

PHYS213 Paper

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Abstract

Up to now, we only considered, in previous chapters, the quantum mechanics in one dimensional space. We need to extend the quantum idea in more degree of freedom, i.e., for 3D space, as well as the central force for atoms. Further, we aim to distinguish the *sharp* observables.

1 PARTICLE IN A THREE-DIMENSIONAL BOX

We consider a Cubic box whose length L . Inside this box a free particle collide with *smooth* elastically with box' walls, preserving the magnitude of each momentum component, in addition to the total energy. This means that the particle occupies the region $0 < x, y, z < L$.

Since this is a three dimensional coordinate, the wavefunction Ψ is a function of the position vector $\vec{r} = (x, y, z)$. The probability density $|\Psi(\vec{r})|^2$ is a *probability per volume*. Thus, the **Schrödinger's equation** is given by

$$-\frac{\hbar}{2m}\nabla^2\Psi + U(\vec{r}) = i\hbar\frac{\partial\Psi}{\partial t} \quad (1)$$

2 CENTRAL FORCES AND ANGULAR MOMENTUM

In contrast of the Cartesian coordinates, we turn our attention to the spherical coordinates, since it is more convenient while dealing with **central forces**. In atoms situation, the central force is the Coulomb attractive force originating from the nucleus, affecting on electrons. Now the vector position becomes $\vec{r} = (r, \theta, \phi)$, as in Figure 1. It is important to note that in orbiting electron, its angular momentum \vec{L} is only *sharp* along a chosen axis while the others components being

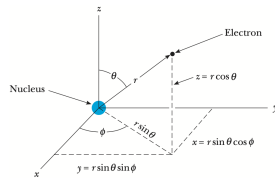


Figure 1: Spherical coordinates for an electron.

"fuzzy". Thus, it is impossible to specify simultaneously any two components of angular momentum, so we take L_z as the sharp component.

Using separation of variables so that the spatial wavefunction becomes $\psi(\vec{r}) = \psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$ so we can find an easy solution for the wavefunction. Then we can find that the sharp observable $|\vec{L}|$, L_z , and E for central force. We have

$$\begin{aligned} |\vec{L}| &= \sqrt{\ell(\ell+1)}\hbar & \ell &= 0, 1, \dots, (n-1) \\ L_z &= m_\ell\hbar & m_\ell &= 0, \pm 1, \dots, \pm\ell \end{aligned}$$

3 SPACE QUANTIZATION

Last time we know that the orientation of the angular momentum vector \vec{L} is specified by the numbers ℓ and m_ℓ . The fact that the direction of \vec{L} is quantized with respect to an axis is called **space quantization**. This naming is because of **this property does not originate from the law of force but derives from the space structure itself**.

4 ATOMIC HYDROGEN

Now we want to consider the easiest real atom, that is hydrogen. Using the Coulomb's law to find the radial potential and the wavefunction for central force, we can conclude the following result for **hydrogen-like ions**

$$\Psi(r, \theta, \phi, t) = R(r) Y_\ell^{m_\ell}(\theta, \phi) e^{-i\omega t} \quad (2)$$

The number n is called the **principal quantum number**. It specifies the **shell**, and for each number $n = 1, 2, 3, \dots$ has a corresponding name K, L, M, \dots so on. Likewise, the **orbital quantum number** $\ell = 0, 1, 2, \dots$ represents the subshells, named with s, p, d, f, \dots so on. In **optical transitions**, photons carry off corresponding energy difference between the states. But not all transitions can occur. To conserve the *total* angular momentum, the angular momentum of the electron must differ by exactly one unit, that is

$$\Delta\ell = \pm 1 \quad \text{and} \quad \Delta m_\ell = 0, \pm 1$$