Massachusetts Institute of Technology

Department of Physics

Physics 8.04 April 20, 1996

Quantum Physics I, Spring 1996

Agenda and **readings** for the week of April 23:

(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).)

- L17 04/23: $\delta-$function potential. Simple Harmonic Oscillator (SHO); dimensional analysis, self-transform, motivate ladder operators (if time permits).
  Readings: think about K #1.4-1, p. 39; CN "Analytic Solutions of TISE: Simple Harmonic Oscillator (SHO)," sections 1 and 2; K2.3.1-2.3.2.
- L18 04/25: SHO power series method.
  Readings: CN "Analytic Solutions of TISE: Simple Harmonic Oscillator (SHO)," sections 1 and 2; K 2.3.3-2.3.4.

Problem Set 8

(Due Friday, April 12 at 5:00 pm sharp.)

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

As we move into the third phase of the course, we now have the opportunity to apply the quantum theory we have developed. This problem set explores four distinct applications.

1 Delta Function "Molecule"

Background: The following potential gives a model of the qualitative features of the bonding in general and the H_2^+ molecule in particular,

$$V(x) = -4e^2\left(\delta(x) + \delta(x-R)\right).$$

Here, each δ-function represents the strong attractive potential concentrated mostly near each of the nuclei, which are at separation R, and e^2 gives a measure of the strength of the potential. Finally, we will imagine that the nuclei in our molecule each have mass M and repel each other with a potential e^2/R and that the molecule contains one electron of mass m.

1.1 Spectrum of the molecule

Determine the bound pure energy states of this potential, and provide a sketch of what the atomic spectrum would look like. Give expressions for all quantities in terms of $\hbar$, R, e^2, and m. A graphical solution is acceptable.

Hint: Exploit the symmetry of the potential about the point $R/2$.

1.2 Predictions about bonding and molecular structure

Skectch the energy of the electron in the molecule as a function of R assuming that the electron is always in the lowest energy bound state. Give physical explainations for the $R \to 0$ and $R \to \infty$ limits of your curves.

Skectch the total energy of the molecule, including the internuclear repulsion, e^2/R. Show that the two atoms prefer to form a bond over being separated at infinite distance by considering the separation $R = \frac{\hbar^2}{me^2}\frac{\alpha}{4}$, where $1/(1+\tanh(3\alpha/4)) = 3/4$.

2 Application of Probability Current: WKB (Wentzel, Kramers, Brillouin) approximation

Background: In this problem you will develop the WKB approximation, which you will use in your next problem set to apply to the problem of the radio active decay of heavy nuclei. (You may wish to consult Kroemer, Ch. 6 for reference.) This problem will explain to you, in quantum mechanical terms, the reason why excited states show an increase in amplitude in regions where the particle's classical velocity is *lower*.

2.1 Mathematics of continuation into the complex plane

Determine the transcendental equation for the pure states of energy in the well in Figure 1 in both cases, where a) $E > V_0$ and b) $E < V_0$. Then, show that both equations are actually the same if we take $k_1 = i\kappa_1$, and explain why this is the case. The fact that you can do this is sometimes referred to as "continuing the solution into the complex plane."

Hint: You may wish to use the definitions:

$$\begin{aligned}
\cos\theta &\equiv \tfrac{e^{i\theta}+e^{-i\theta}}{2} \\
\sin\theta &\equiv \tfrac{e^{i\theta}-e^{-i\theta}}{2i} \\
\cosh\theta &\equiv \tfrac{e^{\theta}+e^{-\theta}}{2} \\
\sinh\theta &\equiv \tfrac{e^{\theta}-e^{-\theta}}{2}
\end{aligned}$$

2.2 Basis for the WKB approximation

Imagine a *stationary* state of energy E as in Figure 2 propagating to the right in a potential varying slowly compared to the wavelength of the state. If the state is *stationary*, show that the current $j(x)$ must be constant with respect to x.

2.3 Basic situation and variation of wavelength

If the potential is slowing varying in space (so that we may ignore reflections), explain qualitatively why near each point x_o in space we may write the state as

$$\Psi(x,t) = A_{x_o} e^{ik_{x_o}x},$$

and give k_{x_o} in terms of E, m, $\hbar$ and $V(x_o)$.

2.4 Variation of amplitude

Use the condition that $j(x)$ is constant with respect to x to determine how A_{x_o} varies as x_o varies. Interpret your result in terms of the classical velocity at the point x_o, $v_{cl} = \hbar k_{x_o}/m$.

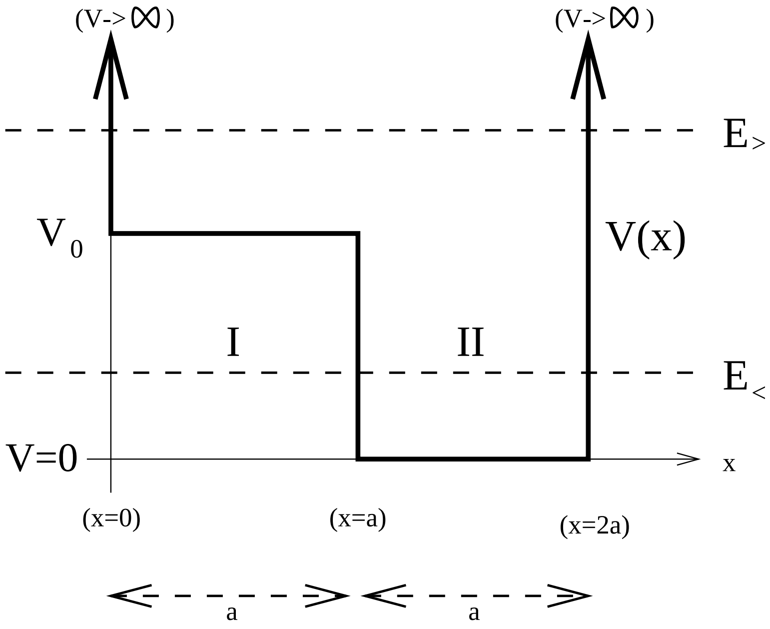

Figure 1: Infinite square well with a bump on one side

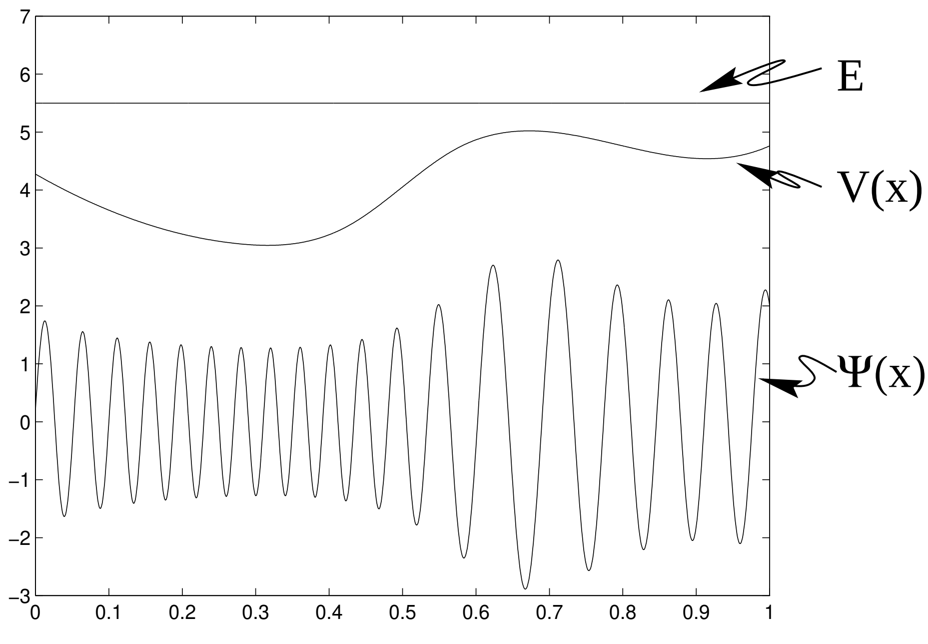

Figure 2: Wave function in classically allowed region of slowly varying potential

2.5 WKB wavefunction in classically allowed regions

Considering the net accumulation of phase as x varies from left to right, and your result for the amplitude of the wave A_x, explain qualitatively the following approximate form for the wavefunction in situations where the potential varies slowly,

$$\psi(x) \approx \frac{N}{\sqrt{E - V(x)}} e^{i \int_{-\infty}^{x} \sqrt{\frac{2m}{\hbar^2}(E - V(x))}\, dx},$$

where N is a normalization constant.

2.6 WKB wavefunction in classically forbidding regions

Use the idea of analytic continuation to write the form you would expect for a wavefunction decaying exponentially as x moves to the right through a classically *forbidden region.*

3 Wavefunctions of the Simple Harmonic Oscillator

A particle of mass m moves in a one-dimensional harmonic oscillator Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m}\partial_x^2 + \frac{m\omega^2}{2}x^2.$$

3.1 First few states and normalization

Using the recursion relation derived in class and in the notes, compute and then normalize the first three states $\psi_0(x)$, $\psi_1(x)$, and $\psi_2(x)$. *Include all relevant dependencies on the constants $\hbar$, m, and ω.* (Do not give simply the results in terms of dimensionless quantities such as $\Psi(X)$.)

Math Hint:
To carry out the integrals in this problem, you may find the following formulas useful:

$$\int_{-\infty}^{\infty} x^n e^{-x^2}\, dx = \int_0^{\infty} y^{\frac{n-1}{2}} e^{-y}\, dy$$

$$\int_0^{\infty} x^{\alpha} e^{-x}\, dx = \alpha!$$

$$\left(\frac{-1}{2}\right)! \equiv \sqrt{\pi}, \quad (n+1)! = (n+1)n! \quad \Rightarrow \quad \left(\frac{1}{2}\right)! = \frac{1}{2}\sqrt{\pi}, \quad \left(\frac{3}{2}\right)! = \frac{3}{4}\sqrt{\pi}.$$

3.2 Time dependence of a superposition of states – should look familiar

A particle is initially in the state $\Psi(x, t=0) = \frac{1}{\sqrt{2}}\psi_1(x) + \frac{1}{\sqrt{2}}\psi_2(x)$. Compute the probability distribution for later times $\mathcal{P}(x, t > 0)$ and compute the expectation of $< x >$ for times $t > 0$.

3.3 Periodicity in the SHO

If a particle is initially in a state which is an even functions of x ($\Psi(x, t=0) = \Psi(-x, t=0)$), *not necessarily* an eigenstate, how much time will pass before the probability distribution *first* returns to its initial shape $\mathcal{P}(x, t) = \mathcal{P}(x, t=0)$? How long is this repeat time for initial states which are arbitrary *odd* functions of x? How long for *completely* arbitrary initial states?

3.4 Illustration of the WKB amplitudes

Use the recursion relation to compute the wavefunction for the tenth excited state $\Psi_{10}(X)$. For simplicity, carry this part out with dimensionless quantities, and use the normalization where $\Psi_{10}(x=0)=1$. Plot the associated probability distribution. On the same graph, plot the function $1/\sqrt{1-x^2/21}$. Use the WKB rule to explain the coincident features of these two two curves on your plot.

4 Pressure in a one dimensional gas of electrons

Background: Many modern electronic structure calculations deal with the fact most molecules contain many electrons by treating the electrons collectively as a special fluid or "gas". Using results known for the electron gas in simple situations such as particles in a box, we can make fairly good estimates of the behavior of electrons in more complicated situations. In this problem, you will explore this idea using the solutions for allowed energies which we have developed in 8.04.

4.1 Total density of electrons in a box

Suppose that N electrons of mass n are placed in a "box," or infinite square well which contains the particles in the region $0 < x < L$. Suppose that there are three electrons in the box, each occupying one of the three lowest pure energy states $\{\psi_n\}_{n=1,2,3}$ of the box. Plot the function $\rho(x) = \mathcal{P}_1(x) + \mathcal{P}_2(x) + \mathcal{P}_3(x) = |\psi_1(x)|^2 + |\psi_2(x)|^2 + |\psi_3(x)|^2$, which represents the average *total* density of electrons in the box. It turns out that when $N >> 1$ (many electrons in the box), the oscillations which you see become quite small and the density appears nearly constant across the box.

4.2 Energy of the electrons in the box

In this and all subsequent parts of this problem, you need keep only terms to leading order in N. That is you may take, for example, $(N+1)/N \approx 1$.

Compute the total energy of $N >> 1$ electrons of mass m in a square well of width L assuming that each allowed energy state is occupied by just one electron and that the electrons occupy the lowest available energy states. From your result, give a formula for $\epsilon(\rho)$ the kinetic energy energy *per particle* of an electron gas of constant density $\rho \equiv N/L$.
Hint: Note that your expression for the energy per particle ϵ should depend only on the density of electrons. Also, you will find the following sum useful,

$$\sum_{n=1}^{N} n^2 = \frac{N\,(N+1)\,(2\,N+1)}{6}.$$

4.3 Force on the sides of the box

The "gas" of electrons in the box push against the sides; they can lower their kinetic energy and thus do work if the sides of the box move outward as L expands. By considering the rate at which the energy of the electron gas E decreases as the size of the box L increases, compute the *force* F exerted on the side of the box at $x = L$ in terms of the average density of electrons, $\rho \equiv N/L$.

4.4 Density of the electron gas in a harmonic oscillator

Assume that now the $N >> 1$ electrons are placed in a harmonic oscillator potential $V(x) = \frac{1}{2}m\omega^2 x^2$ instead. They are again assumed to occupy the lowest N states of the potential. Using the classical turning points of the electron with the highest energy, estimate the size $L(\omega, N)$ of the region into which the N electrons are localized and compute from this the average density of this electron gas as a function of ω and N, $\rho(\omega, N) \equiv N/L(\omega, N)$.

4.5 Energy of the electron gas in the harmonic oscillator

Compute the total energy of the N electrons in the oscillator of frequency ω in terms of N and ω by summing the energies of the occupied states.

Now, estimate this value using the electron gas picture, evaluating the energy of a gas of N electrons in a box at density $\rho = N/L(\omega, N)$. What is the ratio of your electron gas result to the exact result you calculated in the previous section?

Hint: To compute the energy E of the gas of electrons in the SHO, you will find the following sum useful,

$$\sum_{n=1}^{N} n = \frac{N\,(N+1)}{2}.$$

Background note: The good agreement here is partly fortuitous. We ignored two things. First, the actual density profile in the SHO is not constant, and second, we ignored the potential energy of the gas in the SHO.