Massachusetts Institute of Technology

Department of Physics

Physics 8.04 April 30, 1996

Quantum Physics I, Spring 1996

Agenda and **readings** for the week of April 30:

(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).)

- L19 04/30: Intro to scattering; continuum states, reflection at a step using probability currents.
- L20 05/02: More on stationary phase, reflection at a step with packet description – including time delay and packet spreading.

Readings: K 5.1, 5.2, 5.3

Problem Set 9

(Due Friday, May 3 at 5:00 pm sharp.)

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

1 Dimensional Analysis and Series Solutions

Background: The purpose of this problem is to practice the techniques developed in lecture, but on a slightly different problem. On Problem Set 6, you employed separation of variables to derive the following equation for the radial dependence of the Time Independent Schrödinger Equation (TISE) for the Hydrogen atom:

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

Note: I have combined the $rR(r)$ from the notation on PS6 into a new function called $\psi(r)$. For this problem you may begin with Eq. (1) and not consider $R(r)$ from PS6. The only effect of this redefinition is the new boundary condition that $\psi(r=0)=0$.

1.1 Dimensional analysis

Define your own new system of units in which the mass of the particle, the square of the charge on the electron (either, e^2 or $e^2/4\pi\epsilon_0$ if you are an mks fan) and Planck's constant all have the value 1 so that in your new units, Eq. (1) reads

$$-\frac{1}{2}\partial_R^2\Psi(R)-\frac{1}{R}\Psi(R)=\mathcal{E}\Psi(R).$$

(**Note:** the "R" in this expression is just distance measured in your new units. It has nothing to do with the "R" on PS6.)

Give expressions for your unit of mass, length and time in terms of e, $\hbar$ and m. Evaluate numerically your unit energy, distance and mass in terms the of electron Volt, the Angstroms and the mass of the electron, respectively.

Background: The system of units you have just defined is known as "Atomic Units". The unit energy is called the "Hartree" and the unit distance is called the "Bohr".

1.2 Alternate eigenvalue equation

Now <u>derive</u> the eigenvalue equation satisfied by $F(R)$ defined through

$$\Psi(R) \equiv F(R) e^{-\sqrt{-2\mathcal{E}}R}.$$

1.3 Series solution

<u>Derive</u> the recursion relationship for the series coefficients in $F(R) \equiv \sum_n c_n R^n$ in terms of $\nu \equiv \sqrt{-2\mathcal{E}}$. **To make the problem easier** you consider only the case $\ell = 0$.

<u>Explain</u>, in terms of the boundary conditions, why c_0 must be zero. For what values of ν does the remaining series terminate? In terms of m, e and $\hbar$, what are the corresponding allowed energies E?

2 Ladder Operators and the SHO – yes, from Quiz II

Background: In this problem you will use the raising and lowering operators, which came naturally in lecture from the self-transform properties of the pure energy states of the SHO, to find the pure energy states and associated energies of the SHO directly without any complicated power series solutions or messy Gaussian normalization integrals! The "raising" and "lowering" operators are defined respectively through

$$\begin{aligned} \hat{R} &\equiv \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_o} - x_o\frac{i}{\hbar}\hat{p}\right) \\ \hat{L} &\equiv \frac{1}{\sqrt{2}}\left(\frac{\hat{x}}{x_o} + x_o\frac{i}{\hbar}\hat{p}\right), \end{aligned}$$

with x_o defined as

$$x_o \equiv \sqrt{\frac{\hbar}{m\omega}}.$$

2.1 Basic properties of the operators

Using the forms given above for $\hat{R}$ and $\hat{L}$ prove the following basic algebraic facts:

$$\begin{aligned} [\hat{L}, \hat{R}] &= \hat{1} \\ \hat{H} &= \hbar\omega(\hat{R}\hat{L} + 1/2) \\ (\psi, \hat{R}\phi) &= (\hat{L}\psi, \phi) \\ (\hat{R}\psi, \phi) &= (\psi, \hat{L}\phi) \end{aligned}$$

Hints: For the first two, you may wish to begin by computing $\hat{R}\left(\hat{L}\psi(x)\right)$ and $\hat{L}\left(\hat{R}\psi(x)\right)$. For the third and fourth use the Hermiticity of $\hat{x}$ and $\hat{p}$.

2.2 Ground state

<u>Prove</u> that if $\hat{L}\psi_0(x) = 0$, then $\psi_0(x)$ is a pure state of energy and <u>give</u> the associated value of the energy. <u>Solve</u> the *first order* differential equation $\hat{L}\psi_0(x) = 0$ for $\psi_0(x)$. Be sure to <u>give</u> $\psi_0(x)$ in its properly normalized form.

2.3 Raising and lowering properties

Using the properties you showed in 2.1, <u>show</u> that if $\psi(x)$ is a pure state of energy of energy E, then 1) $\hat{R}\psi(x)$ is a pure state of energy $E + \hbar\omega$ <u>and</u> 2) $\hat{L}\psi(x)$ is a pure state of energy $E - \hbar\omega$.

Background: This energy "raising" and "lowering" properties of the $\hat{R}$ and $\hat{L}$ operators explains the origin of their names.

2.4 Normalization considerations

Using the properties you showed in 2.1, compute $(\hat{L}\psi, \hat{L}\psi)$ and $(\hat{R}\psi, \hat{R}\psi)$ in terms of (ψ, ψ). Again, assume that $\psi(x)$ is a pure state of energy of energy E.

Background: Note that this establishes that if $\hat{L}\psi(x)$ is *not* normalizable then *neither was* $\psi(x)$.

2.5 Avoiding falling through the bottom

Explain how we know that there are no normalizable solutions for $E < 0$. Use this fact to show that if $\psi(x)$ is normalizable then the sequence $\hat{L}\psi(x)$, $\hat{L}^2\psi(x)$, $\hat{L}^3\psi(x)$ must eventually yield $\hat{L}^n\psi(x) = 0$. What does this imply about the allowed values of the energy?

2.6 Generating wavefunctions

Use your results from 2.3 to generate the first two excited states of the SHO from your $\psi_0(x)$. Give only properly normalized results by using 2.4 to determine the normalization constants without having to do any Gaussian integrations.

3 Quantum tunnelling through a potential barrier

Background: This problem set contains only three problems. Problems 3 and 4 from this problem set are actually a single problem broken into two parts for grading purposes.

In this problem you will consider particles of mass m in a quantum state approaching, from the left hand side, a potential barrier of height V_0 and length L. See Figure 1. The state of the particles is that of a Gaussian probability distribution with momentum centered about kinetic energy $E \equiv \hbar^2 k_0^2/2m$. Although *classically*, the particles do not have enough energy to enter the barrier region $0 < x < L$, *quantum mechanically* there is a non-zero probability that the particles will appear on the other side of the barrier. This phenomenon is referred to as "quantum tunneling". In this problem you will consider not only the probability of an event of quantum tunneling, but also consider such issues as the time spent inside the forbidden region (often thought to be zero in science fiction stories and thus allowing faster than light travel!) and the effects of the tunneling process on the wave packet emerging on the other side.

3.1 Scattering states

Determine the scattering states of the well pictured in Figure 1 for plane waves of energy $E \equiv \frac{\hbar^2 k^2}{2m}$ incident from the left moving towards the right.

3.2 Transmission and Reflection Coefficients

By considering the current densities of your solutions, determine the transmission T and reflection R probabilities for plane waves approaching this barrier. Verify *explicitly* that your probabilities sum to unity, $T + R = 1$.

3.3 WKB approximation

Compute what you would expect for transmission coefficient from the decay in the WKB approximation,

$$T_{WKB} \sim \left| e^{-\int_0^L \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}\, dx} \right|^2 .$$

Show that in the limit $L \to \infty$, your exact result in 3.2 approaches is the product of the WKB result and the appropriate factors accounting for reflections generated by the sharp potential steps at $x = 0$ and $x = L$.

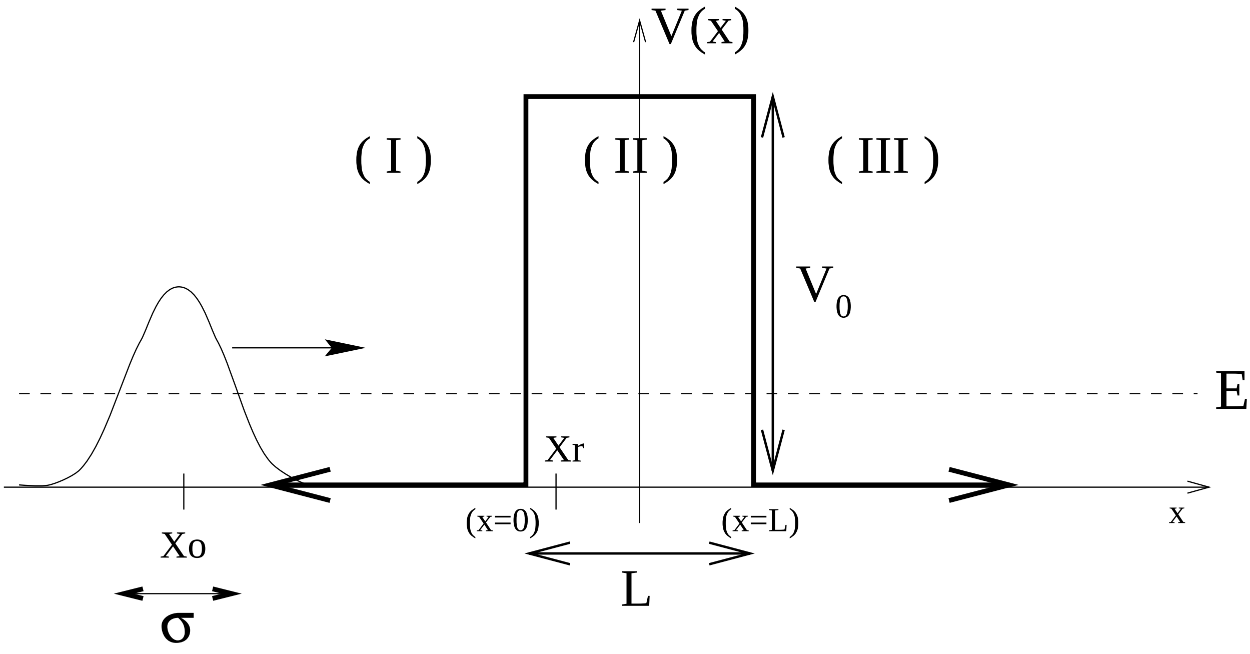

Figure 1: Quantum tunneling problem

Hint: You may continue the transmission coefficients for potential steps computed in lecture into the complex plane.

4 Quantum tunnelling through a potential barrier cont'd

4.1 Professor tunneling through a wall

Estimate the tunneling probability for an $m = 70\,kg$ professor approaching an $L = 10\,cm$ thick wall at a top speed of $9\,m/s$. You may take the height of the potential barrier V_0 to be given by the energy of interspersing my molecules amongst those of the wall, resulting in an energy on the order of $1\,eV$ per molecule. I am consist primarily of water with a molecular weight of $18\,gm/mole$.

Explain why, in this case, you should ignore the step correction terms and consider only the WKB decay.

4.2 Wave packet description

Using your pure states from 3.1, write down a general solution to the TDSE, valid in all three regions, which begins very nearly as a Gaussian of rms width σ centered at position $x_o << 0$ at time $t = 0$.

4.3 Reflected packet

Use the method of stationary phase to consider the behavior of the reflected packet. In particular, determine the time T_r at which the center of the reflected pack returns to the point x_o. From T_r and the speed of the center of the packet, determine the effective point of reflection x_r. Is there any appreciable spreading of the reflected packet beyond what you would expect from the Heisenberg Uncertainty principle?

4.4 Transmitted packet

Use the method of stationary phase to consider the behavior of the transmitted packet. In particular, determine the time T_t at which the center of the reflected pack reaches the point $-x_o > 0$. From T_t and the speed of the center of the packet in the classically allowed regions, determine the effective amount of time spent in the forbidden region, T_f, and the effective velocity in that region, $v_f \equiv L/T_f$. What energy does this velocity correspond to classically? Is there any appreciable spreading of the reflected packet beyond what you would expect from the Heisenberg Uncertainty principle?