Massachusetts Institute of Technology

Department of Physics

Physics 8.04 April 6, 1996

Quantum Physics I, Spring 1996

Agenda and **readings** for the week of April 2:

(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).)

- L13 04/02: TDSE demos and interpretation, Conservation of Probability, Ehrenfest's Theorem.
  CN "General Features of the Time Dependent Schrodinger Equation (TDSE)"
- L14 04/04: WKB approximation/Rule, Eigenstate representation, Variational Principle, Virial Theorem (if time permits).
  CN "General Features of the Time *In*dependent Schrodinger Equation (TDSE)"

Problem Set 6

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

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

1 Conservation of Probability

1.1 Probability Current

Background: This problem refers back to Problem 4 of the previous problem set. It helps to complete your physical picture of the "flow" of probability.

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 square well in Problem 4 of Problem Set 5. Integrate your result from $t = 0$ to $t = t_0$ and compare with your answer for 4.3 of Problem Set 5.

1.2 Probability current density for coherent states of the SHO

Background: This problem refers back to Problem 3 of the previous problem set. It illustrates the power of physical concepts such as the conservation of probability.

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.

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.)

Hint: The key to this problem is to stay organized and manage your algebra. I suggest arranging things so that you can reuse your result for $\psi(x,t)\psi^*(x,t)$ from last lecture.

2 Ehrenfest's Theorem

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 Schrodinger's Equation, which generally requires much more work. This problem also illustrates the fact that our theory satisifies the demands put on it by the JJ Thomson experiments which measured e/m, namely that the motion of the centers of quantum wavepackets 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:

2.1 Apply Ehrenfest's Theorem

2.1.1 Generate the equations

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

2.1.2 Solve the equations

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

2.1.3 Interpret your results

<u>Comment</u> on the similarity of your result to what you expect classically.

2.2 Full Solution

2.2.1 Generate the equations

<u>Show</u> that if the wavefunction 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

$$\begin{aligned} i\hbar\frac{d}{dt}A(t) &= -\frac{2\,\hbar^2\,(A(t))^2}{m} \qquad (1) \\ i\hbar\frac{d}{dt}B(t) &= -\frac{2\,\hbar^2 A(t)B(t) + Fm}{m} \\ i\hbar\frac{d}{dt}C(t) &= -\frac{\hbar^2\left(2\,A(t) + (B(t))^2\right)}{2\,m} \end{aligned}$$

2.2.2 Solve the equations

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

$$\begin{aligned}
\Re\{A(t)\} &= -\frac{1}{4\left[\sigma^2 + \left(\frac{\hbar(t-t_0)}{2m\sigma}\right)^2\right]} \\
\Re\{B(t)\} &= \frac{\frac{1}{2}\frac{F}{m}(t-t_0)^2 + v_0(t-t_o) + x_0}{2\left[\sigma^2 + \left(\frac{\hbar(t-t_0)}{2\sigma m}\right)^2\right]}
\end{aligned}$$

Throughout the rest of this problem, you may take the integration constant t_0 to be zero.

2.2.3 Interpret your results

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

Explain the physical significance of A. Does $A(t)$ behave in the way you would expect from our discussions earlier in the term?
Hint: Keep in mind that $\mathcal{P}(x) \propto \exp(-x^2/(2\sigma^2))$ is a Gaussian of standard deviation $\Delta x = \sigma$.

Use your results for $A(t)$ and $B(t)$ to compute $< x >$ for the wavefunction $\psi(x,t)$ and verify that the results you found in section 2.1.2 using Ehrenfest's Theorem were indeed correct.

3 Separation of Variables

Background: The problem develops further experience with the method of separation of variables, and will become useful when we treat the formal quantum mechanics of the Hydrogen atom.

The Time Independent Schrödinger Equation (TISE) for the Hydrogen atoms reads, in spherical coordinates,

$$-\frac{\hbar^2}{2m}\left(\frac{1}{r}\,\partial_r^2(r\psi) + \frac{1}{r^2\sin\theta}\,\partial_\theta(\sin\theta\,\partial_\theta\psi) + \frac{1}{r^2\sin^2\theta}\,\partial_\phi^2\psi\right) - \frac{e^2}{r}\psi = E\psi.$$

Assignment:

Use the method of separation of variables to show that if we assume the form $\psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$, then the functions $R(r)$, $\Theta(\theta)$, and $\Phi(\phi)$ must obey the equations

$$\Phi''(\phi) = -m^2\Phi(\phi)$$

$$-\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\,\Theta'(\theta)\right) + \frac{m^2\,\Theta(\theta)}{\sin^2\theta} = \ell(\ell+1)\,\Theta(\theta)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\left(rR(r)\right) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\left(rR(r)\right) - \frac{e^2}{r}\left(rR(r)\right) = E\left(rR(r)\right),$$

where m and $\ell(\ell+1)$, for now, are the names given to arbitrary constants produced by the separation procedure.

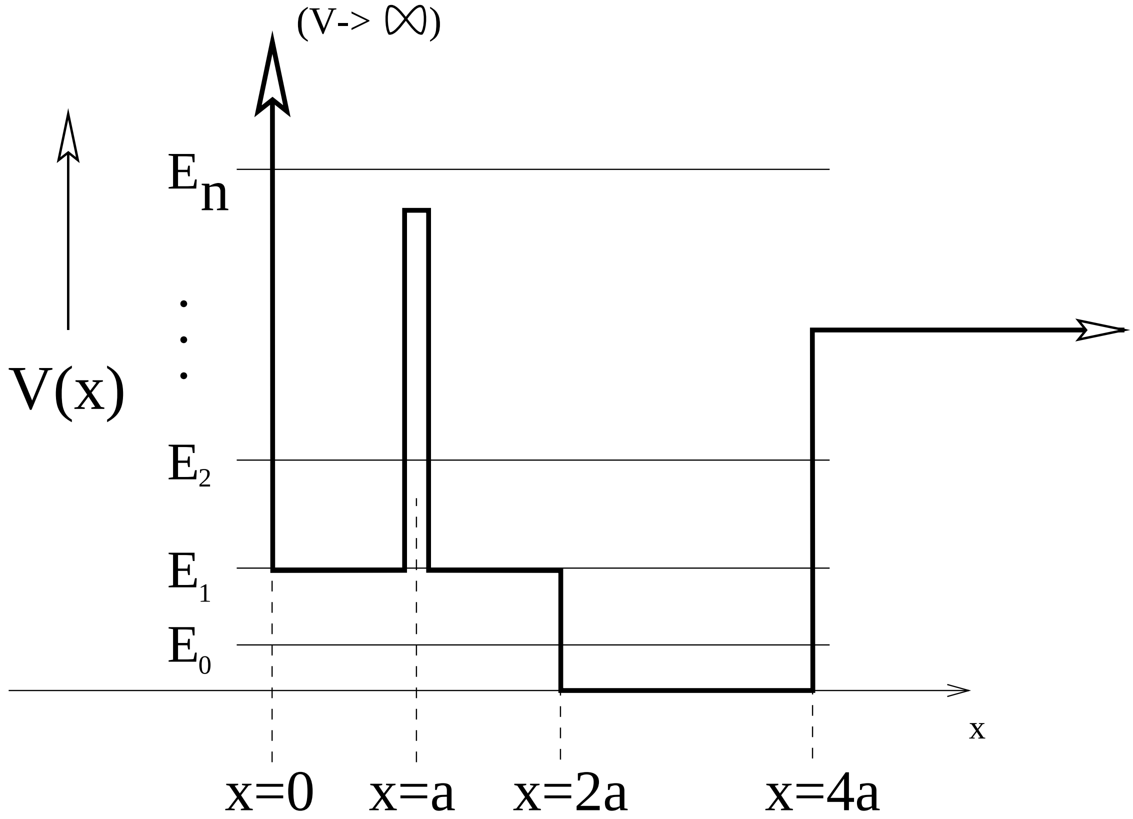

Figure 1: Potential function $V(x)$

4 Qualitative Sketches of Wavefunctions

Background: Qualitative sketches not only develop a physical feel for the salient features of the solutions of the Time Independent Schrödinger Equation (Problem 4.1), they also give an appreciation for the complexity of the solutions to the TDSE (Problem 4.2), and allow us to improve our Bohr-Sommerfeld quantization condition (Problem 4.3).

4.1 Piecewise constant Potential

Make qualitative sketches of the wavefunctions for a particle subjected to the potential in Figure 1. Sketch the ground state, E_0, the first two excited states, E_1 and E_2, and some highly excited state, E_n, with energies as shown in the figure.

Be as precise as you can be with respect to relative curvature, amplitude, continuity, the location of nodes, etc. You may wish to make written comments highlighting salient features, particularly if your artistic skills are wanting.

4.2 Eigenstates for the constant force problem

Sketch for various energies the solutions for the TISE for $V(x) = -Fx$, the potential from Problem 2. How do the shapes of the solutions change with their energy?

4.3 Eigenstates for the Simple Harmonic Oscillator (SHO)

Sketch the first *three* eigenstates for the potential $V(x) = \frac{1}{2}m\omega^2 x^2$. By counting the number of wavelengths which occur in a *complete* orbit between the classical turing points, give a better estimate (than that they simply be integer multiples of Planck's constant h) of the expected values of the classical action integral of the SHO, $\oint p\, ds = \pi\sqrt{2mE}\sqrt{2E/(m\omega^2)}$, in allowed orbits. What does your amended Bohr-Sommerfeld condition give for the allowed energies of the SHO?