

Problem Set 5 Solutions

Problem 1

The energy difference between the ground state (lowest energy level) and first excited state (next level up) in a hydrogen atom is about 10 eV. The diameter of a hydrogen atom is about $1\text{\AA} = 10^{-10}\text{m}$. If we model a hydrogen atom as a 1-D box with hard walls, then what is the length of the box to get the same energy level spacing between the ground state and the first excited state as in hydrogen? How good do you think this analogy is? Can we get the energy level spacing right between the higher energy levels as well?

The energy levels of the square well are given by:

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$

And we want that the energy spacing between the first and second levels is equal to 10eV:

$$\Delta E = 10\text{eV} = \frac{(4-1)\hbar^2 \pi^2}{2mL^2}$$

And solving for L, we have:

$$L = \sqrt{\frac{3\hbar^2 \pi^2}{2m\Delta E}} \approx 0.34\text{nm}$$

A hint: Use Google to calculate this...

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sqr( (3 * hbar^2 * pi^2) / (2 * m_e * 10eV) )
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Problem 2

Consider a particle of mass = m sitting in the ground state of a box of length = L . Suppose that one wall of the box is suddenly moved out so that the length of the box becomes length = 3L .

a) If the energy of the particle is measured right after moving the wall, then what is the probability that the particle will be found in the n = 10 state of the new box?

The wavefunction of the particle immediately after the expansion will be unchanged with respect to the wavefunction before the expansion:

$$\psi_1(x) = \begin{cases} \sqrt{\frac{2}{\pi}} \sin \frac{\pi x}{L} & x \in [0, L] \\ 0 & x \notin [0, L] \end{cases}$$

We wish to calculate the overlap of this wavefunction with the n = 10 excited state of the new well.

$$\Psi_{10}(x) = \begin{cases} \sqrt{\frac{2}{\pi}} \sin \frac{10\pi x}{3L} & x \in [0, 3L] \\ 0 & x \notin [0, 3L] \end{cases}$$

This overlap is:

$$\begin{aligned} \int_0^L \psi_1^*(x) \Psi_1^*(x) &= \int_0^L \frac{2}{\pi} \sin \frac{\pi x}{L} \sin \frac{10\pi x}{3L} \\ &= \frac{9\sqrt{3}L}{91\pi^2} \end{aligned}$$

b) How does this probability change with time?

It doesn't! The probability of being found in a particular eigenstate of the system is independent of time (if the Hamiltonian is not changing).

Problem 3

a) Show that

$$e^{-i\theta\alpha} = \cos \theta I - i \sin \theta \alpha$$

where $\alpha \in \{I, X, Y, Z\}$ is a Pauli matrix is a Pauli matrix.

We can do this by expanding the exponent in a power series:

$$\begin{aligned} e^{-i\theta\alpha} &= I + (-i\theta\alpha) + \frac{1}{2} (-i\theta\alpha)^2 + \frac{1}{6} (-i\theta\alpha)^3 + \dots \\ &= \left(I - \frac{1}{2} (\theta\alpha)^2 + \frac{1}{4!} (\theta\alpha)^4 + \dots \right) - i \left((\theta\alpha) - \frac{1}{3!} (\theta\alpha)^3 + \frac{1}{5!} (\theta\alpha)^5 + \dots \right) \\ &= I \cos(\theta) - i\alpha \sin(\theta) \end{aligned}$$

Where we have used that

$$\alpha^n = \begin{cases} \alpha & n \text{ even} \\ I & n \text{ odd} \end{cases}$$

b) Show that

$$XYX = -Y$$

where X and Y are the Pauli matrices. Write the rotation operator $R_y(\gamma) = e^{-i\gamma Y/2}$ in terms of linear functions of the Pauli matrices. Use these two results to show that

$$XR_y(\gamma)X = R_y(-\gamma)$$

The first thing is the identity above. This can be shown using the anticommutation relations for the Pauli matrices:

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}I$$

Plugging in X, Y, we have

$$XY + YX = 0$$

And multiplying on the right by X (recalling that $X^2 = I$), we have:

$$XYX + YXX = XYX + Y = 0$$

Thus,

$$XYX = -Y$$

Now we can write the rotation operator using the results from part (a):

$$R_y(\gamma) = e^{-i\gamma Y/2} = I \cos(\gamma/2) - iY \sin(\gamma/2)$$

Thus,

$$\begin{aligned} XR_y(\gamma)X &= Xe^{-i\gamma Y/2}X \\ &= XIX \cos(\gamma/2) - iXYX \sin(\gamma/2) \\ &= I \cos(\gamma/2) + iY \sin(\gamma/2) \\ &= I \cos(-\gamma/2) - iY \sin(-\gamma/2) \\ &= R_y(-\gamma) \end{aligned}$$

c) Write the one-qubit operations X and Y in terms of the rotation operators $R_\alpha(\theta)$, $\alpha \in \{x, y, z\}$ on the Bloch sphere, specifying the angles of rotation. [Hint: you may consider their action on the state $|0\rangle$]

Notice the form of the rotation operator:

$$R_\alpha(\theta) = I \cos(\theta/2) - i\alpha \sin(\theta/2)$$

The first thing we notice, is that we want the coefficient of I to be zero, so $\theta = \pm\pi$, giving:

$$R_\alpha(\pm\pi) = \mp i\alpha$$

If we let $\alpha = X$, then we get what we wanted, up to a constant phase of $-i$. The same trick works for Y !