

5.73 Midterm

This exam is open book, open notes. However, you should not consult other people about your solutions to these problems. Any questions (particularly questions that will clarify the intent of a question) should be directed to the Instructor or Graders. The exam should be turned in no later than 5 pm Friday, Oct. 28th.

1. Previously, in Problem Set 3, we considered scattering off of a repulsive δ -function potential of strength V_0 . In particular, we found that the transmitted and reflected fluxes were ($\hbar = m = 1$):

$$T = \frac{k^2}{1+k^2} \quad \text{and} \quad R = \frac{1}{1+k^2}$$

where $k = \frac{\sqrt{2E}}{V_0}$. Here, we consider scattering off of two repulsive

δ -functions of strength V_0 . One

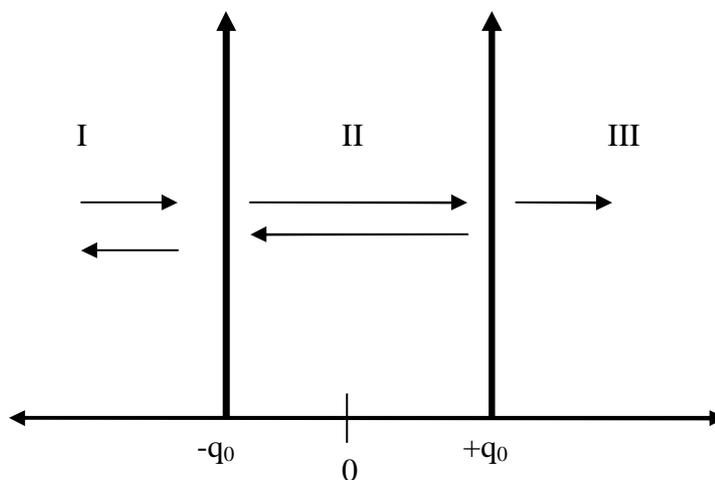
would naively expect that the probability of transmission through **two** barriers would always be *less* than for one (i.e.

only particles that make it across the

first barrier can make it across the second). In this problem you will show that this is not necessarily the case and develop an explanation for this. Therefore, consider the potential:

$$V(q) = V_0 \delta(q - q_0) + V_0 \delta(q + q_0)$$

- a. Assume that our particle is incident from the left with energy E . Divide the system up into three regions as shown above and determine the appropriate scattering state by matching the allowed wavefunctions in the three regions. The algebra is a bit tedious here. You will need to keep careful track of the derivative discontinuity at each



delta function, which becomes a bit painful. You may wish to use a program like Mathematica to do some of the algebra for you. If so, I highly recommend the “Solve[...]” and “Simplify[...]” commands.

- b. Compute the total transmission and reflection probabilities as a function of E, q_0 and V_0 . That is, compute the probability flux of particles in region I moving to the left (reflected particles) and that in region III moving to the right. Verify that flux is conserved.
- c. Show that, for some values of E, q_0 and V_0 the transmitted flux is greater when the particle scatters off two delta functions than one. Develop an explanation for this phenomenon. It may prove useful to plot the real part of the wavefunction for one of the offending choices of E, q_0 and V_0 . For fixed E and $V_0 = 1$ what separation gives maximum transmittance?

2. The time evolution operator $\hat{K}(t)$ for the Harmonic oscillator is given by

$$\hat{K}(t) = e^{-i\hat{H}t/\hbar} = e^{-i\hbar\omega(a^\dagger a + 1/2)t/\hbar} = e^{-i\omega(a^\dagger a + 1/2)t}$$

- a. Consider the operators

$$\tilde{a} = \hat{K}^\dagger(t)a\hat{K}(t) \quad \tilde{a}^\dagger = \hat{K}^\dagger(t)a^\dagger\hat{K}(t)$$

What is the physical meaning of these operators? That is, what does $\langle \tilde{a} \rangle$ mean?

- b. By calculating their action on the Harmonic oscillator states $|\varphi_n\rangle$ find expressions for \tilde{a} and \tilde{a}^\dagger in terms of the raising and lowering operators.
- c. Calculate the operators \tilde{p} and \tilde{q} obtained via

$$\tilde{p} = \hat{K}^\dagger(t)\hat{p}\hat{K}(t) \quad \tilde{q} = \hat{K}^\dagger(t)\hat{q}\hat{K}(t)$$

How can these relations be interpreted? Show, in particular, that

$$\tilde{H} \equiv \frac{\tilde{p}^2}{2m} + \frac{1}{2}m\omega^2\tilde{q}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 = \hat{H}.$$

d. Show that $\hat{K}\left(\frac{\pi}{2\omega}\right)|q\rangle$ is an eigenstate of \hat{p} and specify its eigenvalue. Similarly, show that $\hat{K}\left(\frac{\pi}{\omega}\right)|q\rangle$ is an eigenstate of \hat{q} and specify its eigenvalue. What is going on here?

3. This problem concerns the Morse potential applied to the H_2 molecule. Here, we use the standard Morse form:

$$V(\hat{q}) = D(1 - \exp(-\beta(q - q_0)))^2$$

with the specific choices $D = 4.7 \text{ eV}$, $\beta = 2.1 \text{ \AA}^{-1}$, $q_0 = .741 \text{ \AA}$ and $m = .5 \text{ a.m.u.}$ With these parameters, the Morse potential is a good approximation to the potential energy associated with the stretching of a single, isolated H_2 molecule.

a. Use DVR to determine the bound state energies of this potential, keeping careful track of your units. Here, the bound states are all those stationary states with energy less than the dissociation energy D . Note that there are a finite number of bound states and you should choose your DVR basis so that all are accurately predicted. Fit your results to the standard vibrational form:

$$E(n) = E_0 + \omega_e\left(n + \frac{1}{2}\right) - \omega_e x_e\left(n + \frac{1}{2}\right)^2 + \omega_e y_e\left(n + \frac{1}{2}\right)^3 + \dots$$

Do you notice anything special about the coefficients?

b. Determine the average potential energy, $\langle V(\hat{q}) \rangle$, and the average position, $\langle \hat{q} \rangle$, for each of the bound states. How different is $\langle V(\hat{q}) \rangle$ from $V(\langle \hat{q} \rangle)$? Are there any interesting trends in these averages as energy increases?

c. Perform the same calculation with $m = 1 \text{ a.m.u.}$ (corresponding to D_2) and $m = 1.5 \text{ a.m.u.}$ (corresponding to T_2). What happens to the *number* of bound states as you increase the mass? Is this sensible?