Group Problems #36 - Solutions

Monday, November 28

Problem 1 *Transition Selection Rules*

An electron is in the ground-state of a 1D infinite square well:

$$U(x) = \begin{cases} \infty, & \text{for } x \le -L/2, \\ \infty, & \text{for } x \ge L/2, \\ 0, & \text{for } -L/2 < x < L/2. \end{cases} \tag{1}$$

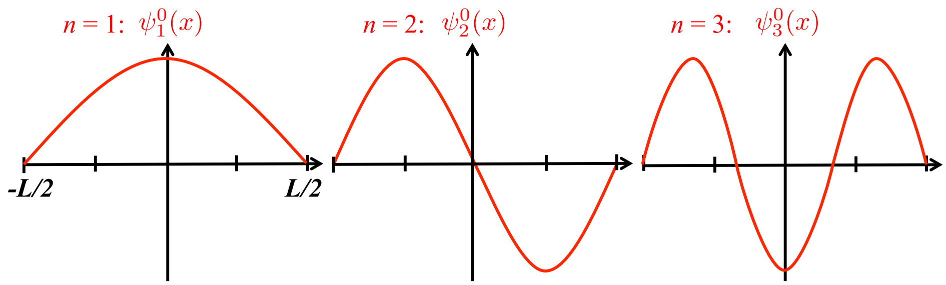
(a) What are the general solutions for the *unperturbed* Hamiltonian, $\psi_n^0(x)$? (Pay attention to the symmetry of the potential!!!)

The general solutions for this potential (note that the potential is centered around $x = 0$ in this case, $-L/2 < x < L/2$) are given by:

$$\psi_n^0(x) = \begin{cases} \sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L}, & \text{for } n = 1, 3, 5, ... \\ \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}, & \text{for } n = 2, 4, 6, ... \end{cases} \tag{2}$$

These solutions are equivalent to those we found when the well extended over $0 < x < L$.

(b) Draw the first three solutions of the unperturbed Hamiltonian, $\psi_1^0(x)$, $\psi_2^0(x)$, and $\psi_3^0(x)$.

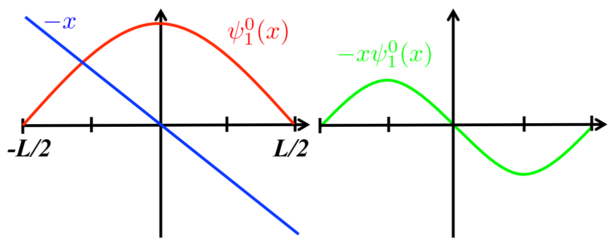


(c) At time $t = 0$ an electric field $\hat{\xi} = \xi\hat{x}$ is switched on for duration Δt. After the perturbation has been applied, the wavefunction can be approximated by,

$$\psi_{\mathrm{t=\Delta t}}(x) \simeq A\psi_1^0(x) + \psi_{\mathrm{pert}}(x,t) \tag{3}$$

$$= A\psi_1^0(x) - \frac{i\Delta t}{\hbar} W\psi_1^0(x), \tag{4}$$

where $W = e\xi x$ is the perturbation term caused by application of the electric field. Draw $\psi_{\mathrm{pert}}(x)$ for this case. (Ignore the "i" for now.)



(d) What can you deduce by graphical comparison of $\psi_{\mathrm{pert}}(x)$ and $\psi_2^0(x)$?

The similarity between $x\psi_1^0(x)$ and $\psi_2^0(x)$ indicates that the perturbation primarily induces a transition between the initial ground state ($n = 1$) and the 1st excited state ($n = 2$). Note that the amplitude of the perturbation part of the wavefunction depends on the duration it is applied, Δt, and also on the strength of the electric field, ξ.

(e) What is the transition probability between states $n = 2$ and $n = 3$?

As given in the lecture, the generic expression for the transition probability from state n to state m is given by:

$$\mathrm{P}(n \to m) = \left(\frac{\Delta t}{\hbar}\right)^2 \left|\int_{-\infty}^{\infty} \psi_m^*(x)\, W\, \psi_n(x)\, dx\right|^2. \tag{5}$$

For $n = 2$, $m = 3$, and $W = e\xi x$, we have:

$$\mathrm{P}(2 \to 3) = \left(\frac{\Delta t}{\hbar}\right)^2 \frac{4}{L^2} \left|\int_{-L/2}^{L/2} \cos(3\pi x/L)\, e\,\xi\, x\, \sin(2\pi x/L)\, dx\right|^2 \tag{6}$$

$$= \frac{4}{L^2}\left(\frac{e\,\xi\,\Delta t}{\hbar}\right)^2 \left(-\frac{24L^2}{25\pi^2}\right)^2 \tag{7}$$

(f) What is the transition probability between states $n = 2$ and $n = 4$?

For $n = 2$ and $m = 4$, we have:

$$\mathrm{P}(2 \to 4) = \left(\frac{\Delta t}{\hbar}\right)^2 \frac{4}{L^2} \left|\int_{-L/2}^{L/2} \sin(4\pi x/L)\, e\,\xi\, x\, \sin(2\pi x/L)\, dx\right|^2 \tag{8}$$

$$= 0. \tag{9}$$

The integral is null since both $\sin(2\pi x/L)$ and $\sin(4\pi x/L)$ are both odd functions of x, whereas $e\xi x$ is obviously an odd function of x. Thus the integrand is an odd function of x and integration over symmetric bounds will identically yield zero.

(g) Can you deduce a general "selection rule" for this perturbation?

The selection rule arises from Eq. 5: the integrand must be an even function of x. For the current perturbation, $W = e\xi x$, this means that ψ_n and ψ_m must have opposite parity (i.e., if one is even the other must be odd) so that the integrand is even. Note that the product of two even functions is even, the product of two odd functions is even, and the product of an even and an odd function is odd.

(h) How does the selection rule depend on the form of the perturbation?

As just described, the integrand in Eq. 5 must be even for the transition probability to be nonzero. Thus, if the perturbation W is odd (as it is in this example: $W = e\xi x$) then the initial and final states must have opposite parity. In contrast, if W is even, then the initial and final states must have the *same* parity. Finally if W is of mixed parity (e.g., $W = Ax^2 + Bx$), then no transitions are excluded by parity.