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Homework 1 Professor: Dr. Jaimes

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Contents

1	Problem 4.2	1
2	Problem 4.3	2
3	Problem 4.13	2
4	Problem 4.14	3
5	Problem 4 23	9

1 Problem 4.2

Use separation of variable in *cartesian* coordinates to solve the infinite *cubical* well (or particle in a box):

$$V(x,y,z) = \begin{cases} 0, & \forall x,y,z \in [0,a] \\ \infty, & \forall x,y,z \notin [0,a] \end{cases}$$

- 1. Find the stationary states, and the corresponding energies.
- 2. Call the distinct energies E_1, E_2, \ldots in order of increasing energy. Find E_1, E_2, E_3, E_4, E_5 and E_6 . Determine their degeneracies (that is, the number of different states that share the same energy).
- 3. What is the degeneracy of E_{14} , and why is this case interesting?

Solution 1: Stationary states

To find the stationary states of the infinite cubical well, we are going to solve the time independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\nabla\psi=E\psi,\ \forall x,y,z\in[0,a],$$

with the following boundary conditions $\psi(0,0,0) = \psi(a,a,a) = 0$. To solve the equation we are going to use the method of separation of variables, that is, that we assume that the solution of the differential equation has the following form $\psi(x,y,z) = X(x)Y(y)Z(z)$. Substituting this solution to the differential equation, we can perform

Quantum Optics March 10, 2024

some algebraic manipulation,

$$\begin{split} -\frac{\hbar^2}{2m}\nabla\psi &= E\psi\\ \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) X(x)Y(y)Z(z) = -\frac{2m}{\hbar^2} EX(x)Y(y)Z(z)\\ Y(y)Z(z)\frac{\partial^2}{\partial x^2} X(x) + X(x)Z(z)\frac{\partial^2}{\partial y^2} Y(y) + X(x)Y(y)\frac{\partial^2}{\partial z^2} Z(z) = -\frac{2m}{\hbar^2} EX(x)Y(y)Z(z)\\ \frac{1}{X(x)}\frac{\partial^2}{\partial x^2} X(x) + \frac{1}{Y(y)}\frac{\partial^2}{\partial y^2} Y(y) + \frac{1}{Z(z)}\frac{\partial^2}{\partial z^2} Z(z) = -\frac{2m}{\hbar^2} E \end{split}$$

2 Problem 4.3

Use

$$P_l^m(x) \equiv \left(1 - x^2\right)^{|m|/2} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^{|m|} P_l(x)$$

$$P_l(x) \equiv \frac{1}{2l!} \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^l \left(x^2 - 1\right)^l$$

$$Y_l^m(\theta, \phi) = \epsilon \sqrt{\frac{(2l+1)}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}} e^{im\phi} P_l^m(\cos[\theta])$$

to construct Y_0^0 and Y_2^l . Check that they are normalized and orthogonal.

3 Problem 4.13

- Find $\langle r \rangle$ and $\langle r^2 \rangle$ for an electron in the ground state of hydrogen. Express your answers in terms of the Bohr radius.
- Find $\langle x \rangle$ and $\langle x^2 \rangle$ for an electron in the ground stat of hydrogen. *Hint:* this requires no noew integration-note that $r^2 = x^2 + y^2 + z^2$, and explot the symmetry of the ground state.
- Find $\langle x^2 \rangle$ in the state n=2, l=1, m=1. Warning: This state is not symmetrical in x, y, z. Use $x=r\sin\theta\cos\phi$.

Quantum Optics March 10, 2024

4 Problem 4.14

What is the *most probable* value of r, in the ground state of hydrogen? (The answer is not zero!) *Hint:* First ypu must figure out the probability that the electron would be found between r and r + dr.

5 Problem 4.23

In problem 4.3 you showed that

$$Y_2^l(\theta,\phi) = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{i\phi}.$$

Apply the raising operator to find $Y_2^2(\theta,\phi)$. Use equation $A_l^m = \hbar\sqrt{l(l+1) - m(m\pm 1)} = \hbar\sqrt{(l\mp m)(l\pm m+1)}$ to get the normalization.

[heading=bibintoc,title=References]