PHYS 3317 Fall 2012
Homework 2 Time Evolution and Tunneling

Additional references: propagation matrix approach to computing tunneling probabilities is covered in Chapter 11 of Miller and Chapter 4 of Levi. Other topics covered are a part of the standard QM formalism review (see previous homework for chapters in books), in particular Chapter 8 of Tannor.

1. Fun with functions of operators and commutators

If $\hat{A}$ and $\hat{B}$ do not commute, then $\hat{B}$ does not commute with an arbitrary function of $\hat{A}$. The most important example of this is the product of exponential operators:

$$e^{\hat{A}}e^{\hat{B}} \neq e^{\hat{A}+\hat{B}} \text{ when } [\hat{A},\hat{B}] \neq 0.$$

Instead, we should use:

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}}e^{[\hat{A},\hat{B}]/2}.$$

Prove this formula.

2. Continuity equation

Prove the continuity equation for the expectation values of 1D charge and current densities:

$$\frac{\partial}{\partial t}\langle\rho\rangle = -\frac{\partial}{\partial x}\langle j_x\rangle .$$

(Hint: ψ satisfies the time-dependent Schrödinger equation (TDSE). The proof amounts to taking TDSE and its complex conjugate, multiplying each by ψ^* or ψ then subtracting the two. After that you need to recognize the density and the current).

Few remarks: this is nothing other than the conservation of charge (or probability). There is a neat theorem in theoretical physics due to Noether that gives a one-to-one correspondence between each conserved quantity in physics and some continuous (differentiable) symmetry. Emmy Noether, who came up with these theorems in the early 20th century, has been described by many at the time (including Einstein) as "the most important woman in the history of mathematics". You are probably familiar with the fact that, say, conservation of momentum is a consequence of shift symmetry in space (or space homogeneity), i.e. $x' \mapsto x + a$ does not change the laws of motion. Similarly, homogeneity of time and rotation leads to conservation of energy and angular momentum. Well, it turns out that the conservation of charge (probability) is a consequence of phase shift invariance of the wavefunction: that is an extra phase factor $\psi' \mapsto \psi e^{i\theta}$ does not affect observables. Good stuff!

3. Time evolution movie of quantum tunneling

As they say, "a picture is worth a thousand words", and using this logic — a movie, being a sequence of many pictures, should be worth on the order of million words or so. In this exercise, you will create an animation of time evolution for quantum state of an electron tunneling through a barrier. To avoid minus signs here and there due to negative charge of the electron, assume electron's charge to be positive (and the field's direction reversed). The initial state is given by a Gaussian wave packet (not an eigenstate, and therefore a superposition of stationary states).

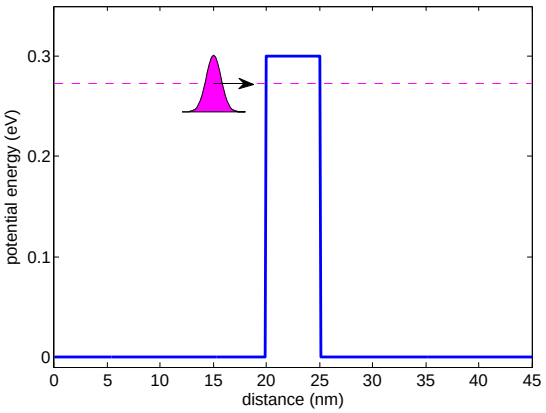

Figure 1: Potential $V(x)$ and initial Gaussian wave packet $|\psi(x, t = 0)|^2$ of an electron.

Your results should include: (i) a printout of the final computer program you used (no need to attach `schrod.m` program as it has not changed); (ii) three computer-generated plots as requested below (with appropriately labeled axes) along with any answers to the questions below.

(a) Code in the potential as shown in the Figure 1 by modifying your MATLAB code from the previous homework assignment. Set the width of the box to $L = 45\,\text{nm}$ with $\Delta x = 0.1\,\text{nm}$ by specifying `len = 45; npoints = 450;` in the program. Prepare the initial state ψ_0 that corresponds to a Gaussian packet with the position expectation $x_0 = 15\,\text{nm}$, variance $(\Delta x_0)^2 = 0.5\,\text{nm}^2$, and the velocity expectation $v_0 = 0.3\,\text{nm/fs}$. Normalize the state and check that it returns correct x_0, $(\Delta x_0)^2$, and v_0. Note: if you copy physical constants `hbar`, `echarge`, and `emass` from `schrod.m`, then sticking to units of nm ($= 10^{-9}\,\text{m}$) for position, fs ($= 10^{-15}\,\text{s}$) for time, and electron-volt (eV) for energy will work everywhere without extra powers of 10.

(b) Next, you need to decompose the function into the eigenbasis of stationary states $|\phi_n(x)\rangle$. Decompose $|\psi_0\rangle = \sum_n c_n |\phi_n\rangle$ by finding $c_n = \langle\phi_n|\psi_0\rangle$. Numerically, we have to truncate the sum at some $n_{\max}$. We can identify the criterion for choosing $n_{\max}$ if we note that $\sum_{n=1}^{\infty} |c_n|^2 = 1$, so if we choose $n_{\max}$ sufficiently large, we expect $\epsilon = 1 - \sum_{n=1}^{n_{\max}} |c_n|^2 \ll 1$. Choose the number of eigenstates

$n_{\max}$ to be sufficiently large so that the error due to the sum truncation is small (say less than $\sim 10^{-6}$). Produce a graph of the spectrum for ψ_0, that is $|c_n|^2$ vs. the eigenenergy E_n on a log-log scale. Label the axes. Indicate what $n_{\max}$ you chose and what your residual error ϵ is. Side note #1: in principle, you can simply find *all* eigenvectors (a complete set) and always decompose any ψ_0 this way. MATLAB operates efficiently on vectors and matrices so if your code is written in terms of vector/matrix operations it will often execute with nearly the same speed regardless of how many modes you chose for decomposition. But when you program in `C++` for example, it will not be the case. Side note #2: in real life you ought to always "mistrust" simulations and expect some numerical "artifacts". E.g. a good check here whether your simulations "hold water" is to double the number of sample points `npoints` and check whether any physical quantities you compute have changed (for example, the energy of the electron). If the change is small enough, the mesh size is adequate, otherwise you need to keep increasing the number of mesh points.

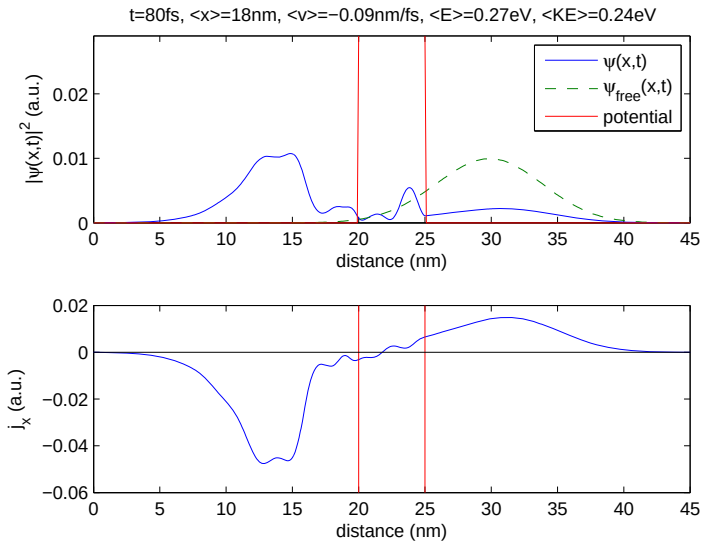

Figure 2: A snapshot of $|\psi(x)|^2$ and local current $j_x(x)$ evolving in time.

(c) You are now ready to evolve the $\psi(x,t)$ since you know how the stationary states evolve in time in which basis you have just represented ψ_0. Put a `for` loop that increments time from 0 to 80 fs with 1 fs steps (incidently, if you wait longer the wave packet will eventually start bouncing off the impenetrable walls at $x = 0$ and $x = L$, something we are not interested in this problem). Inside the loop, plot the probability density function of finding the electron $|\psi(x,t)|^2$ vs. x. Use MATLAB's `title` command to supply additional information about each frame such as time t, the expectation values for the position $\langle x(t)\rangle$, velocity $\langle v(t)\rangle$, total energy $\langle E(t)\rangle$, and the kinetic energy $\langle \mathrm{KE}(t)\rangle$. Other useful

commands for labeling your plots are `xlabel`, `ylabel`, and `legend`. To force MATLAB to display updated plots use `drawnow`. Additionally you can add `pause()` statement to the body of the loop, which will cause the program to wait until you push a key before incrementing the time and updating the plot.

(d) Let's add another Gaussian wave packet for a better comparison: one that is identical to ψ_0 at $t = 0$ but is drifting freely without any barrier. Plot $|\psi_{\text{free}}(x,t)|^2$ with dashed line so you can see the difference between tunneling and free space propagation. Add $V(x)$ to the same plot to underscore the spatial boundaries of the barrier. Use MATLAB's `hold on/off` commands for adding new curves to the same figure.

(e) In practical semiconductor devices, we would be typically way more interested in current (density) than in the expectation value of the electron's position. Produce the current density plot $j_x(x,t) \propto i(\psi\, d\psi^*/dx - \psi^* d\psi/dx)$ vs. x for each time step in a subplot below $|\psi(x,t)|^2$ (use MATLAB's `subplot(...)` function). Whew! Now you can enjoy the movie. Your final "movie frame" should look similar to Figure 2. Print it out for submission. The local current vanishes at some moments and some positions, $j_x(x,t) = 0$. Explain why.

(f) In class we said that another way to evolve a state is through the time evolution operator $\hat{U} = e^{-i\hat{H}t/\hbar}$. Obtain $\psi(x, t = 80\,\text{fs})$ this way using MATLAB's `expm()` function to build the time evolution operator directly from the Hamiltonian. Plot $|\psi(x, t = 80\,\text{fs})|^2$ vs. x from both methods (by decomposition and the time evolution operator) on the same plot, e.g. one solid curve and the other one with dots. Cautionary note #1: Hamiltonian matrix is of different size than the wavefunction because $\psi(x = 0) = \psi(x = L) = 0$ are assumed. Cautionary note #2: `expm()` is computationally 'expensive' and will be quite a bit slower for the large number of sample points while the decomposition method can still be plenty fast.

(g) Let's reflect on some of the cool physics going on here. Observe the transmitted portion of the wave packet to the right of the barrier. Which of the two pulses, the free propagating one or the one that saw the barrier, arrives first as judged by the location of the peak of the (transmitted) wave packet? If in doubt, either zoom in/out or look at the plot of $j_x(x)$. For most combinations of the barrier height, width, and the initial electron energy the tunneled-through electron arrives later than its free propagating counterpart as we would intuitively expect (after all, the whole "idea" of the barrier is to provide some resistance to the particle and, therefore, slow it down). But, for a properly chosen combination of parameters, the tunneled particle can arrive ahead of the free traveling one even though both started out with the same initial velocity! This takes on a really bizarre form when the particle happens to be a photon traveling

at the speed of light and a tunneled-through photon can be *measured* ahead of the free one (faster than the speed of light)! Does it mean that Einstein's special relativity is violated? The short answer is no, it does not. A longer answer could be a potentially very interesting seminar about superluminal velocities: when it can happen and when it can't. See A.M. Steinberg et al., "Measurement of the single-photon tunneling time", Physical Review Letters, **71** (1993) 708 for more details.

That's it. Of course, you can investigate any combinations of the barrier width and height, the initial wave packet's velocity/energy, width, etc. Such movies are a great way to build up your intuition for the quantum mechanical behavior. And this behavior can be truly weird.

4. Resonant tunneling diode

This will be our first real application of QM in this course. The specific device you will simulate is called *resonant tunneling diode* (RTD). These diodes have an interesting current-voltage characteristic with regions of *negative (differential) resistance*. In other words, the current increases when the voltage decreases. This property is useful for building devices such as oscillators, amplifiers, frequency mixers, and so on. Additionally, RTD's are one of the fastest electronic components available responding to changing signals with the frequency of up to THz (meaning that they can be used in RF circuitry). *Terahertz* here means that the response time of the device is in *sub-picoseconds*.

RTD's are all about quantum tunneling. *Resonant* part of 'RTD' refers to the fact that the tunneling barrier is actually made of two barriers with a well trapped in the middle. As a result, there are quasi-bound (resonant) states in the well with corresponding peaks in transmission (*resonant tunneling*). For example, Figure 3 shows one such geometry: two thin barriers are made of AlGaAs (1.5 nm thick) while the well is GaAs (5 nm thick). Each barrier is about 0.3 eV high. By applying an external voltage between the cathode and the anode region (30 nm thick), the barrier potential region gets skewed (see the right figure for $V_D = 0.5$ volts). Refer to the animation at nanohub.org web-site to see RTD in action.

We can model an RTD ourselves using the same tunneling theory we covered in class.

(a) Download `tunnel.m` from the Blackboard (under *Simulations*). This program is based on the lecture notes and uses propagation matrices to compute tunneling probabilities. Take a look at the program to see how it is implemented. Code in the potential as seen in Figure 3. Build a function that takes voltage as its input argument and "applies" the voltage to the potential as shown in the figure. IMPORTANT: use the effective mass $m^* = 0.07 \times m_0$ throughout, with m_0 being electron's mass in vacuum (electrons in GaAs and AlGaAs respond

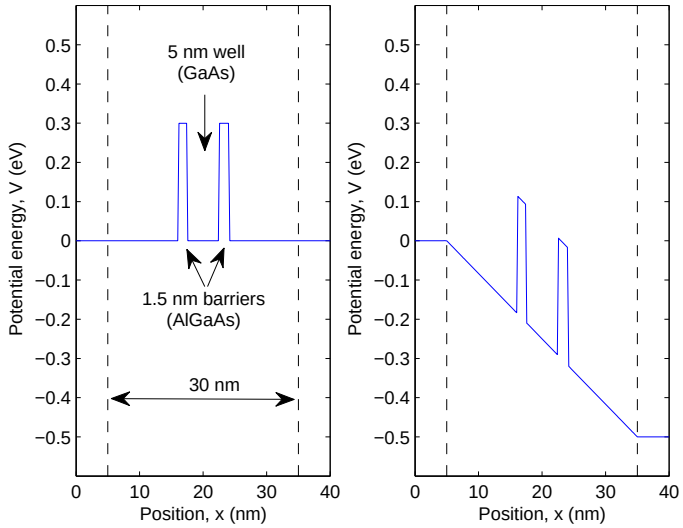

Figure 3: Potential of a resonant tunneling diode: (left) no voltage applied; (right) with 0.5 V applied.

to fields as if they were very 'light'). Produce two plots with the energy E of the incoming electron (varying E between 0 and 1 eV) on the y-axis and the transmission coefficient $T(E)$ on the x-axis for $V_D = 0$ and 0.5 volts. What is the energy of the quasi-bound state at $V_D = 0$ V? Can you estimate the lifetime in femtoseconds of an electron "stuck" in this quasi-bound state (Hint: use the uncertainty principle).

(b) To compute the total current going through the diode we need to take into account the fact that inside a semiconductor there are many carriers and states participating, not just a single electron. This part is getting a bit ahead of ourselves in this course, so we will simply use the result below deferring more detailed explanations to a later point when we shall talk about solid state physics. The result is that the current can be computed by the following integral (known as Tsu-Esaki formula):

$$J \propto \int_0^\infty T(E)N(E)dE,$$

where $T(E)$ is the transmission coefficient that `tunnel.m` computes. (You will probably want to "wrap" `tunnel.m` into a function that returns the quantities we are interested in as output arguments). The function $N(E)$ is known as a *supply function*, – which effectively tells us how many carriers are available to participate in the current transfer. We will use the following result:

$$N(E) = \ln\left\{\frac{1+\exp[(E_F - E)/k_BT]}{1+\exp[(E_F - E - V_D)/k_BT]}\right\},$$

where E_F is the Fermi energy (highest occupied electron level at absolute zero $T = 0\,\mathrm{K}$), V_D is the voltage applied across the diode and k_B is Boltzmann constant. We will have much to say about Fermi energy later in this course. Compute the current $J(V_D)$ for the diode voltage $0 \leq V_D \leq 0.5\,\mathrm{V}$ assuming for the sake of this exercise that the Fermi energy is $E_F = 0.1\,\mathrm{eV}$ (that is relative to the *conduction band*, which, technically speaking, would categorize this material as a *degenerate semiconductor*. More about it later!). Use the room temperature $k_B T = 0.025\,\mathrm{eV}$ (this number is worth memorizing!). Recall that an integral is simply a glorified sum, so use `sum()` times the energy increment to find its value. To evaluate the integral you will also need to truncate its upper limit somewhere (cannot integrate all the way to infinity). Luckily to us, $N(E)$ is significant only up to about 0.3 or 0.4 eV. Make a plot of $J(V_D)$ vs. V_D. The negative resistance region that you are supposed to obtain is due to the resonant quantum tunneling.