Lecture 11:3D Problems

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QM I _ Fall 2019

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- [ ] 3D Problems in Cartesian Coordinates

- [ ] 3D Problems in Spherical Coordinates
  - Radial Schrödinger's eq
  - Harmonic Oscillator
  - Hydrogen Atom

Cartesian Coordinates

$$\vec{P} = (\hat{P}_x, \hat{P}_y, \hat{P}_z) \quad , \quad \vec{R} = (\hat{X}, \hat{Y}, \hat{Z})$$

$$V(\vec{R}) = V(\hat{X}) + V(\hat{Y}) + V(\hat{Z})$$

Assumptions

* Independent of time

* Seprable terms → No $\hat{X}\hat{Y}$ terms

$$V(\vec{R}) = V(\hat{X}) + V(\hat{Y}) + V(\hat{Z})$$

$$= V(X) \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes V(Y) \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes V(Z)$$

$$\Rightarrow \quad H = H_x \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes H_y \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes H_z$$

$$H_x = \frac{\hat{P}_x^2}{2m} + \hat{V}(x)$$

$$H(z) = \frac{\hat{P}_z^2}{2m} + \hat{V}(z)$$

$$H_y = \frac{\hat{P}_y^2}{2m} + \hat{V}(y)$$

To find the eigenvectors of H, we can seperately find the eigen vectors:

$$H\,|\psi_n\rangle = E_n|\psi_n\rangle \Rightarrow |\psi_n\rangle = |\psi_n^x\rangle \otimes |\psi_n^y\rangle \otimes |\psi_n^z\rangle$$

$$: \quad H_x|\psi_n^x\rangle = E_n^x|\psi_x\rangle$$

$$H_y|\psi_n^y\rangle = E_n^y|\psi_y\rangle \qquad E_n = E_n^x + E_n^y + E_n^z$$

$$H_z|\psi_n^z\rangle = E_n^z|\psi_z\rangle$$

Similar to any time-indep Hamiltonian

$$\psi_n(\vec{r},t) = \psi_n(\vec{r})\, e^{-i\frac{E_n t}{\hbar}}$$

But $\psi_n(r) = \langle \vec{r}\,|\,\psi_n\rangle = \underbrace{\langle x|\psi_n^x\rangle}\,\underbrace{\langle y|\psi_n^y\rangle}\,\underbrace{\langle z|\psi_n^z\rangle}$

$$\psi_n(x,y,z) = X_n(x)\; Y_n(y)\; Z_n(z)$$

So, to find $\psi_n(x,y,z)$, we need to find

$$X_n(x) = \langle x|\psi_n^x\rangle \longrightarrow |\psi_n^x\rangle$$

$$X_n(x) = \langle x | \psi_n^x \rangle \rightarrow |\psi_n^x\rangle$$

$$Y_n(y) = \langle y | \psi_n^y \rangle \rightarrow |\psi_n^y\rangle$$

$$Z_n(z) = \langle z | \psi_n^z \rangle \rightarrow |\psi_n^z\rangle$$

We can also solve the time-indep Schrödinger's eq.

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}(x)\right] X_n(x) = E_n^x X_n(x)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dy^2} + \hat{V}(y)\right] Y_n(y) = E_n^y Y_n(y)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2} + \hat{V}(z)\right] Z_n(z) = E_n^z Z_n(z)$$

Examples

* Free particle in 3D:

$$\hat{V}_x = \hat{V}_y = \hat{V}_z = 0$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} X(x) = E^x X(x) \Rightarrow X(x) = A e^{-ik_x x} + B e^{ik_x x}$$

Similarly for y & z:

Similarly for y & z:

$$\psi_{\vec{k}}(x,y,z,t) = A\, e^{i(\vec{k}\cdot\vec{r} - \omega t)}$$

$$|k| = \sqrt{k_x^2 + k_y^2 + k_z^2} \rightarrow \text{infinite degeneracy.}$$

Could travel in any direction with the same energy.

$$A = \sqrt{\frac{1}{(2\pi)^3}} \Rightarrow \langle \psi_{\vec{k}}(t) | \psi_{\vec{k}'}(t) \rangle = \delta(\vec{k} - \vec{k}')$$

$\rightarrow$ We could also have wavepackets.

Potential Well in 3D. Potential Box

$$V(x,y,z) = \begin{cases} 0 & 0<x<a,\ 0<y<b,\ 0<z<c \\ \infty & \text{else} \end{cases}$$

$$\Rightarrow X_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi x}{a}\right)$$

$$Y_n(x) = \sqrt{\frac{2}{b}} \sin\left(\frac{n_y \pi y}{b}\right)$$

$$Z_n(z) = \sqrt{\frac{2}{c}} \sin\left(\frac{n_z \pi z}{c}\right)$$

$$E_n = \frac{\hbar^2 \pi^2}{2m} \left[\left(\frac{n_x}{a}\right)^2 + \left(\frac{n_y}{b}\right)^2 + \left(\frac{n_z}{c}\right)^2 \right]$$

degeneracy for the potential box $(a=b=c)$

$(n_x, n_y, n_z) = (1,1,1) \longrightarrow E_1 = \frac{3}{2} \frac{\hbar^2 \pi^2}{ma^2}$ $\quad g=1$

$(1,1,2) = (2,1,1) = (1,2,1) = \frac{3\hbar^2\pi^2}{ma^2}$ $\quad g=3$

$(2,2,1) : \frac{9}{2} \frac{\hbar^2 \pi^2}{ma^2}$ $\quad g=3$

(A) For large enough $E(n)$, find dn, the number of states that are between E & $E+dE$.

Hint: $dn = \rho(n)\, dE$

ρ ↓ density of states

Harmonic Oscillator

$$V(\vec{R}) = \frac{1}{2} m\omega_x^2 \hat{X}^2 + \frac{1}{2} m\omega_y^2 \hat{Y}^2 + \frac{1}{2} m\omega_z \hat{Z}^2$$

$$\Rightarrow X_n(x) : \left(\frac{P^2}{2m} + \frac{1}{2} m\omega_x^2 \hat{X}^2\right) X_n(x) = E_n^x X_n(x)$$

Similarly for $Y_n(y)$ & $Z_n(z)$.

$$\Rightarrow E_n = \hbar\omega_x (n_x + 1/2) + \hbar\omega_y (n_y + 1/2) + \hbar\omega_z (n_z + 1/2).$$

Isotropic HO : $\omega_x = \omega_y = \omega_z$

$$E_n = \hbar\omega \left(n_x + n_y + n_z + 3/2 \right)$$

$$g_0 = 1 \Rightarrow E_0 = \frac{3}{2}\hbar\omega$$

$$g_1 = 3 \Rightarrow E_1 = \frac{5}{2}\hbar\omega \qquad (1,0,0), (0,1,0), (0,0,1)$$

$$g_2 = 6 \Rightarrow E_2 = \frac{7}{2}\hbar\omega \qquad (110), (101)(011)(200)(020)(002)$$

$$\vdots$$

(A) Show that for H.O.

$$g_n = \frac{1}{2}(n+1)(n+2).$$