Free Study Material from All Lab Experiments

All Lab Experiments

Quantum Mechanics & Applications Some Important Questions (Solved)

SOME SOLVED EXAMPLES

Problem 1. A particle has the wave function

$$\psi(r) = Ne^{-\alpha r}$$

where N is a normalization factor and α is a known real parameter.

(a) Calculate the factor N.

(b) Caculate the expection values.

$$\langle x\rangle, \langle r\rangle, \langle r^2\rangle$$

in this state.

Solution: (a) The normalization factor is determined from the normalization condition.

$$1 = \int d^3r\,|\psi(r)|^2 = \int_0^\infty dr\, N^2 e^{-1\alpha r} = \frac{\pi N^2}{\alpha^3}$$

which gives

$$N = \sqrt{\frac{\alpha^3}{\pi}}$$

We have used the integral $(n \geq 0)$

$$\int_0^\infty dx\, x^n e^{-x} = \gamma(n+1) = n!$$

(b) The expectation value $\langle x\rangle$ vanishes owing to spherical symmetry. For example,

$$\langle x\rangle = N^2 \int d^3r\, re^{-2\alpha r} = N^2 \int_0^\infty dr\, r^3 e^{-2\alpha r} \int_{-1}^{1} d\cos\theta \sin\theta \int_0^{2\pi} d\phi \cos\phi$$

The expectation value of the radius is

$$\langle r\rangle = N^2 \int d^3r\, re^{-2\alpha r} = 4\pi N^2 \int_0^\infty dr\, r^3 e^{-2ar} = \frac{3}{2\alpha}$$

The expectation value of the radius is

$$\langle r\rangle = \langle r^2\rangle = N^2 \int d^3r\, r^2 e^{-2\alpha r} = 4\pi N^2 \int_0^\infty dr\, r^4 e^{-2ar} = \frac{3}{\alpha^2}$$

Problem 2. Find the probability of finding the praticle between 0.1 to 0.2 of potential well of length L_z.

Solution: The normalization wavefunctions of the various different levels in the potential well are

$$\psi_n(z) = \sqrt{\frac{2}{L_z}}\sin\left(\frac{n\pi z}{L_z}\right)$$

The lowest energy state is $n = 1$, and we are given $L_z = 1\ nm$.

The probability of finding the electron between 0.1 and 0.2 nm from on eside of the well is, using nanometer units for distance.

$$P = \int_{0.1}^{0.2} |\psi_1(z)|^2\, dz = \int_{0.1}^{0.2} 2\sin^2(\pi z) dz$$

$$= \int_{0.1}^{0.2} |\psi_1(z)|^2\, dz = \int_{0.1}^{0.2} [1-\cos(1\pi z)]dz$$

$$= 0.1 - \int_{0.1}^{0.2} \cos(2\pi z) dz$$

$$= 0.1 - \frac{1}{2\pi}[\sin(2\pi\times 0.2) - \sin(2\pi\times 0.1)]$$

$$= 0.042$$

Problem 3. Consider first the commutator $[\hat{z}, \hat{p}_z]$ operating on an arbitary function $|f\rangle$ in the position representation.

Solution: We have

$$[\hat{z},\hat{p}_z]|f\rangle = -i\hbar z\frac{\partial f(z)}{\partial z} + i\hbar\frac{\partial}{\partial z}\{zf(z)\}$$

$$= -i\hbar z\frac{\partial f(z)}{\partial z} + i\hbar z\frac{\partial f(z)}{\partial z} i\hbar f(z)\frac{\partial z}{\partial z}$$

$$= i\hbar|f\rangle$$

and so we can state

$$[\hat{z},\hat{p}_z] = i\hbar$$

Problem 4. A particle moving in one dimension is in a stationary state whose wave funtion

$$\psi(x) = \begin{cases} 0, & x < -a, \\ A\left(1+\cos\frac{\pi x}{a}\right), & -a \le x \le a, \\ 0, & x > a, \end{cases}$$

where A and a are real constant,

(a) Is this a physically acceptable wave funtion? Explian.

(b) Find the magnitude of A so that $\psi(x)$ is normalized.

Solution: (a) Since $\psi(x)$ is square integrable, single-valued, continuous, and has a continuous first derivative, it is physically acceptable.

(b) Normalization of $\psi(x)$: using the relation $\cos^2 y = (1 + \cos 2y)/2$, we have

$$1 = \int_{-\infty}^{+\infty} |y(x)|^2 dx = A^2 \int_{-a}^{a} dx\left[1 + 2\cos\frac{\pi x}{a} + \cos^2\left(\frac{\pi x}{a}\right)\right]$$

$$= A^2 \int_{-a}^{a} dx\left[\frac{3}{2} + 2\cos\frac{\pi x}{a} + \frac{1}{2}\cos\frac{2\pi x}{a}\right]$$

$$= \frac{3}{2}A^2 \int_{-a}^{a} dx = 3aA^2;$$

hence $A = 1/\sqrt{3a}$.

Problem 5. Consider a particle of mass m moving freely between x = 0 and x = a inside an infinite square well potential.

(a) Calculate the expection values $\langle \hat{X} \rangle_{n_2}$ $\langle \hat{P} \rangle_{n_2}$ $\langle \hat{X}^2 \rangle_{n_2}$ and $\langle \hat{P}^2 \rangle_{n_2}$ **and compare them with their classical counterparts.**

Solution: $$\langle \psi_n | \hat{X} | \psi_n \rangle = \int_0^a \psi_n^*(x) x \psi_n(x) dx = \frac{2}{a}\int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx$$

$$= \frac{1}{a}\int_0^a x\left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right] dx = \frac{a}{2},$$

$$= \frac{2}{a}\int_0^a x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{1}{a}\int_0^a x^2\left[1 - \cos\left(\frac{2n\pi x}{a}\right)\right] dx$$

$$= \frac{a^2}{3} - \frac{1}{a}\int_0^a x^2 \cos\left(\frac{2n\pi x}{a}\right) dx$$

$$= \frac{a^2}{3} - \frac{1}{2n\pi} x^2 \sin\left(\frac{2n\pi x}{a}\right)\Bigg|_{x=0}^{x=a} + \frac{1}{n\pi}\int_0^a x \sin\left(\frac{2n\pi x}{a}\right) dx$$

$$= \frac{a^2}{3} - \frac{a}{2n^2\pi^2},$$

$$\left\langle \psi_n \left| \hat{P}^2 \right| \psi_n \right\rangle = -\hbar^2 \int_0^a \psi_n^*(x) \frac{d^2\psi_n(x)}{dx^2} dx$$

$$= \frac{n^2\pi^2\hbar^2}{a^2} \int_0^a |\psi_n(x)|^2 \, dx = \frac{n^2\pi^2\hbar^2}{a^2}.$$

In deriving the previous three expresssion, we have used integrations by parts. Since $E_n = n^2\pi^2\hbar^2/(2ma^2)$, we may write

$$\left\langle \psi_n \left| \hat{P}^2 \right| \psi_n \right\rangle = \frac{n^2\pi^2\hbar^2}{a^2} = 2mE_n.$$

Problem 6. Using $\left[\hat{X}, \hat{P}\right] = i\hbar$, calculate the various commutation relations between the following operatores[2].

$$\hat{T}_1 = \frac{1}{4}\left(\hat{P}^2 - \hat{X}^2\right), \quad \hat{T}_2 = \frac{1}{4}\left(\hat{X}\hat{P} + \hat{P}\hat{X}\right), \quad \hat{T}_3 = \frac{1}{4}\left(\hat{P}^2 + \hat{X}^2\right).$$

Solution: The operators $\hat{T}_1$, $\hat{T}_2$, and $\hat{T}_3$ can be viewed as describing some sort of collective vibrations; $\hat{T}_3$ has the structure of a harmonic oscillator Hamoltonian. The first commulator can be calculated as follows:

$$\left[\hat{T}_1, \hat{T}_2\right] = \frac{1}{4}\left[\hat{P}^2 - \hat{X}^2, \hat{T}_2\right] = \frac{1}{4}\left[\hat{P}^2, \hat{T}_2\right] - \frac{1}{4}\left[\hat{X}^2, \hat{T}_2\right],$$

where, using the commutation relation $\left[\hat{X}, \hat{P}\right] = i\hbar$, we have

$$\left[\hat{P}^2, \hat{T}_2\right] = \frac{1}{4}\left[\hat{P}^2 - \hat{X}\hat{P}\right] + \frac{1}{4}\left[\hat{P}^2, \hat{P}\hat{X}\right]$$

$$= \frac{1}{4}\hat{P}\left[\hat{P}, \hat{X}\hat{P}\right] + \frac{1}{4}\left[\hat{P}, \hat{X}\hat{P}\right]\hat{P} + \frac{1}{4}\hat{P}\left[\hat{P}, \hat{P}\hat{X}\right] + \frac{1}{4}\left[\hat{P}, \hat{P}\hat{X}\right]\hat{P}$$

$$= \frac{1}{4}\hat{P}\left[\hat{P}, \hat{X}\right]\hat{P} + \frac{1}{4}\left[\hat{P}, \hat{X}\right]\hat{P}^2 + \frac{1}{4}\hat{P}^2\left[\hat{P}, \hat{X}\right] + \frac{1}{4}\hat{P}\left[\hat{P}, \hat{X}\right]\hat{P}$$

$$= -\frac{i\hbar}{4}\hat{P}^2 - \frac{i\hbar}{4}\hat{P}^2 - \frac{i\hbar}{4}\hat{P}^2 - \frac{i\hbar}{4}\hat{P}^2 = -i\hbar\hat{P}^2$$

$$\left[\hat{X}^2, \hat{T}_2\right] = \frac{1}{4}\left[\hat{X}^2, \hat{X}\hat{P}\right] + \frac{1}{4}\left[\hat{X}^2, \hat{P}\hat{X}\right]$$

$$= \frac{1}{4}\hat{X}\left[\hat{X}, \hat{X}\hat{P}\right] + \frac{1}{4}\left[\hat{X}, \hat{X}\hat{P}\right]\hat{X} + \frac{1}{4}\hat{X}\left[\hat{X}, \hat{P}\hat{X}\right] + \frac{1}{4}\left[\hat{X}, \hat{P}\hat{X}\right]\hat{X}$$

$$= \frac{1}{4}\hat{X}^2\left[\hat{X},\hat{P}\right] + \frac{1}{4}\hat{X}\left[\hat{X},\hat{P}\right]\hat{X} + \frac{1}{4}\hat{X}\left[\hat{X},\hat{P}\right]\hat{X} + \frac{1}{4}\left[\hat{X},\hat{P}\right]\hat{X}^2$$

$$= \frac{i\hbar}{4}\hat{X}^2 + \frac{i\hbar}{4}\hat{X}^2 + \frac{i\hbar}{4}\hat{X}^2 + \frac{i\hbar}{4}\hat{X}^2 = i\hbar\hat{X}^2,$$

hence

$$\left[\hat{T}_1,\hat{T}_2\right] = \frac{1}{4}\left[\hat{P}^2 - \hat{X}^2,\hat{T}_2\right] = \frac{1}{4}\left(i\hbar\hat{P}^2 + i\hbar\hat{X}\right) = -i\hbar\hat{T}_3$$

The second commutator is calculated as follows:

$$\left[\hat{T}_2,\hat{T}_3\right] = \frac{1}{4}\left[\hat{T}_2,\hat{P}^2 + \hat{X}^2\right] = \frac{1}{4}\left[\hat{T}_2,\hat{P}^2\right] + \frac{1}{4}\left[\hat{T}_2,\hat{X}^2\right],$$

where $\left[\hat{T}_2,\hat{P}^2\right]$ and $\left[\hat{T}_2,\hat{X}^2\right]$ were calculated in (5.290) and (5.291):

$$\left[\hat{T}_2,\hat{P}^2\right] = i\hbar\hat{P}^2,\ \left[\hat{T}_2,\hat{X}^2\right] = -i\hbar\hat{X}^2.$$

Thus, we have

$$\left[\hat{T}_2,\hat{T}_3\right] = \frac{1}{4}\left(i\hbar\hat{P}^2 - i\hbar\hat{X}^2\right) = i\hbar\hat{T}_1.$$

The third commutator is

$$\left[\hat{T}_3,\hat{T}_1\right] = \frac{1}{4}\left[\hat{T}_3,\hat{P}^2 - \hat{X}^2\right] = \frac{1}{4}\left[\hat{T}_3,\hat{P}^2\right] - \frac{1}{4}\left[\hat{T}_3,\hat{X}^2\right],$$

where

$$\left[\hat{T}_3,\hat{P}^2\right] = \frac{1}{4}\left[\hat{P}^2,\hat{P}^2\right] + \frac{1}{4}\left[\hat{X}^2,\hat{P}^2\right] = \frac{1}{4}\left[\hat{X}^2,\hat{P}^2\right] = \frac{1}{4}\hat{X}\left[\hat{X},\hat{P}^2\right] + \frac{1}{4}\left[\hat{X},\hat{P}^2\right]\hat{X}$$

$$= \frac{1}{4}\hat{X}\hat{P}\left[\hat{X},\hat{P}\right] + \frac{1}{4}\hat{X}\left[\hat{X},\hat{P}\right]\hat{P} + \frac{1}{4}\hat{P}\left[\hat{X},\hat{P}\right]\hat{X} + \frac{1}{4}\left[\hat{X},\hat{P}\right]\hat{P}\hat{X}$$

$$= \frac{i\hbar}{4}\left(2\hat{X}\hat{P} + 2\hat{P}\hat{X}\right) = \frac{i\hbar}{4}\left(\hat{X}\hat{P} + \hat{P}\hat{X}\right)$$

$$\left[\hat{T}_3,\hat{X}^2\right] = \frac{1}{4}\left[\hat{P}^2,\hat{X}^2\right] + \frac{1}{4}\left[\hat{X}^2,\hat{X}^2\right] = \frac{1}{4}\left[\hat{P}^2,\hat{X}^2\right] = -\frac{i\hbar}{2}\left(\hat{X}\hat{P} + \hat{P}\hat{X}\right);$$

hence

$$\left[\hat{T}_3,\hat{T}_1\right] = \frac{1}{4}\left[\hat{T}_3,\hat{P}^2\right] - \frac{1}{4}\left[\hat{T}_3,\hat{X}^2\right] = \frac{i\hbar}{8}\left(\hat{X}\hat{P} + \hat{P}\hat{X}\right) + \frac{i\hbar}{8}\left(\hat{X}\hat{P} + \hat{P}\hat{X}\right)$$

$$= \frac{i\hbar}{8}\left(\hat{X}\hat{P}+\hat{P}\hat{X}\right) = i\hbar\hat{T}_2.$$

These relation are similar to those of ordinary angular momentum, save for the minus sigh in $\left[\hat{T}_1, \hat{T}_2\right] = -i\hbar\hat{T}_3$.

Problem 7. In a region of space, a particle with mass m and zero energy has a time-independent wave function

$$\psi(x) = Axe^{-x^2/L^2} \qquad ...(1)$$

where A and L constant.

• **Determine the potential energy $U(x)$ of the particle?**

Solution. Time independent Schrodinger eqution for the wavefunction $\psi(x)$ of a particle of mass m in a potential $U(x)$.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x) = E\psi(x) \qquad ...(2)$$

When a particle a particle with zero energy has wavefunction $\psi(x)$ given bh Eq. (1), it follows on substitution into Eq. (2) that

$$U(x) = \frac{2\hbar^2}{mL^4}\left(x^2-\frac{3L^2}{2}\right) \qquad ...(3)$$

$U(x)$ is a parabola centred at $x = 0$ with $U(0) = -3\hbar^2 mL^2$.

Problem 8. A proton is confined in an infinite square well of width 10 fm. (The nuclear potential that binds protons and neutrns in the nucleus of an atom is often approximated by an infinite square well potential.

- **Calculatethe energy and wavelength of the photon emitted when the proton undergoes a transition from the furst excited state (n = 2) to the groun d state (n = 1).**
- **In what region of the electromagnetic spectrum does this wavelength belong?**

Solution. Energy E_n of a photon of mass in the nth energy state of an infinite square well potential with width L.

$$E_n = \frac{n^2\hbar^2}{8mL^2}$$

The energy E and wavelength λ of a photon emitted as the particle makes a transition from the n = 2 state to the n = 1 state are

$$E = E_2 - E_1 = \frac{3\hbar^2}{8mL^2}$$

$$\lambda = \frac{\hbar c}{E}$$

For a proton (m = 938 MeV/c^2), E = 6.15 MeV and λ = 202fm. The wavelength is in the gamma ray region of the spectrum.

Problem 9. A 1.00 g marble is constrained to roll inside a tube of length L = 1.00 cm. The tube is capped at both ends.

Solution:

- Modsling this as a one-dimensional infinite square well, determine the value of the quantum number n if the marble is initially given an energy of 1.00 mJ.
- Calculate the exitation energy required to proton the marble to the next available energy state.

The allowed energy values E_n for a particle of mass m in a one-dimensional infinite square well potential of width L are given

$$n = 4.27 \times 10^{28}$$

when E_n = 1.00 mJ.

The excitation energy E required to promote the marble to thr next availabel enrgy state is

$$E = E_{n+1} - E_n = \frac{(2n+1)\hbar^2}{8mL^2} = 4.69 \times 10^{-23} J.$$

This example illustrates the large quantum number and small energy differences associated with the behavior of macroscopic objects.

Problem 10. The wave function

$$\psi(x) = Axe^{-\alpha x^2}$$

describe a state of a harmonic oscillator provided the constant α is chosen appropriately.

- **Using the Schrondinger Eq., determine an expression for α in terms of the oscillator mass m and the classical frequency of vibration ω.**
- **Determine the energy of this state and noumalize the wave function.**

Solution. Schrodinger equation for a harmonic oscillator when

$$U(x) = \frac{1}{2}Kx^2 = \frac{1}{2}m\omega^2 x^2 \text{ where } \omega = \omega_{\text{classical}} = \sqrt{\frac{K}{m}}$$

$\psi(x)$ given by Eq. (53) satisfies Eq. (20) when

$$\alpha = \frac{m\omega}{2\hbar} \text{ and } E = \frac{3}{2}\hbar\omega$$

Eq. gives the wave function of the excited state of the harmonic oscillator. Requiring that

$$\int_{-\infty}^{+\infty} \left|\psi(x)^2\right| dx = 1$$

yeilds $$|A| = \left(\frac{32\alpha^3}{\pi}\right)^{1/4}$$

Problem 11. An electron is describe by the wave function

$$\psi(x) = \begin{cases} 0 & \text{for } x < 0 \\ Ce^{-x}(1-e^{x}) & \text{for } x > 0 \end{cases}$$

where x is in nm and C is a constant.

- **Determine the value of C that normalizes $\psi(x)$.**
- **Where is the electron must likely to be found? That is, for what value of x is the probability of finding the electron the largest?**
- **Calculate the average position $\langle x \rangle$ for the electron. Compare this result the most likely position, and comment on the difference.**

Solution: An electron is described by the wave function $\psi(x)$ given by Eq. normalization contion-yields-

$$|C| = 2\sqrt{3}nm^{-1/2}$$

The most likely place x_m for the electron to be is where $|\psi(x)|^2$ is maximum or, in this case, where $\psi(x)$ is maximum. It follows from Eq. (58) that

$$x_m = 1n\ 2nm = 0.693\ nm$$

It follows from Eqs. that the average position $\langle x \rangle$ of a particle state $\psi(x)$ is

$$\langle x \rangle = \int_{-\infty}^{+\infty} x|\psi(x)|^2 dx$$

It follows from Eqs. (58) and (61) that

$$\langle x \rangle = \frac{13}{12}nm \simeq 1.083nm.$$

$\langle x \rangle > x_m$ because, according to given equation, values of $\langle x \rangle > x_m$ are weighted more heavily in determining $\langle x \rangle$.

Problem 12. Find LS spectral terms for non-equivalent electrons (npnd) and also show what LS & JJ coupling schemes are the same. [Important]

Solution:

- *npnd*, i.e., *p* & *d* optically active electrons:
- $L = |l_1 - l_2| ...(l_1 + l_2)$ but $l_1 = 1, l_2 = 2 \Rightarrow L = 1, 2, 3$
- $S = |s_1 - r_2| ... (s_1 + s_2) \Rightarrow S = 0, 1\ (s_1 = s_2 = ½)$

$S = 0$ $L = 1$ ${}^1P$
$S = 0$ $L = 2$ ${}^1D$
$S = 0$ $L = 3$ ${}^1F$
$S = 1$ $L = 1$ ${}^3P$
$S = 1$ $L = 2$ ${}^3D$
$S = 1$ $L = 3$ ${}^3F$

- Produce 6 terms: ${}^1P$, ${}^1D$, ${}^1F$, ${}^3P$, ${}^3D$, ${}^3F$
- Taking J into account in each case
- $J = |L - S| \ldots (L + S)$
- e.g., for ${}^3F$, $L = 3$, $S = 1 \Rightarrow J = 2, 3, 4$
  thus full levels are ${}^3F_2$, ${}^3F_3$, ${}^3F_4$
  $S = 0$ $L = 1$ $J = 1$ ${}^1P_1$
  $S = 0$ L $= 2$ $J = 2$ ${}^1D_2$
  $S = 0$ $L = 3$ $J = 3$ ${}^1F_3$
  $S = 1$ $L = 1$ $J = 0, 1, 2$ ${}^3P_0$, ${}^3P_1$, ${}^3P_2$
  $S = 1$ $L = 2$ $J = 1, 2, 3$ ${}^3D_1$, ${}^2D_2$, ${}^3D_3$
  $S = 1$ $L = 3$ $J = 2, 3, 4$ ${}^3F_2$, ${}^3F_3$, ${}^3F_4$
- In total there are 12 levels for the 6 terms ${}^1P$, ${}^1D$, ${}^1F$, ${}^3P$, ${}^3D$, ${}^3F$

Both approaches LS and JJ are the same. As you can find in this example. All the spectral terms are same. Do this examples if anybody asks to prove that the LS and JJ coupling are the same.

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