Massachusetts Institute of Technology

Department of Physics

Physics 8.04 March 14, 1996

Quantum Physics I, Spring 1996

Agenda and **readings** for the week of March 19:

(Note: The abbreviations for the readings are RH = *Resnick and Halliday*, K = *Kroemer*, FT = *French and Taylor*, CN = class notes given out after lecture (also appears on web after lecture).)

- L11 03/19: Quantum Operators and Expectations, Dynamics and Schrödingers Equation, Computer demos and interpretation of solutions of the TDSE
  Readings: CN "Quantum Averages and Operators"
- L12 03/21: Conservation of Probability, Ehrenfest's Theorem; and (time permitting) Separation of Variables, Time Independent Schrödinger Equation (TISE).
  CN "General Features of the Time Dependent Schrodinger Equation (TDSE)", CN "Derivation and Features of the Time Independent Schrodinger Equation (TISE)"

Problem Set 5

(Due Friday, March 22 at 5:00 pm sharp.)

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

1 Derivation of Operators from the de Broglie Hypothesis

1.1 Completing the basic set from lecture

Background: In lecture, we found representations for the operators for x and p in the position representation ($\hat{x} \to x$ and $\hat{p} \to \frac{\hbar}{i}\partial_x$, respectively), and for the momentum operator in the position representation $\hat{p} \to p$.

Complete the set by deriving the representation for the position operator $\hat{x}$ in the *momentum* representation.

1.2 Powers of x and p

Beginning with the definitions of the operators $\hat{x^n}$ and $\hat{p^n}$,

$$< x^n >= \int dx\, \psi^*(x) x^n \psi(x) \equiv < \psi|\hat{x^n}|\psi >$$

$$< p^n >= \int dp\, \tilde{\psi}^*(p) p^n \tilde{\psi}(p) \equiv < \psi|\hat{p^n}|\psi >,$$

derive position and momentum space representations for $\hat{p^n}$ and $\hat{x^n}$.

1.3 Arbitrary functions of x and p

Imagining an analytic function with the power series expansion, $f(x) \equiv \sum_{n=0}^{\infty} a_n x^n$.

Beginning with the definitions of the operators $\hat{f(x)}$ and $\hat{f(p)}$,

$$< f(x) >= \int dx\, \psi^*(x) f(x) \psi(x) \equiv < \psi | \hat{f(x)} | \psi >$$

$$< f(p) >= \int dp\, \tilde{\psi}^*(p) f(p) \tilde{\psi}(p) \equiv < \psi | \hat{f(p)} | \psi >,$$

derive position and momentum space representations for $\hat{f(p)}$ and $\hat{f(x)}$ respectively.

Hint: You should find $\hat{f(p)} = f(\hat{p})$ and $\hat{f(x)} = f(\hat{x})$.

1.4 Beyond one dimension

Taking the de Broglie hypothesis in three dimensions to be that $e^{i\vec{k}\cdot\vec{x}}$ represents a pure state of momentum $\vec{p} = \hbar\vec{k}$, derive representations for the *three dimensional* momentum and position operators $\hat{\vec{p}}$ and $\hat{\vec{x}}$ in *both* the position and momentum representations.

1.5 Hamiltonian Operators

Derive, in the position representation, the Hamilton $\hat{H}$ (total energy) operator for a single particle moving with energy $E = \frac{\vec{p}^2}{2m} + V(\vec{x})$ from the condition that the average energy of the particle computed from $< \psi | \hat{H} | \psi >$ match the average energy computed from the position and momentum operators $\hat{\vec{x}}$ and $\hat{\vec{p}}$.

1.6 Hamiltonian for the Simple Harmonic Oscillator (SHO)

In problem 3, you will need the Hamiltonian operator for the SHO. Explain the form for that operator.

2 Uncertainty Principle

Background: In this problem you will prove that the Heisenberg Uncertainty Principle (HUP) follows directly from the operator formalism which we developed from the de Broglie hypothesis!!! You may regard this proof as either one confirmation that our formalism is consistent with our experimental observations of the HUP or as the precise mathematical link between the Davisson-Germer/G.P. Thomson observations that $\lambda = h/p$ and the HUP statement that $\Delta x\, \Delta p_x \geq \hbar/2$.

2.1 Shift away the mean values

Let $\hat{\rho}$ and $\hat{\chi}$ be two new operators defined as $\hat{\rho} \equiv \hat{p} - < \hat{p} >$ and $\hat{\chi} \equiv \hat{x} - < \hat{x} >$. Show

$$(\Delta p)^2 = (\hat{\rho}\psi, \hat{\rho}\psi),$$

and

$$(\Delta x)^2 = (\hat{\chi}\psi, \hat{\chi}\psi).$$

2.2 Generate an inequality

Use the Schwartz Inequality from the Problem Set 4 with $f = \hat{\rho}\psi$ and $g = \hat{\chi}\psi$ to show

$$(\Delta x)^2 (\Delta p)^2 \geq | < \hat{\rho}\hat{\chi} > |^2.$$

2.3 Separation of the terms

Show that

$$\hat{\rho}\hat{\chi} = \frac{1}{2}\{\hat{\rho}, \hat{\chi}\} + \frac{1}{2}[\hat{\rho}, \hat{\chi}],$$

where $[\hat{x}, \hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x}$ and $\{\hat{x}, \hat{p}\} \equiv \hat{x}\hat{p} + \hat{p}\hat{x}$.

Next, use the properties of the Hermitian inner product to show that if we then take $< \{\hat{\rho}, \hat{\chi}\} >$, we get a purely real number, whereas if we take $< [\hat{\rho}, \hat{\chi}] >$ we get a purely imaginary number. *Do not use any* specific *properties of the $\hat{x}$ or $\hat{p}$ operators in this step!*

2.4 Two General Uncertainty Principles

From your results show both,

$$\begin{aligned} \Delta x\, \Delta p &\geq \frac{1}{2}| < [\hat{x}, \hat{p}] > | \\ \Delta x\, \Delta p &\geq \frac{1}{2}| < \{\hat{x}, \hat{p}\} > |, \end{aligned}$$

where $[\hat{x}, \hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x}$ and $\{\hat{x}, \hat{p}\} \equiv \hat{x}\hat{p} + \hat{p}\hat{x}$.

At this point analyze your proof in steps 2.1 through 2.4 critically for dependencies on the specific properties of $\hat{x}$ and $\hat{p}$ and give the most general statement(s) with which you are comfortable for the spread in results $\Delta A\, \Delta B$ of the measurements of an arbitrary pair of observables A and B.

2.5 Application to x and p

Compute $[\hat{x}, \hat{p}]$ and $\{\hat{x}, \hat{p}\}$, and use whichever form is appropriate to complete the proof of the specific form of Heisenberg Uncertainty Principle (HUP) stated in the first phase of the course,

$$\Delta x\, \Delta p \geq \hbar/2.$$

3 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 Schrodinger 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. Find the value $A(t)$, which controls the width of the wavefunction, for which the solution for $A(t)$ 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 Correspondence Principle/Ehrenfest's Theorem

Show,

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

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

(**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 wavepacket 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: Using your results from Problem Set 4 for the Fourier Transform of a Gaussian, you should be able to find $\tilde{\psi}(k,t)$ readily. With $\psi(x,t)$ and $\tilde{\psi}(k,t)$ in hand, you should be able to evaluate the integrals for $< x >$ and $< p >$ very quickly by symmetry.

3.5 Probability current density

Compute the probability current from your expression for $\psi(x,t)$ using the result from lecture

$$\begin{aligned} j(x,t) &\equiv \frac{\hbar}{2im}\left(\psi(x,t)^*\partial_x\psi(x,t) - \psi(x,t)\partial_x\psi(x,t)^*\right) \\ &= \frac{\hbar}{m}\Im\{\psi(x,t)^*\partial_x\psi(x,t)\}, \end{aligned}$$

where $\Im\{z\}$ is defined to be the imaginary part of the complex number z.

Hint: The key to this problem is to stay organized and manage your algebra. I suggest keeping things in terms of A, B, and C until the last possible moment when you finally substitute your expressions from subsection 3.2.

3.6 Conservation of probability

Verify that your results satisfy

$$\partial_t P(x,t) + \partial_x j(x,t) = 0.$$

(**Background:** Note that this verifies that the probability $\mathcal{P}(x,t) \equiv |\psi(x,t)|^2$ is conserved.)

4 Time Dependent Solutions in the Square Well

Background: This problem is designed to help you better visualize the "flow" of probability.

At a particle of mass m in an infinite square well of width L is in a state described by

$$\psi(x,t) = \frac{1}{\sqrt{L}} \left(\left(\sin \frac{\pi}{L} x \right) e^{-i\frac{\hbar\pi^2}{2mL^2}t} - \left(\sin \frac{2\pi}{L} x \right) e^{-i\frac{2\hbar\pi^2}{mL^2}t} \right).$$

Assignment:

4.1 Verification of TDSE

Substitute the above wavefunction directly into the TDSE and verify that it is a solution.

4.2 Probability density

Sketch a plot of the probability distribution $\mathcal{P}(x,t)$ for $t=0$ and $t = t_0 \equiv \frac{2}{3}\frac{mL^2}{\pi\hbar}$.

4.3 Net flow of probability

How much probability has "flowed" from the left half of the well, $x < L/2$, to the right half of the well, $x > L/2$, during the interval $0 < t < t_0$?

4.4 Probability Current

Use the probability current to compute as a function of time t the rate $I(t) \equiv \frac{d\mathcal{P}}{dt}$ at which probability flows across the point $x = L/2$ from the left half to the right half of the well. Integrate this result from $t=0$ to $t=t_0$ and compare with your answer for 4.3.