# Quantum Mechanics 115C: Homework 3

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## 3.1 Symmetrical double well potential: toy model of ammonia molecule

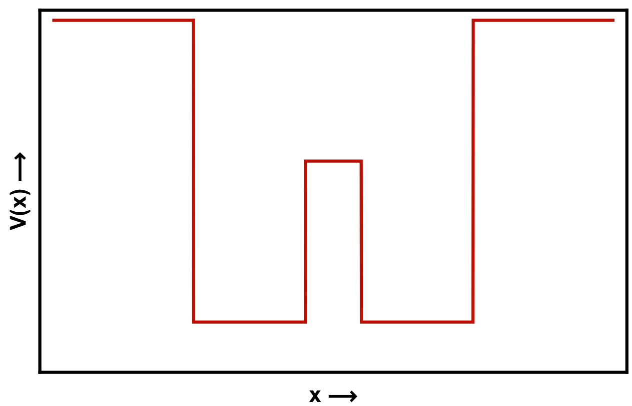


Figure 1: Double symmetrical potential well

Imagine a double potential well, something like the one shown in Fig. 1, where the walls at the ends are infinite. As you can see, the Hamiltonian for this problem has parity symmetry about the center.

**(a)** Draw, in a qualitative way, the ground state and the first excited state wavefunctions for this system. Is the ground state parity symmetric or anti-symmetric? Is the first excited state parity symmetric or anti-symmetric? Why is this the case?

**(b)** Draw the ground state and first excited state wavefunctions for a central barrier height of (i) infinity and (ii) zero. What determines the splitting in energy between the ground state and the first excited state for part **(a)**? When will the splitting be large, and when will it be zero?

**(c)** In the case where the splitting is zero, the ground state and the first excited state wavefunctions, $\psi_0(x)$ and $\psi_1(x)$, respectively, become degenerate. Linear combinations of these states then become stationary states with the same energy eigenvalue, $E_0$. Draw the wavefunctions for the following linear combinations:

$$\psi_\pm(x) = \frac{1}{\sqrt{2}}(\psi_0(x) \pm \psi_1(x)) \tag{1}$$

**(d)** Are the $\psi_\pm(x)$ wavefunctions from part **(c)** parity symmetric? Is the Hamiltonian parity symmetric?

**(e)** Is the expectation value of $x$ zero or non-zero in the following cases: $\langle\psi_+|\, x \,|\psi_+\rangle$, $\langle\psi_-|\, x \,|\psi_-\rangle$, $\langle\psi_0|\, x \,|\psi_0\rangle$ and $\langle\psi_1|\, x \,|\psi_1\rangle$? Explain your answer; you do not necessarily have to do a calculation.

**(f)** Let's now return to the case of finite barrier height, as depicted in Fig. 1. In this case, the ground and excited states are non-degenerate. Are the $|\pm\rangle$ states stationary states? Why or why not?

**(g)** Suppose that a particle starts out in a superposition of the ground state and first excited state, so that:

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{2}$$

where $|0\rangle$ and $|1\rangle$ represent the ground and first excited states respectively. The other superposition state is:

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \tag{3}$$

At time $t = 0$, the system is prepared the state $|+\rangle$. Write down the state vector at time $t$, $|+(t)\rangle$, given that $H|0\rangle = E_0|0\rangle$ and $H|1\rangle = E_1|1\rangle$, where $H$ is the Hamiltonian.

**(h)** At time $t$, what is the probability that the particle is in state $|-\rangle$, given that it was in state $|+\rangle$ at time $t = 0$? How long does it take for a particle in state $|+\rangle$ to turn into the state $|-\rangle$ for the first time?

**(i)** As the barrier height is raised to infinity, how long does it take for a particle in state $|+\rangle$ to turn into the state $|-\rangle$ for the first time?

This problem represents a simple model of the ammonia molecule, $NH_3$, which was used as the "gain medium" for the first maser. The molecule has two states, that with the nitrogen atom above the triangular plane formed by the three hydrogen atoms and that with the nitrogen atom below. These are analogous to the $|+\rangle$ and $|-\rangle$ states of this problem. The natural oscillation frequency of the ammonia molecule is roughly 24 GHz or 24 billion times a second.[1]

**(j)** Can you estimate the energy difference between the ground state and excited state in the ammonia molecule based on the frequency given above? In what range of the electromagnetic spectrum would this oscillatory motion emit light (e.g. visible, UV, X-ray, etc.)?

**(k)** On the other hand, $AsH_3$, which has the same structure as $NH_3$, has a natural oscillation frequency of approximately 160 $\mu$Hz. How long does it take for the As atom to tunnel to the other side of the $H_3$ triangular plane? What does this tunneling time tell you about the barrier height for $AsH_3$ compared to $NH_3$?

**(l)** Would you say that $NH_3$ possesses a dipole moment? Would you say that $AsH_3$ possesses a dipole moment? Why or why not? Justify your answer.

### 3.2 Particle on a circle: toy model of a superconducting qubit

Consider a free particle, but one that is constrained to move in a circle of length $L$ (you can imagine that space has periodic boundary conditions if that makes visualization easier). The stationary states for this problem can be written in the form $\psi(x) = Ne^{ikx}$, where $x$ is the position coordinate and the momentum $p = \hbar k$.

[1] Feynman's Lectures on Physics Vol. III has an extensive account of the use of the ammonia molecule for the first maser. It's a great read for those who are interested.

**(a)** Show that the periodic boundary condition implies that

$$\hbar k_n = \frac{2\pi\hbar n}{L} \qquad \text{with} \qquad n = 0, \pm1, \pm2, ... \tag{4}$$

**(b)** Show that the normalized eigenfunctions are given by:

$$\psi_n(x) = \frac{e^{ik_n x}}{\sqrt{L}}. \tag{5}$$

**(c)** What are the energy eigenvalues? Are there degenerate eigenvalues? If so, which states have the same eigenvalues?

**(d)** Now consider a perturbation of the form:

$$H' = -\beta p, \tag{6}$$

where $\beta$ is a constant and $p$ is the momentum operator. (This perturbation is meant to qualitatively mimic the effect of a magnetic field.) What are the "good states" for this perturbation? Can you explain how you know the states you wrote down are the "good states"?

**(e)** Find the first-order correction to the energy levels due to the perturbation $H'$.

**(f)** Does the lifting of degeneracy affect each degenerate pair in the same way? Draw the splitting of the energy level for the first three degenerate states with

$$\beta = \frac{2\pi\hbar}{2mL}. \tag{7}$$

**(g)** Show that when $\beta$ is tuned to $2\pi\hbar n/2mL$, there is a new degeneracy in the problem. Which energy levels become degenerate for these values of $\beta_n$?

**(h)** Is perturbation theory even valid for these values of $\beta_n$? Why or why not? It may be helpful to refer to **Problem 2.3** in your previous homework assignment.

**(i)** Is there a reason to think that the result obtained from perturbation theory for this problem might work regardless of the restrictions placed by part **(h)**?

**(f)** Find the first-order correction to ground state for arbitrary $\beta$.

**(g)** Find the second-order correction to the energy levels due to the perturbation $H'$. Can you explain your answer? Do you think that higher order corrections will yield non-zero results? Why or why not?

### 3.3 Particle on a circle II

Consider a particle confined to a circle as in **Problem 3.2**. In this problem, we will consider a perturbation of the form:

$$H' = V \sin\left(\frac{4\pi x}{L}\right). \tag{8}$$

**(a)** Use degenerate perturbation theory to calculate the first order shift to the lowest energy degenerate states. *Hint: You may be able to guess the "good states" which is a valid way of completing this problem, but by no mean is this necessary.*

**(b)** What are the "good states" for part **(a)**?

**(c)** Use degenerate perturbation theory to calculate the first order shift to the second lowest degenerate energy levels.

**(d)** By how much have the energies split in parts **(a)** and **(c)**?

**(e)** From parts **(a)** and **(c)** can you guess whether the degeneracy will be lifted for the higher energy degenerate states? Explain your answer.

**(f)** How would changing the wavelength (or wavevector) of the perturbation to, say, $L/4$ (or $8\pi/L$) change which set of degenerate states experience an energy splitting? Explain your answer.