Massachusetts Institute of Technology

Department of Physics

Physics 8.04 March 20, 1997

Quantum Physics I, Spring 1997

Problem Set 6

(Due Friday, April 4 at 5:00 pm sharp.)

Agenda and **required readings** for the weeks of March 31:

The abbreviations are RH = *Resnick and Halliday* (section numbers), G = *Gasiorowicz* (section(s) contained within the given range of pages), H = *Heisenberg* (section numbers), FT = *French and Taylor* (section numbers), CN = class notes provided on the web.

- L13, 04/01: Conservation Laws in Quantum Dynamics, Proof of $F = ma$ (Ehrenfest's Theorem)
  Readings: CN "Notes on General Features of the Time Dependent Schrödinger Equation (TDSE)", G 43-46, 125-128
- L14, 04/03: Separation of Variables, Gaussian Wave Packets, Scattering
  Readings: Section 1 of CN "Notes on Derivation and Features of the Time Independent Schrödinger Equation (TISE)," Sections 1-2 of CN "Notes on Scattering Theory," G 30-32, 74-78

Work requested of the students is highlighted by either a question mark (?) or underlining.

Contents

1 Practice with Mathematical Manipulations

The formalism of quantum mechanics requires familiarity with several new types of mathematical operations. The problems below are designed to help you develop these skills.

1.1 Hermitian Inner Product

In lecture we defined the Hermitian inner product between two functions $f(q)$ and $g(q)$ to be given by

$$< f|g >\equiv \int dq\, f^*(q)g(q).$$

Note that this operation is very analogous to the familiar vector dot product

$$\vec{f}\cdot\vec{g}\equiv\sum_{i=1}^{3} f_i g_i.$$

Demonstrate that the following properties hold for the Hermitian inner product *and* state the analogous property for the vector dot product. In the statements below f, g and h will be functions, whereas lower case Greek letters will be constants, so that, for instance, αg means $\alpha g(q)$.
Mathematicians call any operation $< | >$ holding the four properties listed below a Hermitian inner product. Because mathematicians take great care in their definitions, most of the properties of the operation we have defined for $< | >$ follow from just these four basic properties. You may use this analogy as a guide for any proofs you may need to give involving the Hermitian inner product. Because they are so analogous to the properties of the ordinary vector inner product (dot product), these relations should be easy to remember.

a)

$$< f|g >^* = < g|f >$$

b)

$$< f, \alpha g + h >= \alpha < f|g > + < f|h >$$

c)

$$< \alpha f + h, g >= \alpha^* < f|g > + < h|g >$$

d)

$$< f|f > \text{ is a real number and } < f|f >> 0 \text{ unless } f = 0$$

Note: c) above is redundant and not needed to define the Hermitian Inner Product (HIP). I include it to remind you that pulling a constant out of the left hand side of a HIP generates the complex conjugate of the constant.

1.2 Hemiticity of Operators

Use the fact that any physical operator $\hat{\mathcal{O}}$ must be Hermitian ($<\hat{\mathcal{O}}\psi|\phi> = <\psi|\hat{\mathcal{O}}\phi>$ for all functions ψ and ϕ) to show that the wave funcions $\psi_{\mathcal{O}_0}(x)$ and $\psi_{\mathcal{O}_1}(x)$ of any two pure states with respect to the observable $\mathcal{O}$ of *different* values $\mathcal{O}_0 \neq \mathcal{O}_1$ must obey $<\psi_{\mathcal{O}_0}(x)|\psi_{\mathcal{O}_1}(x)> = 0$. This property is known as "orthogonality."

Hint: Consider the relationships among $<\psi_{\mathcal{O}_0}(x)|\psi_{\mathcal{O}_1}(x)>$, $<\psi_{\mathcal{O}_0}(x)|\hat{\mathcal{O}}\psi_{\mathcal{O}_1}(x)>$, and $<\hat{\mathcal{O}}\psi_{\mathcal{O}_0}(x)|\psi_{\mathcal{O}_1}(x)>$ and be sure to use the fact that $\hat{\mathcal{O}}$ is Hermitian.

1.3 Manipulation of Fourier Integrals

Prove the Fourier Convolution Theorem of Problem 4-3.4 (problem 3.4 of Problem set 4),

$$\mathcal{F}^{-1}\left[\psi(x)\phi(x)\right] = \int \frac{dk'}{\sqrt{2\pi}} \tilde{\psi}(k')\tilde{\phi}(k-k').$$

Hint: Substitute the appropriate definitions for $\psi = \mathcal{F}[\tilde{\psi}]$ and $\phi = \mathcal{F}[\tilde{\phi}]$ into the left-hand side, write all Fourier transforms as integrals, and then manipulate the order of integration so as to obtain a Dirac δ-function.

1.4 Pure States

Using the quantum purity test for the momentum representation of the position operator which you derived in Problem Set 5, determine by solving the resulting differential equation $\tilde{\psi}_{x_0}(k)$, the momentum representation of a pure state with respect to position which always yields the position x_0 when measured. Show explicitly that your form for $\tilde{\psi}_{x_0}(k)$ is a pure state of position of position x_0 by transforming your result into real space to determine $\psi_{x_0}(x)$.

2 Computer Assignment

Log in into your Athena account on any Silicon Graphics, SUN (Sparc5's are best, classics are too slow), or Linux workstation, execute the following commands, and then follow the instructions from there:

add 8.04
solver

When you are done the assignment use the final command

8.04grade

3 A Wave Packet in Simple Harmonic Motion: Coherent State of Simple Harmonic Oscillator

Background: Without the general tools for solving the Time Dependent Schrödinger Equation (TDSE) which we will learn in the coming lectures, direct solutions to the TDSE are difficult but not impossible to find. In this problem, you will consider one such solution, the "Coherent States" of a Simple Harmonic Oscillator (SHO) of frequency ω. We will use the solution to this problem to illustrate the general principles of the Correspondence Principle and the Conservation of Probability discussed in lecture.

Consider a particle of mass m in a one-dimension simple Harmonic oscillator of frequency ω. The Hamiltonian for this system is then given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2.$$

We begin with trial solutions of the form

$$\psi(x,t) = \exp\left(-A(t)x^2 + B(t)x + C(t)\right). \tag{1}$$

Assignment:

3.1 Effective equations for A(t), B(t) and C(t)

Write down the time dependent Schrödinger equation which $\psi(x,t)$ obeys in this problem. Show that there are solutions of the form (1) provided that A, B and C obey the differential equations,

$$A'(t) = \frac{i}{2\hbar m}\left(m^2\omega^2 - 4\hbar^2 A(t)^2\right)$$

$$B'(t) = -\frac{2\hbar i}{m}A(t)B(t)$$

$$C'(t) = \frac{i\hbar}{2m}\left(B(t)^2 - 2A(t)\right).$$

3.2 Solutions of constant width

Some of the solutions to the TDSE for the SHO maintain their shape as they move through time. The function $A(t)$ controls the width of the solution $\psi(x,t)$. Find the value of A such that $A(t)$ is a constant and does not vary with time. Find general solutions for $B(t)$ and $C(t)$ when $A(t)$ takes this special constant value, A_0. Do not use the symbol "A_0" in your answers but rather the value of A_0 in terms of m, ω and $\hbar$.

3.3 Rigid shape of the probability distribution

Compute $\mathcal{P}(x,t) = |\psi(x,t)|^2$ from your solution and show that we may write $\mathcal{P}$ in the form $\mathcal{P}(x,t) = \mathcal{P}\left(x - x_0\cos(\omega t + \phi_0)\right)$, where x_0 and ϕ_0 are constants independent of time. (**Background:** Note that this means that the probability distribution does not change shape but simply shifts rigidly back and forth as a function of time. The fact that the distribution keeps its shape as a function of time is related to why these solutions are called "Coherent States".)

3.4 Conservation of probability

Show that if $\int dx\, \mathcal{P}(x, t=0) = 1$, then $\int dx\, \mathcal{P}(x,t) = 1$ for all $t > 0$.

Hint: This should be trivial given the result of Problem 3.3.

3.5 Correspondence Principle/Ehrenfest's Theorem

Show that for your wave function

$$\frac{d}{dt} < x > = < \frac{p}{m} >$$

$$\frac{d}{dt} < p > = < -\frac{d}{dx} V > .$$

(**Background:** Note that this shows that your results are consistent with the correspondence principle part of the de Broglie hypothesis, namely that average behavior of the wave packet evolves according to Newton's Laws. The result you find here is a specific case of Ehrenfest's theorem which we will prove in lecture.)

Hint: You should be able to determine $< x >$ just from the symmetry of $\mathcal{P}(x)$. To determine $< p >$, consider carefully the two alternatives of a) using the momentum operator to compute the average and b) using your previous results for the Fourier transforms of Gaussians to get $\tilde{\psi}(k,t)$ and then determine the average value of k from where $\tilde{\psi}(k,t)$ is centered.

3.6 Connection to Problem 2

Which one of the scenarios from Problem 2 does this solution most closely represent?

4 A Wave Packet Moving with Constant Acceleration

Background: This problem shows how Ehrenfest's Theorem may be used to make precise statements about the behavior of quantum expectations, giving results equivalent to those expected from solving the full Time Dependent Schrödinger's Equation, which generally requires much more work. This problem also illustrates the fact that our theory satisfies the demands put on it by the JJ Thomson experiments which measured e/m, namely that the motion of the centers of quantum wave packets follow trajectories which may be described using the familiar equations from 8.01.
In this problem, you will consider a particle subjected to a constant force ($V(x) = -Fx$), so that its Hamiltonian is given by

$$H = \frac{p^2}{2m} - Fx.$$

Assignment:

4.1 Apply Ehrenfest's Theorem

4.1.1 Generate the equations

Apply Ehrenfest's Theorem to this specific problem to generate a pair of differential equations for $< x >$ and $< p >$.

4.1.2 Solve the equations

Solve your equations to give $< x >$ as a function of time t.

4.1.3 Interpret your results

How do these results compare to the classical behavior of a particle subjected to a constant force?

4.2 Full Solution

4.2.1 Generate the equations

Show that if the wave function has the form,

$$\psi(x,t) = \exp\{A(t)x^2 + B(t)x + C(t)\},$$

and satisfies the TDSE for this problem that then A, B and C obey the equations

$$\begin{aligned} i\hbar \frac{d}{dt} A(t) &= -\frac{2\,\hbar^2\,(A(t))^2}{m} \\ i\hbar \frac{d}{dt} B(t) &= -\frac{2\,\hbar^2 A(t)B(t) + Fm}{m} \\ i\hbar \frac{d}{dt} C(t) &= -\frac{\hbar^2\left(2\,A(t) + (B(t))^2\right)}{2\,m} \end{aligned} \tag{2}$$

4.2.2 Solve the equations

Show that the *real parts* of the solutions for $A(t)$ and $B(t)$ may be written in the following forms

$$\begin{aligned} \Re\{A(t)\} &= -\frac{1}{4}\frac{1}{\sigma^2 + \left(\frac{\hbar t}{2m\sigma}\right)^2} \\ \Re\{B(t)\} &= \frac{m\sigma^2 t\,(Ft + 2\,v_0\,m)}{4\,\sigma^4 m^2 + \hbar^2 t^2}, \end{aligned}$$

where σ and v_0 are combinations of the constants of integration generated while solving the differential equations.

4.2.3 Interpret your results

Explain the physical significance of C and why the solution for C is not important in determining $< x >$.

Use your results for $A(t)$ and $B(t)$ to determine $< x >$ for the wave function $\psi(x,t)$ and verify that the results you found in section 4.1.2 using Ehrenfest's Theorem were indeed correct.

Show that the width of the packet exhibits the precise minimal spreading allowed under the HUP: a) generalize your derivation of Problem 3-1 (problem 1 from Problem Set 3) to the case of particles moving not in free space but under a constant force and b) show that Δx for your wave function follows this behavior exactly
Hint: Keep in mind that $\mathcal{P}(x) \propto \exp(-x^2/(2\sigma^2))$ is a Gaussian of standard deviation $\Delta x = \sigma$.

Finally, determine $\Delta p(t)$ the width of the distribution in momentum as a function of time. Give a classical explanation for the behavior which you find.
Hint: You have at least three choices: a) transform your wave function to momentum space and pick off the width of the Gaussian distribution $\tilde{\mathcal{P}}(k)$, b) normalize your wave function and then use the momentum operator to compute $\Delta p^2 =< \psi|\hat{p}^2\psi > - < \psi|\hat{p}\psi >^2$, or c) knowing that $\tilde{\psi}(k)$ must also be a Gaussian form, write

$$\tilde{\psi}(k,t) = \exp\left(\tilde{A}(t)k^2 + \tilde{B}(t)k + \tilde{C}(t)\right)$$

and then generate equations for $\tilde{A}(t)$, $\tilde{B}(t)$, $\tilde{C}(t)$ from the TDSE in *momentum space*. (Note that in this case $\hat{\tilde{H}} = \frac{\hbar^2 k^2}{2m} - Fi\partial_k$.) Think through your options carefully and then choose the best one for you.

4.3 Connection to Problem 2

Which one of the scenarios from Problem 2 does this solution to the TDSE most closely represent?