Homework 9

Due in class Nov. 6

1. Consider the following:

(a) A particle of mass m is in the ground state of the potential

$$V(x) = -V_0 \ell \delta(x).$$

Assume V_0 and ℓ are positive, real constants. At $t = 0$ the strength V_0 of the potential is suddenly doubled. This process happens very fast — approximately instantaneously. Calculate the probability that long after $t = 0$ the system is in the ground state of the new potential. How fast must the change take place for this "instantaneous" assumption to be valid?

(b) Assume now that the particle is in an infinite square well of width a. The left wall is suddenly moved such that the width of the well becomes $2a$. Without doing any calculations, argue which energy is most likely to be measured long after the wall was moved. How fast must the change take place for this "instantaneous" assumption to be valid?

(c) For the infinite well in (b), assume that the well's width is suddenly halved. Can you apply an analysis similar to (a) and (b)? Describe what you think would happen physically.

2. A particle in an infinite square well of width a is subjected to the following perturbation

$$V(x,t) = Q\left(\frac{x}{a}\right)^2 e^{-\alpha|t|}\sin\omega t.$$

Take all constants to be positive and real.

(a) If the system is initially in the ground state, to what final states are transitions possible in first order perturbation theory? And if it's initially in the first excited state?

(b) If the system is initially in the ground state, to what final states are transitions possible in second order perturbation theory?

(c) Using first order perturbation theory, calculate the transition probabilities from the ground state to the two lowest states you identified in (a). If you wanted to maximize the population of the lower of these two states *and* minimize the population of the upper one, how would you choose the parameters for V?

(d) Assume now that the system is initially in the middle state from (a) and (c). Using first order perturbation theory, calculate the transition probabilities back to the ground state and to the highest state from (a). If you wanted to maximize the population of the ground state while minimizing the population of the highest state, how would you choose the parameters for V?

3. A hydrogen atom is placed in a weak, static electric field of magnitude $\mathcal{E}_0$. The resulting Hamiltonian can be written as

$$\begin{aligned} H = {} & |1s\rangle E_{1s}\langle 1s| + |2s\rangle E_{2s}\langle 2s| + |2p\rangle E_{2p}\langle 2p| \\ & + d_{1s,2p}\mathcal{E}_0\big[|1s\rangle\langle 2p| + |2p\rangle\langle 1s|\big] \\ & + d_{2s,2p}\mathcal{E}_0\big[|2s\rangle\langle 2p| + |2p\rangle\langle 2s|\big]. \end{aligned}$$

Assume all constants are positive and real. The dipole matrix elements $d_{i,j}$ are defined as

$$d_{i,j} = \langle i|\hat{d}|j\rangle.$$

Note: You may use atomic units for this problem: $\hbar = m_e = e = 1$.

(a) Find the matrix representation of H in the $\{|1s\rangle, |2s\rangle, |2p\rangle\}$ basis. Is your **H** Hermitian?

(b) Find the eigenenergies and eigenstates for this Hamiltonian approximately using perturbation theory. Take your calculations to the lowest non-vanishing order. Clearly define both the unperturbed Hamiltonian and the perturbation.

(c) Plot the eigenenergies you found in (b) as a function of an appropriate perturbation parameter. For what values of this parameter are your energies valid?

(d) At $t = 0$, the system is in the state $|2s\rangle$. Based on your approximate eigenstates from (b), what energies can be measured at a later time t and with what probabilities?

(e) Let's again assume the system is in the state $|2s\rangle$ at $t = 0$. Now, though, the perturbation

$$\hat{V} = \hat{d}\mathcal{E}_1 e^{-\left(\frac{t}{\tau}\right)^2}\cos(\omega t)$$

is applied. All constants here are positive and real, and you may take $\omega = \frac{3}{8}$ in atomic units. At $t \to \infty$, what energies can be measured and with what probabilities? Would your answer change if $\mathcal{E}_0 = 0$? What would it be? Identify the origin of any differences.

4. A delta function potential is actually not a bad model for the H^- atom: both have only one bound state and the potential between the "outer" electron and H is short ranged like the delta function. So, let's explore this model a little, but reduced to 1D for simplicity.

When working with electrons in atoms, it's handy to use atomic units. In these units, $\hbar = m_e = e = 1$. So, H^- is represented by the Hamiltonian (in atomic units)

$$H_0 = -\frac{1}{2}\frac{d^2}{dx^2} - \kappa\delta(x)$$

where κ is a real positive number. This Hamiltonian describes the motion of the electron in the presence of an H atom. We will expose our H^- to a laser pulse whose electric field is given by

$$\mathcal{E}(t) = \mathcal{E}_0 e^{-\left(\frac{t}{\tau}\right)^2}\cos\omega_0 t.$$

The perturbation felt by the H^- is thus

$$H_1 = x\mathcal{E}(t)$$

in the dipole approximation. Since there is only one bound state with energy

$$E_0 = -\frac{\kappa^2}{2},$$

the only possible transitions are to the continuum — which frees the electron. This process is known as ionization.

(a) What symmetry should the ground state wave function have? Find the bound state wave function explicitly.

(b) We know that evaluating the matrix elements in perturbation theory is simpler if we can use symmetry. So, let's construct continuum states for H_0 with the highest symmetry possible. In particular, assume the following forms for the continuum states:

$$\psi_E^e(x) = \sqrt{\frac{2}{\pi k}} \begin{cases} \cos(kx + \phi^e) & x < 0 \\ \cos(kx - \phi^e) & x > 0 \end{cases},$$

$$\psi_E^o(x) = \sqrt{\frac{2}{\pi k}} \begin{cases} \sin(kx + \phi^o) & x < 0 \\ \sin(kx - \phi^o) & x > 0 \end{cases},$$

where the subscript E indicates these are energy eigenstates, and the superscript e and o indicates the even and odd solutions, respectively. The constant prefactor is required to energy normalize these states. Verify that these states are indeed even and odd. Calculate ϕ^e and ϕ^o.

(c) Using first order perturbation theory, calculate the ionization probability $P(E)$ for our model H^- as a function of energy. Plot $P(E)$ as a function of energy for $\omega < E_0$, $\omega \approx E_0$, and $\omega > E_0$. Discuss your results physically, and make sure to compare the results for these different ω. In an experiment, this spectrum is exactly what you would measure if you collected all ionized electrons and measured their kinetic energy.

(d) The total ionization probability is found be integrating $P(E)$ over all allowed energies (because $P(E)$ is actually a probability density, like $|\psi(x)|^2$). Find the total ionization probability for the three cases you plotted in (c) (you may find numerical integration useful here). For what values of $\mathcal{E}_0$ are your results valid?