Problem Set #2: Due: Friday, February 2, 11:59pm

You are welcome to use Mathematica or similar tools in doing these problems

1. *Ehrenfest's theorem:.* At the end of the Lecture #4 notes there is a derivation of the first half of Ehrenfest's theorem showing

$$\frac{d\langle\hat{x}\rangle}{dt} = \langle\hat{v}\rangle$$

Please refer to the notes for details. This shows that the expectation value of $\langle\hat{x}\rangle$ follows the classical equation of motion – a manifestation of the correspondence principle. Starting with the corresponding expression for $\langle\hat{p}\rangle$,

$$\langle\hat{p}\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t)dx \qquad \text{(a)}$$

complete Ehrenfest's theorem by deriving the expectation-value analog of Newton's second law.

$$\frac{d\langle\hat{p}\rangle}{dt} = -\langle\frac{\partial V}{\partial x}\rangle$$

You might follow these steps:

a) Take the time derivative of equation (a).

b) Eliminate the time derivatives of $\psi(x,t)$ and $\psi^*(x,t)$ by utilizing the Schroedinger equation and its complex conjugate.

c) Eliminate spatial derivatives of $\psi^*(x,t)$ by partially integrating, under the assumption that surface terms vanish at infinity, then cancel like terms.

2. *The uncertainty principle:* Here you will complete the derivation of the uncertainty principle that is outlined at the end of the notes for Lecture 4. The derivation is based on the Cauchy-Schwarz identity you may recognized from linear algebra where $\vec{u}$ and $\vec{v}$ are vectors in some vector space

$$\vec{u}\cdot\vec{u}\ \vec{v}\cdot\vec{v} \geq |\vec{u}\cdot\vec{v}|^2,$$

generalized to wave functions: recall in class we discussed how, by thinking of dx as some small but finite Δx, we can view wave functions as vectors of infinite dimension, with the corresponding integral over dx (or sum over Δx) giving the dot product of a function with its conjugate. Consequently there is a form of the Cauchy Schwarz identity for functions and their integrals where $\vec{u} \to f(x)$ and $\vec{v} \to g(x)$,

$$\int |f(x)|^2 dx \int |g(x)|^2 dx \ \geq \ \left|\int f^*(x)g(x)dx\right|^2$$

a) Insert into the Cauchy-Schwartz identity $f(x) \to (\hat{x} - \langle\hat{x}\rangle)\psi(x,t)$ and $g(x) \to (\hat{p} - \langle\hat{p}\rangle)\psi(x,t)$, re-expressing the LHS in terms of $(\Delta x)^2 \equiv \langle\hat{x} - \langle\hat{x}\rangle)^2 = \langle\hat{x}^2\rangle - \langle\hat{x}\rangle^2$ and $(\Delta p)^2 \equiv \langle\hat{p} - \langle\hat{p}\rangle)^2 = \langle\hat{p}^2\rangle - \langle\hat{p}\rangle^2$.
b) Show that

$$(\hat{x} - \langle\hat{x}\rangle)(\hat{p} - \langle\hat{p}\rangle) - (\hat{p} - \langle\hat{p}\rangle)(\hat{x} - \langle\hat{x}\rangle) = i\hbar$$

and use this result to simplify the RHS, obtaining

$$\Delta x \ \Delta p \ \geq \ \frac{\hbar}{2}$$

3. *Phases and beats:* We showed that the general solution for the time-dependent Schrödinger equation, assuming no time dependence in the potential $V(x)$, is

$$\Psi(x,t) = \sum_i c_i \phi_i(x) e^{-iE_i t/\hbar}$$

where the sum extends over the complete set of stationary states $\{\phi_i(x)\}$ with corresponding energies $\{E_i\}$.
a) Derive an expression for the probability distribution $|\Psi(x,t)|^2$ at time t, showing that the phases depend only on the differences of the stationary-state energies.
b) Please rewrite the expression for $|\Psi(x,t)|^2$ in terms of real functions of the various beat phases $\Delta_{ji} = (E_j - E_i)t/\hbar$, that is, in the form

$$\sum_{i,j} [A_{ij} \cos \Delta_{ji} + B_{ij} \sin \Delta_{ij}]$$

where the coefficients A_{ij} and B_{ij} are real (and time independent, so determined by the initial conditions). Recall that, if $z = x + iy$ is a complex number (so x and y real), then $\mathrm{Re}[z] \equiv x = (z + z^*)/2$ and $\mathrm{Im}[z] \equiv y = -i(z - z^*)/2$.
c) The energy levels of a 1D harmonic oscillator have energies, in ascending order, of $\frac{1}{2}\hbar\omega$, $\frac{3}{2}\hbar\omega$, $\frac{5}{2}\hbar\omega, \cdots$. At time t=0 a general wave packet is formed, expressed as a sum over many stationary states. At time $t_0 > 0$ the initial state has evolved back into its $t = 0$ form. What time is it?
d) The stationary states of the 1D harmonic oscillator carry a parity quantum number, meaning that these states are either even or odd under reflection about the origin. The ground state, second excited state, fourth excited state, etc., have even parity. The other stationary states have odd parity. Answer question c) if the initial wave packet formed is a state of good parity.

4. *The prime directive:* A simple system consists of just two stationary states that we can express as vectors

$$\phi_1 \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ with } E_1 = +E_0 \qquad\qquad \phi_2 \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ with } E_2 = -E_0$$

The inner products are just the usual one for vectors: $\phi_1 \cdot \phi_1 = \phi_2 \cdot \phi_2 = 1$ and $\phi_1 \cdot \phi_2 = 0$.

a) At time $t = 0$ we have a wave packet described by

$$\Psi \equiv \Psi(t=0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \phi_1$$

That is, we start off with with a wave packet that is a stationary state. Derive an expression for $\Psi(t),\ t > 0$. Measuring time in units of $\hbar/E_0$ plot the probability that $\Psi(t)$ is in the state $\Psi(t=0)$ as a function of t. On the same graph plot the probability that $\Psi(t)$ is in the orthogonal state

$$\Psi' = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \equiv \phi_2.$$

b) Repeat part a) above, but with

$$\Psi \equiv \Psi(t=0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \text{and} \qquad \Psi' = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

c) Repeat part a) above, but with

$$\Psi \equiv \Psi(t=0) = \frac{1}{2} \begin{pmatrix} \sqrt{3} \\ 1 \end{pmatrix} \qquad \text{and} \qquad \Psi' = \frac{1}{2} \begin{pmatrix} -1 \\ \sqrt{3} \end{pmatrix}$$

Did you notice any differences in the three cases?

(Note: You have just explored the phenomena of vacuum neutrino oscillations. There are two neutrino bases. The first corresponds to the free-space stationary states $\{\phi_1, \phi_2\}$, which are the neutrino states of definite mass. States of definite mass propagate in free space without changing. There is second neutrino basis, the neutrinos of definite flavor, say electron and muon type, represented here by $\{\Psi, \Psi'\}$. Both bases span the same two-dimensional space. Weak interactions produce flavor eigenstates: the problem asks you to calculate how flavor eigenstates evolve as they

travel away from the source. In case a) we assumed the flavor basis and the mass basis coincide. In neutrino-speak, the mixing angle θ that describes how one rotates the flavor basis into the mass eigenstate basis is zero: no rotation is needed because the bases coincide. The propagating neutrino does not change: it remains the same mass/flavor eigenstate for all time. Case b) corresponds to the assumption that the flavor eigenstate produced is an equal combination of the two mass eigenstates – the mixing angle is maximal, $\theta = 45°$. In this case the initial flavor eigenstate Ψ oscillates entirely into the orthogonal flavor state Ψ' at certain points. One has complete flavor conversion. Case c) corresponds to a mixing angle $\theta = 30°$. The oscillation is strong but never complete: the mixing angle deduced from studies of solar neutrinos is about $33.6°$, so close to this value.)

5. *Continuous and discrete probability distributions and the Lanczos algorithm:* The Lanczos algorithm (also known as the Davidson algorithm in chemistry) is a procedure by which one can simplify a complicated probability distribution, replacing it with a simpler discrete distribution (points and weights) that has the same moments as the original distribution. In quantum mechanics it is often used when one is trying to find the stationary states in a huge Hilbert space – e.g., one of dimension $\sim 10^{11}$ – where it is impossible to diagonalize the Hamiltonian $\hat{H}$. The algorithm recursively maps $\hat{H}$ into smaller matrices, of dimension n=1,2,3,...., in such a way that certain exact information of the original matrix is preserved, namely the $2n-1$ moments of $\hat{H}$. The basis for the small matrix is constructed recursively, producing a tri-diagonal approximate representation of $\hat{H}$. After 50 to 100 iterations, if one diagonalizes the small matrix, one recovers almost exactly the ground state and first few excited states of the large matrix (energies and wave functions). This method of moments can also be used to calculate Green's functions and responses functions, other quantities of great interest in quantum mechanics.

Here we use the method to replace a continuous probability distribution by a simpler discrete one, such that the lowest moments of an operator are preserved. Instead of choosing some $\hat{H}$ as that operator, we instead take $\hat{x}^2$.

a) Consider the probability distribution defined by $\psi_0(x)$,

$$\psi_0(x) = \frac{\sqrt{2}}{\pi^{1/4}} e^{-x^2/2} \qquad \int_0^\infty |\psi_0(x)|^2 dx = 1$$

Calculate, by direct integration, the six lowest moments $(\hat{x}^2)^i$ of this distribution,

$$\int_0^\infty (x^2)^i \ |\psi_0(x)|^2 dx, \quad i = 0, 1, ..., 5$$

(The zeroth moment checks the normalization.)

b) Now use $\psi_0(x)$ as a "seed" for a series of operations

$$\begin{aligned} x^2\psi_0(x) &= \alpha_0\psi_0(x) + \beta_0\psi_1(x) \\ x^2\psi_1(x) &= \beta_0\psi_0(x) + \alpha_1\psi_1(x) + \beta_1\psi_2(x) \\ x^2\psi_2(x) &= \qquad\qquad \beta_1\psi_1(x) + \alpha_2\psi_2(x) + \beta_2\psi_3(x) \\ &.... \end{aligned}$$

Here ψ_1 and ψ_2 must be constructed so they satisfy the same normalization condition as ψ_0. This procedure is recursive. In the first step one calculates the part of $x^2\psi_0(x)$ that is proportional to $\psi_0(x)$ from

$$\alpha_0 = \int_0^\infty \psi_0^*(x) x^2 \psi_0(x) dx$$

Then $\beta_0\psi_1(x)$ is the orthogonal remainder, and the requirement that $\psi_1(x)$ be normalized determines β_0. Then move on to the second line. The part proportion to β_0 is given by the first line, as

$$\int_0^\infty \psi_1^*(x) x^2 \psi_0(x) dx = \int_0^\infty \psi_0^*(x) x^2 \psi_1(x) dx$$

as all quantities are real. Then α_1 and the remainder $\beta_1\psi_2(x)$ are determined as before. Then repeat for the third line, except that you do not need to calculate β_2 (the term in red) . Instead you truncate the algorithm by discarding this contribution.

c) In the recursively constructed basis $\{\psi_0, \psi_1, \psi_2\}$ one now has the (approximate) matrix representation

$$\hat{x}^2 = \begin{pmatrix} \alpha_0 & \beta_0 & 0 \\ \beta_0 & \alpha_1 & \beta_1 \\ 0 & \beta_1 & \alpha_2 \end{pmatrix}$$

Diagonalize this matrix (you can use Mathematica, Wolfram Alpha, MatLab, etc.). (Make sure your routine returns normalized eigenvectors.) Denote the three eigenvalues as x_j and the corresponding eigenvectors as ϕ_j. Define the weights $w_j = \langle\psi_0|\phi_j\rangle$. That is, these are given by the first component

of each respective eigenvector.

d) We now recalculate the moments of part a) with the replacement

$$\int_0^\infty (x^2)^i \ |\psi_0(x)|^2 dx \quad \Rightarrow \quad \sum_{j=1}^{3} (x_j^2)^i \ w_j^2, \quad i = 0, 1, ..., 5$$

What do you find?