## Homework 6

Due in class Oct. 9

1. By now, you know the potential

$$V(x) = -V_0 a\left[\delta(x-a) + \delta(x+a)\right]$$

very well ($a$ and $V_0$ are positive, real constants). We want to revisit its solutions, this time for the resonant states. You should assume $\hbar = m = 1$, $a = 1$, and $V_0 = 5$ (in appropriate units).

To solve this problem, you will need a convention for normalizing the continuum states. One standard convention is called "momentum normalization" (we have talked about this before). It implies that the orthonormality relation is

$$\int_{-\infty}^{\infty} dx \psi_{p'}^*(x)\psi_p(x) = \delta(p-p').$$

This is accomplished by writing

$$\psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ipx}{\hbar}\right)$$

In practice, one imposes this normalization by making sure the wave function has the same amplitude as this momentum eigenstate *asymptotically.*

(a) What are the approximate conditions for a resonance to occur? At what energies will they (approximately) appear?

(b) Locate the first transmission resonance and plot its wave function. Make sure to normalize it as described above. Do the same for the third resonance. Compare these two wave functions and answer the following:

(i) How many nodes do they have between $x = -a$ and $x = +a$? Explain why they have the number they do. (Keep in mind that there might be bound states!)

(ii) How do their amplitudes in this region compare? Explain this physically, making sure to connect with the behavior of the transmission and reflection probabilities.

(iii) Based on these observations, sketch the wave function for the fourth and fifth resonances. Make sure to reproduce their key characteristics semi-quantitatively.

(c) Assume the system is initially in the state

$$\psi(x,0) = \begin{cases} \mathcal{N}\cos^2\left(\frac{\pi x}{2a}\right) & |x| \le a \\ 0 & \text{otherwise} \end{cases}.$$

Find the time-dependent wave function and examine its time evolution (the probability density is probably a useful thing to study). Calculate the quantity $|\langle\psi(0)|\psi(t)\rangle|^2$. What does this quantity represent physically?

(d) Assume now that the system is initially in the state

$$\psi(x,0) = \begin{cases} \mathcal{N}\cos^2\left(\frac{\pi x}{a}\right) & |x| \le \frac{a}{2} \\ 0 & \text{otherwise} \end{cases}.$$

Find the time-dependent wave function and examine its time evolution. Calculate the quantity $|\langle\psi(0)|\psi(t)\rangle|^2$.

(e) Now we want to try to understand your results from (c) and (d). Show some characteristic plots of $|\psi(x,t)|^2$ and/or describe their behavior. Plot $|\langle\psi(0)|\psi(t)\rangle|^2$ for each case and describe them physically. HINT: Resonances probably play an important role.

2. Let us now consider a more realistic model for a molecular potential:

$$V(x) = V_0\left[\left(\frac{x}{\alpha}\right)^2 - 1\right]^2$$

where $\alpha$ and $V_0$ are positive, real constants. A potential of this form is a good model for the position $x$ of the nitrogen atom in ammonia, $NH_3$. The shape of ammonia can be pictured as a pyramid with a triangular base — the H's lie at the corners of the base, and the N at the top. There is no reason, however, for the nitrogen to stay above the H's, and it can tunnel through the base to be on bottom.

(a) Sketch or plot the potential. What symmetries does it possess? Sketch your guess for the ground and first excited state wave functions. What do these symmetries and wave functions represent physically for the $NH_3$, *i.e.* positions of the nuclei?

(b) For a particle localized on one side of the barrier, the potential appears nearly harmonic near the minimum. Find the effective harmonic potential for such a particle.

(c) Construct an approximate ground and first excited state wave function as a linear combination of the ground states of the right- and left-side simple harmonic oscillator (SHO) potentials from (b). [Just like you did in 2(c) above for the square wells.] Calculate the energies of your approximate states from the expectation value of the Hamiltonian with the full potential. Use $V_0 = \frac{6\hbar^2}{m\alpha^2}$ and $V_0 = \frac{8\hbar^2}{m\alpha^2}$. Explain the change in energies between these two values of $V_0$. The energies of the SHO states were the same — why are the energies of your approximate states different?

(d) Estimate the time it takes for a particle localized to the left of the barrier to appear on the right side [use the values of $V_0$ from (c)]. [HINT: Your approximate eigenstates will evolve approximately in time with a phase $e^{-iEt/\hbar}$ where $E$ is the energy you calculated in (c)].

3. For a simple harmonic oscillator, compute the following using raising and lowering operators:

(a)

$$\langle n'|\hat{X}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left[\sqrt{n+1}\,\delta_{n',n+1} + \sqrt{n}\,\delta_{n',n-1}\right]$$

$$\langle n'|\hat{P}|n\rangle = i\sqrt{\frac{m\hbar\omega}{2}}\left[\sqrt{n+1}\,\delta_{n',n+1} - \sqrt{n}\,\delta_{n',n-1}\right].$$

(b) $\langle\hat{X}\rangle$ and $\langle\hat{P}\rangle$ for an arbitrary state $|n\rangle$

(c) $\langle\hat{X}^2\rangle$ and $\langle\hat{P}^2\rangle$ for an arbitrary state $|n\rangle$

(d) $\langle \hat{T} \rangle$ and $\langle \hat{V} \rangle$ for an arbitrary state $|n\rangle$ and verify that the virial theorem is satisfied.

4. Project the relation

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$$

on the position basis and derive the recursion relation

$$H_n^{'}(y) = 2nH_{n-1}(y)$$

for Hermite polynomials where $y = \sqrt{(m\omega/\hbar)}x$.

5. The initial state of a simple harmonic oscillator is

$$|\psi(0)\rangle = \alpha|0\rangle + \beta|1\rangle.$$

(a) Find the expansion coefficients that maximize $\langle \hat{X} \rangle(0)$.

(b) Using your coefficients from (a), find $\langle \hat{X} \rangle(t)$. Explain your result physically (illustrations using the coordinate space probability density might help).

(c) If the energy were measured at some time $t$, what values could be obtained and with what probabilities?

(d) If the initial state were instead a linear combination of $|1\rangle$ and $|2\rangle$, discuss qualitatively how your answer to (b) would change.

(e) Repeat (d) for an initial linear combination of $|0\rangle$ and $|2\rangle$.