d^2\psi(x_j)}{dx^2} \approx \frac{\psi(x_{j+1}) - 2\psi(x_j) + \psi(x_{j-1})}{h_0^2}.$$

Derive this formula using the Taylor expansion of $\psi(x)$ about the point $x = jh_0$, to obtain expressions for $\psi(x_{j\pm1})$. Build the matrix in MATLAB corresponding to this operator and test it by applying to some nontrivial function and comparing with the exact second derivative. Attach a plot of the comparison (no need to show the code).

(b) Write the expression for 1D Schrödinger equation in matrix form. That is to say, the equation only relates sampled wavefunction values $\psi(x_i)$. The operator $\hat{H}$ (in matrix form) acts on the wavefunction represented by a finite column vector $[\psi(x_1)\ \psi(x_2)\ \dots\ \psi(x_{N-1})]^\mathsf{T}$ (values $\psi(x_0) = \psi(x_N) = 0$ as imposed by our choice of boundary conditions). Recognize Hamiltonian matrix elements H_{ij} from the equation, writing the formulas for non-zero elements.

(c) The whole problem is now contained in the matrix $\mathbf{H}$. Eigenvalues and eigenstates can be readily found using standard numerical routines of linear algebra. MATLAB implementation for doing just that is found on the course's website, which simulates an electron in the potential well (go to *Simulations→1D Schrodinger equation* on the web-site). Download both files, and run the code by executing `runschrod.m`. Print out the norm for the eigenfunctions to check whether any additional re-normalization may be required.

(d) Modify `runschrod.m` to simulate 1 nm-wide square infinite potential well. Keep the number of sample points to 200. I.e. `length = 1; npoints = 200;` in the program. We want to use this well-known case in order to compare simulations with the exact analytical formula for allowed energy levels to see whether there are any surprises before calculating wavefunctions of more complicated potentials. What is the maximum number of eigenstates? Make a plot of energy levels (in eV) returned by the program (say, circles) and the analytical result $E_n = n^2\hbar^2\pi^2/(2mL^2)$ (solid line) vs. the quantum number from 1 to the maximum possible in this case. (Note that MATLAB's function `eigs` used in `schrod.m` sometimes returns eigenvalues in the opposite order: the highest eigenvalue listed first. You can use `sort` to avoid confusion.). What rule of thumb can you formulate about when the results of the simulations are trustworthy or when they cannot be trusted?

(e) Here the potential stays the same as in part **(d)**. The electron is now described by the wavefunction $\psi_0(x) \propto -i \times f(x)$ where $f(x)$ is given by a half-cycle of sine: $f(x) = \sin(5\pi(x - 0.2)/L)$ for $0.2 < x(\text{nm}) < 0.4$ and zero outside. Normalize this wavefunction. Compute the expectation values of position and momentum of this state. What is the expectation value of energy? What is the most likely outcome of the energy measurement? As a final exercise, compute and print out the uncertainty $\Delta p_x \Delta x$ in units of $\hbar$ for this state. Remember: anything less than 0.5 is unphysical.