Homework 1

Professor: Dr. Jaimes

Francisco Javier Vázquez Tavares A00827546

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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 perfom some algebraic manipulation,

$$-\frac{\hbar^2}{2m}\nabla\psi = E\psi$$

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)X(x)Y(y)Z(z) = -\frac{2m}{\hbar^2}EX(x)Y(y)Z(z)$$

$$Y(y)Z(z)\frac{\partial^2}{\partial x^2}X(x)+X(x)Z(z)\frac{\partial^2}{\partial y^2}Y(y)+X(x)Y(y)\frac{\partial^2}{\partial z^2}Z(z) = -\frac{2m}{\hbar^2}EX(x)Y(y)Z(z)$$

$$\frac{1}{X(x)}\frac{\partial^2}{\partial x^2}X(x)+\frac{1}{Y(y)}\frac{\partial^2}{\partial y^2}Y(y)+\frac{1}{Z(z)}\frac{\partial^2}{\partial z^2}Z(z) = -\frac{2m}{\hbar^2}E.$$

Now we can re-write this partial differential equation into three diferential equations assumming that $E=\frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)$,

$$\frac{\mathrm{d}^2X(x)}{\mathrm{d}x^2} = -k_x^2X(x) \to X(x) = A_x\sin[k_xx]+B_x\cos[k_xx],$$

$$\frac{\mathrm{d}^2Y(y)}{\mathrm{d}y^2} = -k_y^2Y(y) \to Y(y) = A_y\sin[k_yy]+B_y\cos[k_yy],$$

$$\frac{\mathrm{d}^2Z(z)}{\mathrm{d}z^2} = -k_z^2Z(z) \to Z(z) = A_z\sin[k_zz]+B_z\cos[k_zz].$$

In order to find the expression for the coefficients $A_n,\ B_n$ and k_n, we start by applying the boundary conditions. Since sin and cos are periodic functions, they satisfy $f(0)=f(a)$, however only the sin function satisfy the condition $f(0)=f(a)=0$, hence, we set $B_x=B_y=B_z=0$ leading to,

$$X(x)=A_x\sin[k_xx],\quad Y(y)=A_y\sin[k_yy],\quad Z(z)=A_z\sin[k_zz].$$

Now we recall the fact that x, y and z have units of distance and that the argument of the sin function must be dimensonless, combining this restriction with the property of periodicity we can define the constants k_n as, $k_x=n_x\pi/a,\ k_y=n_y\pi/a,\ k_z=n_z\pi/a$, where $(n_x,n_y,n_z)\in\mathbb{Z}^+$. With this information we can re-write the solution as,

$$\psi(x,y,z)=A_xA_yA_z\sin\left[\frac{n_x\pi}{a}x\right]\sin\left[\frac{n_y\pi}{a}y\right]\sin\left[\frac{n_z\pi}{a}z\right],$$

with

$$E=\frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2+n_y^2+n_z^2\right),\quad (n_x,n_y,n_z)\in\mathbb{Z}^+.$$

Finally, in order to get the expression for A_x, A_y and A_z we apply the normalization restiction to each spatial dimension,

$$\int_0^a A_l^2\sin^2\left[\frac{n_l\pi}{a}s\right]ds = A_l^2\frac{a}{4}\left(2-\frac{1}{\pi n}\sin[2\pi n]\right)=1,$$

since $n\in\mathbb{Z}^+$ we get that $A_l=\sqrt{2/a}$, therefore,

$$\boxed{\psi(x,y,z)=\sqrt{\frac{8}{a^3}}\sin\left[\frac{n_x\pi}{a}x\right]\sin\left[\frac{n_y\pi}{a}y\right]\sin\left[\frac{n_z\pi}{a}z\right],\quad (n_x,n_y,n_z)\in\mathbb{Z}^+}$$

Solution 2: Energy analysis

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 $x = r \sin\theta \cos\phi$.

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.

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