Lesson 10: Schrödinger equation in three dimensions

Clara E. Alonso Alonso

May 3, 2012

Let's assume $V(\vec{r}) = V_x(x) + V_y(y) + V_z(z)$

T. I. Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\bigtriangledown^2 + V_x(x) + V_y(y) + V_z(z)\right]\Psi(\vec{r}) = E\Psi(\vec{r})$$

We search for solutions of type

$$\Psi(\vec{r}) = X(x)\,Y(y)\,Z(z)$$

Separation of variables, Schrodinger Eq. is linear and homogeneous in $\Psi(\vec{r})$

$$-\frac{\hbar^2}{2m}\left[YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2}\right] + YZV_x(x)X + XZV_y(y)Y + XYV_z(z)Z = E\,XYZ$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2}\right] + V_x(x) + V_y(y) + V_z(z) = E$$

Assume that we vary only $x \quad \rightarrow$

$-\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2} + V_x(x) \quad \rightarrow$ does not vary because

$$-\frac{\hbar^2}{2m}\left[\frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2}\right] + V_y(y) + V_z(z) - E$$

does not vary $\quad \rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{X}\frac{d^2X}{dx^2} + V_x(x) = E_x$ constant

analogously $\quad \rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{Y}\frac{d^2Y}{dy^2} + V_y(y) = E_y$ constant

$-\frac{\hbar^2}{2m}\frac{1}{Z}\frac{d^2Z}{dz^2} + V_z(z) = E_z$ constant

where $\quad E_x + E_y + E_z = E$

We have to solve three one-dimensional Schrödinger equations

Let's consider a box with edges $2a,\ 2b$ and $2c$ origin centered

Potential that describes the particle confined in such a box

$$
\begin{aligned}
V_x(x) &= 0 \qquad -a < x < a \quad ; \quad V_x(x) = \infty \quad |x| \geq a \\
V_y(y) &= 0 \qquad -b < y < b \quad ; \quad V_y(y) = \infty \quad |y| \geq b \\
V_z(z) &= 0 \qquad -c < z < c \quad ; \quad V_z(z) = \infty \quad |z| \geq c
\end{aligned}
$$

The solutions are obtained right away since the equations and boundary conditions are the ones of the 1D infinite well

$$X(x) = \frac{1}{\sqrt{a}} \left\{ \begin{array}{c} \cos \\ \sin \end{array} \right\} \frac{n_x \pi x}{2a} \quad ; \quad E_x = \frac{\pi^2 \hbar^2}{8ma^2} n_x^2$$

$$Y(y) = \frac{1}{\sqrt{b}} \left\{ \begin{array}{c} \cos \\ \sin \end{array} \right\} \frac{n_y \pi y}{2b} \quad ; \quad E_y = \frac{\pi^2 \hbar^2}{8mb^2} n_y^2$$

$$Z(z) = \frac{1}{\sqrt{c}} \left\{ \begin{array}{c} \cos \\ \sin \end{array} \right\} \frac{n_z \pi y}{2c} \quad ; \quad E_z = \frac{\pi^2 \hbar^2}{8mc^2} n_z^2$$

$n_x,\ n_y,\ n_z = 1, 2, 3 \cdots$

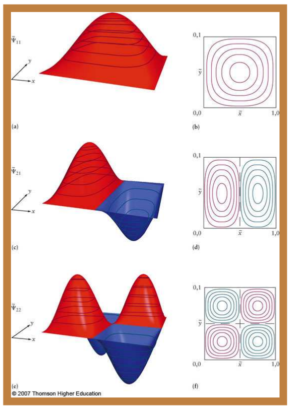
$\cos$ ($\sin$) are related with odd (even) n

$$\Psi_{n_x, n_y, n_z}(x, y, z) = X_{n_x}(x) Y_{n_y}(y) Z_{n_z}(z)$$

$$E = \frac{\pi^2 \hbar^2}{8m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

Ground state $n_x = n_y = n_z = 1$

Figure: $\Psi_{1,1}$ $\Psi_{2,1}$ $\Psi_{2,2}$ 2D square box



2D: Constant probability density surface. (a) and (b) rectangular box, states Ψ_{11} and Ψ_{21}. (c) y (d) square box, degenerate states Ψ_{21} and Ψ_{12}. (e) superposition of Ψ_{21} and Ψ_{12}

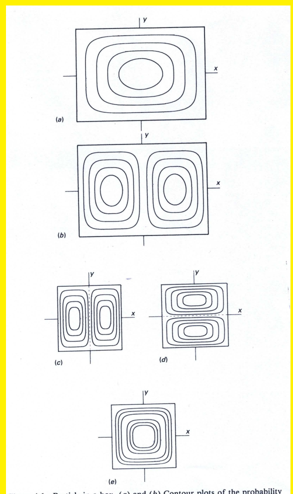


Figure 4.1 Particle in a box. (*a*) and (*b*) Contour plots of the probability densities for the states u_{111}, and u_{211}, for a rectangular box. (*c*) and (*d*) Contour plots for the degenerate eigenstates u_{211} and u_{121}, for a square box. (*e*) Contour plot for an incoherent superposition of u_{211} and u_{121}, which reflects the symmetry of the square box.

Degeneracy in the 3D box

Let's assume $a = b$

$$E = \frac{\pi^2\hbar^2}{8m}\left(\frac{n_x^2 + n_y^2}{a^2} + \frac{n_z^2}{c^2}\right)$$

Ψ_{121} and Ψ_{211} have the same energy and different wave functions $\rightarrow$ there's double **degeneracy**. In general, two states (n_1, n_2, n_3) and (n_2, n_1, n_3) are degenerate. The probability density of one of the states becomes the one of the other changing (x,y) to (y,-x), i.e., under a rotation of angle $\frac{\pi}{2}$ around the z axis

This degeneracy clearly comes from the **symmetry** of the system (this is its origin almost always). When this is not the case, we call it **accidental** degeneracy

10 / 46

Spherical symmetric potentials

11 / 46

$$V(\vec{r}) = V(r)$$

Appropriate coordinates $\rightarrow$ **spherical** ones

$$x = r\ \sin\theta\cos\phi$$
$$y = r\ \sin\theta\sin\phi$$
$$z = r\ \cos\theta$$

$$\vec{\nabla} = \vec{u}_r\frac{\partial}{\partial r} + \vec{u}_\phi\frac{1}{r\ \sin\theta}\frac{\partial}{\partial\phi} + \vec{u}_\theta\frac{1}{r}\frac{\partial}{\partial\theta} \qquad \text{in this order}$$

12 / 46

$$\vec{u}_r = \sin\theta\cos\phi\,\vec{\imath} + \sin\theta\sin\phi\,\vec{j} + \cos\theta\,\vec{k}$$

$$\vec{u}_\phi = -\sin\phi\,\vec{\imath} + \cos\phi\,\vec{j}$$

$$\vec{u}_\theta = \cos\theta\cos\phi\,\vec{\imath} + \cos\theta\sin\phi\,\vec{j} - \sin\theta\,\vec{k}$$

$$\bigtriangledown^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

Schrödinger Eq.

$$-\frac{\hbar^2}{2\mu}\bigtriangledown^2\,\Psi(\vec{r}) + V(r)\Psi(\vec{r}) = E\,\Psi(\vec{r})$$

13 / 46

Angular momentum operator

$$\vec{L} = \vec{r}\times\vec{p} \;\rightarrow\; -i\hbar\,\vec{r}\times\vec{\bigtriangledown}$$

$$L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\hbar\frac{\partial}{\partial\phi}$$

$$\begin{aligned} L^2 &= L_x^2 + L_y^2 + L_z^2 \\ &= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \\ &= \hbar^2\,r^2\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \bigtriangledown^2\right] \end{aligned}$$

14 / 46

$$[L_i,\, x_j] \;=\; i\hbar\epsilon_{ijk}\, x_k$$
$$[L_i,\, p_j] \;=\; i\hbar\epsilon_{ijk}\, p_k$$
$$[L_i,\, L_j] \;=\; i\hbar\epsilon_{ijk} L_k$$

Levi-Civita tensor

$$\epsilon_{ijk} \;=\; \begin{cases} 1 & \text{if ijk even permutation of 123} \\ -1 & \text{if ijk odd permutation of 123} \\ 0 & \text{if in ijk there are repeated indexes} \end{cases}$$

15 / 46

$$\left[L^2,\, \vec{L}\right] \;=\; 0$$

Example

$$\begin{aligned} \left[L^2,\, L_x\right] &= \left[L_y^2,\, L_x\right] + \left[L_z^2,\, L_x\right] \\ &= L_y \left[L_y,\, L_x\right] + \left[L_y,\, L_x\right] L_y + L_z \left[L_z,\, L_x\right] + \left[L_z,\, L_x\right] L_z \\ &= -i\hbar L_y L_z - i\hbar L_z L_y + i\hbar L_z L_y + i\hbar L_y L_z \\ &= 0 \end{aligned}$$

$\left[\vec{L},\, V(r)\right] \;=\; 0$; $L_x,\, L_y,\, L_z$ $\rightarrow$ derivatives with respect to angles, $V(r)$ does not depend on angles

If $\left[\vec{L},\, T\right] \;=\; 0$ $\rightarrow \vec{L}$ is **constant of motion**

16 / 46

$$T \;=\; \frac{p^2}{2\mu} \;=\; \frac{L^2}{2\mu r^2} \;-\; \frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)$$

$\left[L^2,\ \vec{L}\right] \;=\; 0$, the rest of T acts only on r

$$\left[\vec{L},\ T\right] \;=\; 0 \quad \rightarrow \left[\vec{L},\ H\right] \;=\; 0 \quad \rightarrow \left[L^2,\ H\right] \;=\; 0$$

Moreover

$$\frac{\partial \vec{L}}{\partial t} \;=\; 0 \quad ; \quad \frac{\partial L^2}{\partial t} \;=\; 0$$

$$\rightarrow \quad \frac{d\ <\vec{L}>}{dt} \;=\; 0 \quad ; \quad \frac{d\ <L^2>}{dt} \;=\; 0$$

for central forces $\vec{L}$ and L^2 are constants of motion

17 / 46

We can find a set of simultaneous eigenfunctions of $H,\ L^2$ and L_z : $\Psi_\lambda(\vec{r})$

$$H\ \Psi_\lambda(\vec{r}) \;=\; E\ \Psi_\lambda(\vec{r})$$

$$L^2\ \Psi_\lambda(\vec{r}) \;=\; \lambda\hbar^2\ \Psi_\lambda(\vec{r})$$

$$L_z\ \Psi_\lambda(\vec{r}) \;=\; m\hbar\ \Psi_\lambda(\vec{r})$$

$$\left[-\frac{\hbar^2}{2\mu r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \;+\; \frac{L^2}{2\mu r^2} \;+\; V(r)\right]\ \Psi_\lambda(\vec{r}) \;=\; E\ \Psi_\lambda(\vec{r})$$

We factorize $\Psi_\lambda(\vec{r}) \;=\; R(r)\, Y_\lambda(\theta,\phi)$

We get

$$L_z\, Y_\lambda(\theta,\phi) \;=\; m\hbar\, Y_\lambda(\theta,\phi)$$

$$L^2\, Y_\lambda(\theta,\phi) \;=\; \lambda\hbar^2\, Y_\lambda(\theta,\phi)$$

18 / 46

$$\left[-\frac{\hbar^2}{2\mu r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{\lambda\hbar^2}{2\mu r^2} + V(r)\right] R(r) = E\,R(r)$$

With $\quad R(r) = \frac{u(r)}{r}$

$$-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2} + \left[\frac{\lambda\hbar^2}{2\mu r^2} + V(r)\right] u(r) = E\,u(r) \qquad (1)$$

analogous to Schrödinger Eq. in one dim. adding $V(r)$ the term $\frac{\lambda\hbar^2}{2\mu r^2}$ (centrifugal potential)

- (1) is different from Eq. in Cartesian coordinates since $r \geq 0$
- $\Psi_\lambda(\vec{r})$ finite $\rightarrow \quad u(0) = 0 \quad$ ($\Psi_\lambda(\vec{r}) = \frac{u(r)}{r}\,Y_\lambda(\theta,\phi)$)
- In order to get $u(r)$ we need $V(r)$

19 / 46

- In order to get $Y_\lambda(\theta,\phi) \quad \rightarrow$ we do not need $V(r)$, it does not appear in Eqs. which determine it

20 / 46

*** Obtaining $Y_\lambda(\theta,\phi)$

$$L^2\, Y_\lambda(\theta,\phi) \;=\; \lambda\hbar^2 \;\, Y_\lambda(\theta,\phi)$$

$$L_z\, Y_\lambda(\theta,\phi) \;=\; m\hbar \;\, Y_\lambda(\theta,\phi)$$

$$\begin{aligned} L^2 \quad &= \quad -\hbar^2 \left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \;+\; \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right] \\ &= \quad -\hbar^2 \left[-\frac{L_z^2}{\hbar^2\sin^2\theta} \;+\; \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right] \end{aligned}$$

$$\left[\frac{m^2\hbar^2}{\sin^2\theta} - \frac{\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right] \; Y_\lambda(\theta,\phi) \;=\; \lambda\hbar^2 \;\, Y_\lambda(\theta,\phi)$$

Separation of variables $\quad Y_\lambda(\theta,\phi) \;=\; \Theta(\theta)\,\Phi(\phi)$

$$\left[\frac{m^2}{\sin^2\theta} - \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d}{d\theta}\right)\right] \; \Theta(\theta) \quad = \quad \lambda\,\Theta(\theta) \tag{2}$$

$$-i\hbar\frac{d\Phi}{d\phi} = m\hbar\;\Phi \tag{3}$$

*** Obtaining $\Phi(\phi)$ from (3)

$$\Phi_m(\phi) \;=\; e^{im\phi}$$

with the condition $\Phi(\phi) \;=\; \Phi(\phi \,+\, 2\pi)$ (single-valued)

$$e^{i2\pi m} \;=\; 1 \;\;\rightarrow\;\; m \;=\; 0, \pm 1, \pm 2 \cdots$$

m is the magnetic quantum number

Eigenvalues of $L_z \quad \rightarrow \quad 0, \pm\hbar, \pm 2\hbar \cdots$

*** Obtaining $\Theta(\theta)$ from (2)

Change $t \;=\; \cos\theta$

$$\Theta(\theta) \;=\; F(t)$$

$$\frac{d}{d\theta} \;=\; \frac{dt}{d\theta}\frac{d}{dt} \;=\; -\sqrt{1-t^2}\frac{d}{dt}$$

(2) $\rightarrow$ $\frac{d}{dt}\left[(1-t^2)\frac{dF}{dt}\right] - \frac{m^2}{1-t^2}F \,+\, \lambda\, F \;=\; 0$

associated Legendre differential equation

- (a) for $m \;=\; 0$

$$\frac{d}{dt}\left[(1-t^2)\frac{dF(t)}{dt}\right] \,+\, \lambda\, F(t) \;=\; 0 \tag{4}$$

If we make the change $t \rightleftharpoons -t$ in (4)

$$\frac{d}{dt}\left[(1-t^2)\frac{dF(-t)}{dt}\right] + \lambda\, F(-t) = 0 \tag{5}$$

$F(-t)$ is solution of the associated Legendre differential equation if $F(t)$ is

The operator applied to $F(t)$ in (4) is linear $\rightarrow$ the combinations

$$F_e = F(t) + F(-t) \quad \text{(even in t)} \quad \text{and}$$

$$F_o = F(t) - F(-t) \quad \text{(odd in t)}$$

are solutions of the associated Legendre differential equation

25 / 46

Look for F **even** or **odd** in t (since there are such solutions)

$t \rightleftharpoons -t \rightarrow \theta \rightleftharpoons \pi - \theta$

(The change $t \rightleftharpoons -t$ is equivalent to making a reflection about the plane xy $\rightarrow$ change $z \rightleftharpoons -z$)

The **regular** solution (it is not ∞) of (4) can be expanded in power series

$$F(t) = \sum_{k=0}^{\infty} a_k\, t^k$$

By a method analogous to that used in the harmonic oscillator

$$\frac{a_{k+2}}{a_k} = \frac{k(k+1)-\lambda}{(k+2)(k+1)} \qquad \text{recurrence relation}$$

26 / 46

$a_0 \neq 0$; $a_1 = 0$ k even, even series in t

$a_1 \neq 0$; $a_0 = 0$ k odd, odd series in t

If the series does not cut

$$\lim_{k \to \infty} \frac{a_{k+2}}{a_k} = \frac{k}{k+2} \to 1$$

Convergence criterion

$$R = \lim_{n \to \infty} \left| \frac{a_{n+1}}{a_n} t \right| < 1$$

For $|t| = 1 \Rightarrow R = 1 \Rightarrow$ the series does not converge if the series does not cut

We cut the series for $k = l$ (integer ≥ 0) $\to$ polynomial (l even $\Rightarrow$ even polynomial; l odd $\Rightarrow$ odd polynomial)

$$a_{l+2} = 0$$

$$\lambda = l(l+1)$$

Eigenvalues of $L^2 \to l(l+1)\,\hbar^2$

$$l = 0, 1, 2, \cdots$$

$$\lambda = 0, 2, 6, \cdots$$

Solution of (4) $\to$ **Legendre polynomial** $P_l(t)$

They can be obtained from Rodrigues formula

$$P_l(t) = \frac{1}{2^l\, l!} \left(\frac{d}{dt}\right)^l (t^2 - 1)^l$$

Legendre polynomials

$$
\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_2(x) &= \frac{1}{2}(3x^2 - 1) \\
P_3(x) &= \frac{1}{2}\left(5x^3 - 3x\right) \\
P_4(x) &= \frac{1}{8}\left(35x^4 - 30x^2 + 3\right) \\
P_5(x) &= \frac{1}{8}\left(63x^5 - 70x^3 + 15x\right) \\
P_6(x) &= \frac{1}{16}\left(231x^6 - 315x^4 + 105x^2 - 5\right) \\
P_7(x) &= \frac{1}{16}\left(429x^7 - 693x^5 + 315x^3 - 35x\right) \\
P_8(x) &= \frac{1}{128}\left(6435x^8 - 12012x^6 + 6930x^4 - 1260x^2 + 35\right).
\end{aligned} \tag{13}
$$

- (b) $m \neq 0$

$$F(t) \;\to\; P_l^m(t) \;=\; (1-t^2)^{\frac{|m|}{2}} \, \frac{d^{|m|} P_l(t)}{dt^{|m|}}$$

$|m| \leq l$ integer $\quad m \;=\; -l, -l+1, \cdots, l-1, l$

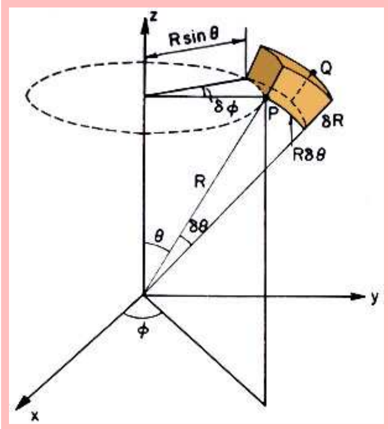
$P_l^m(t)$ **associated Legendre function**

$$Y_{lm}(\theta,\phi) \;=\; \mathcal{N} \Phi_m(\phi) \Theta_l^m(\theta) \quad \text{spherical harmonics}$$

$$1 = \int d\tau \, |\Psi(\vec{r})|^2 = \int_0^\infty dr \; r^2 \, |R(r)|^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi \, |Y_{lm}|^2$$

We impose $\int_0^\infty \, dr \; r^2 \, |R(r)|^2 = 1$ and

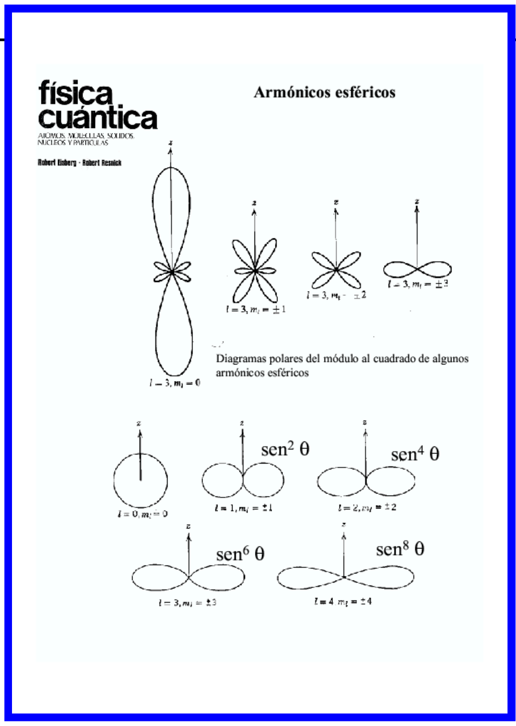
$\int_0^\pi d\theta \; \sin\theta \int_0^{2\pi} d\phi \, |Y_{lm}|^2 = 1$



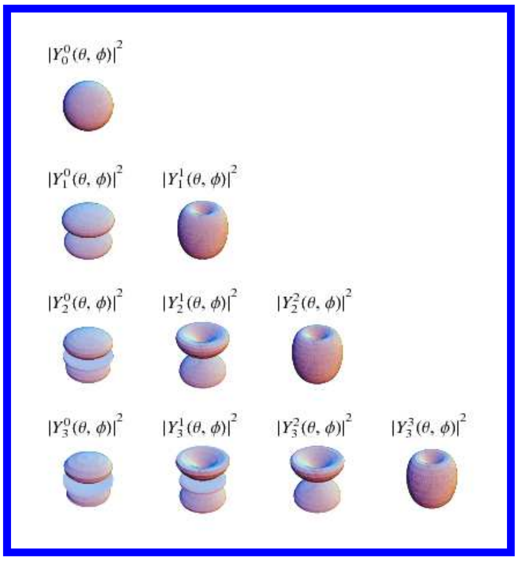
$$d\tau \;=\; dr\; r\, d\theta\; r\;\sin\theta\; d\phi \;=\; r^2\;\sin\theta\; dr\; d\theta\; d\phi \;=\; r^2\; dr\; d\Omega$$

spherical harmonics $Y_l^m \;=\; Y_{lm}$

$Y_0^0 = \sqrt{\frac{1}{4\pi}}$	$Y_1^0 \;= \sqrt{\frac{3}{4\pi}}\cos(\theta)$	$Y_2^0 \;= \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$
	$Y_1^1 \;= -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\mathrm{i}\phi}$	$Y_2^1 \;= -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{\mathrm{i}\phi}$
	$Y_1^{-1} = \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-\mathrm{i}\phi}$	$Y_2^{-1} = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{-\mathrm{i}\phi}$
		$Y_2^2 \;= \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{2\mathrm{i}\phi}$
		$Y_2^{-2} = \sqrt{\frac{15}{32\pi}}\sin^2\theta\, e^{-2\mathrm{i}\phi}$


física cuántica
ATOMOS, MOLECULAS, SOLIDOS, NUCLEOS Y PARTICULAS
Robert Eisberg · Robert Resnick
Armónicos esféricos
$l = 3, m_l = 0$
$l = 3, m_l = \pm 1$
$l = 3, m_l = \pm 2$
$l = 3, m_l = \pm 3$
Diagramas polares del módulo al cuadrado de algunos armónicos esféricos
$l = 0, m_l = 0$
$\mathrm{sen}^2\,\theta$
$l = 1, m_l = \pm 1$
$\mathrm{sen}^4\,\theta$
$l = 2, m_l = \pm 2$
$\mathrm{sen}^6\,\theta$
$l = 3, m_l = \pm 3$
$\mathrm{sen}^8\,\theta$
$l = 4, m_l = \pm 4$

33 / 46


$|Y_0^0(\theta, \phi)|^2$
$|Y_1^0(\theta, \phi)|^2$
$|Y_1^1(\theta, \phi)|^2$
$|Y_2^0(\theta, \phi)|^2$
$|Y_2^1(\theta, \phi)|^2$
$|Y_2^2(\theta, \phi)|^2$
$|Y_3^0(\theta, \phi)|^2$
$|Y_3^1(\theta, \phi)|^2$
$|Y_3^2(\theta, \phi)|^2$
$|Y_3^3(\theta, \phi)|^2$

34 / 46

Y_{lm} are simultaneous eigenfunctions of L^2 and L_z. They are an orthonormal set

$$\int d\Omega\, Y^*_{lm}\, Y_{l'm'} \;=\; \delta_{ll'}\, \delta_{mm'}$$

$$m \geq 0 \qquad Y_{lm}(\theta,\phi) \;=\; \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}(-1)^m e^{im\phi}\, P_l^m(\cos\theta)$$

$$m < 0 \qquad Y_{lm}(\theta,\phi) \;=\; (-1)^m\, Y^*_{l-m}(\theta,\phi)$$

Reflection about the origin

$$\vec{r} \;\rightarrow\; -\vec{r} \;\begin{cases} \phi \;\rightarrow\; \phi \;+\; \pi \\ \theta \;\rightarrow\; \pi - \theta \end{cases}$$

$$e^{im\phi} \;\rightarrow\; (-)^m e^{im\phi} \qquad (e^{im\pi} \;=\; (-)^m)$$

$$P_l^m(\cos\theta) \;\rightarrow\; (-)^{l-m} P_l^m(\cos\theta)$$

$Y_{lm} \;\rightarrow\; (-)^l\, Y_{lm}$ PARITY $\rightarrow\; (-)^l$

Any $f(\theta,\phi) \;\rightarrow$ can be expanded in terms of $Y_{lm}(\theta,\phi)$

Angular momentum $\rightarrow$ any vector operator $\vec{J}$ whose components satisfy the commutation relations:
$[J_i,\, J_j] \;=\; i\hbar\, \epsilon_{ijk}\, J_k$

We define **ladder operators** from its J_x and J_y components

$$J_+ \;=\; J_x \;+\; i\, J_y \quad ; \quad J_- \;=\; J_x \;-\; i\, J_y$$

$$(J_+)^\dagger \;=\; J_-$$

$$[J_z,\, J_+] \;=\; \hbar\, J_+ \;;\; [J_z,\, J_-] \;=\; -\hbar\, J_- \;;\; [J_+,\, J_-] \;=\; 2\,\hbar\, J_z \tag{6}$$

From $[J^2,\, \vec{J}] \;=\; 0 \quad \rightarrow \quad [J^2,\, J_+] \;=\; [J^2,\, J_-] \;=\; [J^2,\, J_z] \;=\; 0$

J^2 can be written

$$J^2 \;=\; \frac{1}{2}\; [J_+ J_- \;+\; J_- J_+] \;+\; J_z^2$$

From (6)

$$J_- J+ \;=\; J^2 \;-\; J_z(J_z \;+\; \hbar) \tag{7}$$

$$J_+ J- \;=\; J^2 \;-\; J_z(J_z \;-\; \hbar) \tag{8}$$

If we call $\mid j\; m >$ a normalized state such that

$$J^2 \;\mid j\; m > = \; j(j+1)\,\hbar^2 \;\mid j\; m >$$

$$J_z \;\mid j\; m > = \; m\,\hbar \;\mid j\; m >$$

(7) $\Rightarrow$

$$\begin{aligned} J_- J_+ \;\mid j\; m > \;&=\; \hbar^2\, [j(j+1) \;-\; m(m+1)] \;\mid j\; m > \\ &=\; \hbar^2\; (j-m)(j+m+1) \;\mid j\; m > \end{aligned}$$

(8) $\Rightarrow$

$$
\begin{aligned}
J_+ J_- \ \mid j\, m > \ &= \ \hbar^2 \left[j(j+1) \ - \ m(m-1) \right] \ \mid j\, m > \\
&= \ \hbar^2 \ (j+m)(j-m+1) \ \mid j\, m >
\end{aligned}
$$

Since $(J_-)^\dagger \ = \ J_+$ and $(J_+)^\dagger \ = \ J_-$, the squares of the norms of $J_+ \ \mid j\, m >$ and $J_- \ \mid j\, m >$ are

$$< j\, m \mid J_- J_+ \ \mid j\, m > = \ (j-m)(j+m+1) \, \hbar^2 < j\, m \mid j\, m >$$

$$< j\, m \mid J_+ J_- \ \mid j\, m > = \ (j+m)(j-m+1) \, \hbar^2 < j\, m \mid j\, m >$$

and must be $\geq \ 0 \quad (j \ \geq \ 0)$

$$(j-m)(j+m+1) \ \geq \ 0 \ \ ; \ \ (j+m)(j-m+1) \geq \ 0$$

40 / 46

$$* \ (j-m) \ \geq \ 0 \ ; \ (j+m+1) \ \geq \ 0 \qquad \text{or}$$

$$\rightarrow\leftarrow \quad (j-m) \ \leq \ 0 \ ; \ (j+m+1) \ \leq \ 0$$

and

$$* \ (j+m) \ \geq \ 0 \ ; \ (j-m+1) \ \geq \ 0 \qquad \text{or}$$

$$\rightarrow\leftarrow \quad (j+m) \ \leq \ 0 \ ; \ (j-m+1) \ \leq \ 0$$

$$\Downarrow$$

$$-j \ \leq \ m \ \leq \ j \tag{9}$$

Zero norm $\rightarrow$ zero vector

$$J_+ \ \mid j\, m > = \ 0 \iff (j-m)(j+m+1) \ = \ 0$$

$$J_- \ \mid j\, m > = \ 0 \iff (j+m)(j-m+1) \ = \ 0$$

41 / 46

From (9)

$$J_+ \mid j\,m> = 0 \iff m = j$$

$$J_- \mid j\,m> = 0 \iff m = -j$$

If $m \neq j$

$$J^2\,J_+ \mid j\,m> = J_+\,J^2 \mid j\,m> = j\,(j+1)\hbar^2\,J_+ \mid j\,m>$$

If $m \neq -j$

$$J^2\,J_- \mid j\,m> = J_-\,J^2 \mid j\,m> = j\,(j+1)\hbar^2\,J_- \mid j\,m>$$

Moreover

$$[J_z,\,J_+] = \hbar\,J_+ \Rightarrow J_z\,J_+ = J_+(J_z + \hbar)$$

Then

$$J_z\,[J_+ \mid j\,m>] = J_+(J_z + \hbar) \mid j\,m> = (m+1)\hbar\,[J_+ \mid j\,m>]$$

On the other hand $[J_z,\,J_-] = -\hbar\,J_- \Rightarrow J_z\,J_- = J_-(J_z - \hbar)$ Then

$$J_z\,[J_- \mid j\,m>] = J_-(J_z - \hbar) \mid j\,m> = (m-1)\hbar\,[J_- \mid j\,m>]$$

All this leads to

- $-j \leq m \leq j$
- for $m = j \Rightarrow J_+ \mid j\,j> = 0$
- for $m \neq j \Rightarrow J_+ \mid j\,m> \propto \mid j\,m+1>$

  Norm of

$$J_+ \mid j\,m> \to \hbar\sqrt{(j-m)(j+m+1)} = \hbar\sqrt{j(j+1)-m(m+1)}$$

- If $m = -j \;\Rightarrow\; J_- \mid j\; -j >= 0$
- If $m \neq -j \;\Rightarrow\; J_- \mid j\, m > \propto \mid j\, m - 1 >$

  Norm of

$$J_- \mid j\, m > \;\rightarrow\; \hbar\sqrt{(j+m)(j-m+1)} \;=\; \hbar\sqrt{j(j+1)-m(m-1)}$$

We set the phases so that

$$J_+ \mid j\, m >= \hbar\sqrt{j(j+1)-m(m+1)} \mid j\, m+1 >$$

$$J_- \mid j\, m >= \hbar\sqrt{j(j+1)-m(m-1)} \mid j\, m-1 >$$

From a state $\mid j\, m >$ can be obtained, by successive application of J_+ and J_-, the others, to have the $2j+1$ compatible with j

Bibliography

[1] A.P.French and E.F. Taylor, “Introducción a la Física Cuántica”

[2] S. Gasiorowicz, “Quantum Physics”, ed. John Wiley, 2003, Apéndice B

[3] D.J. Griffiths, “Introduction to Quantum Mechanics”, ed. Pearson Education Inc., 2005

[4] D. Park, “Introduction to the Quantum Theory”, ed. McGraw-Hill, 1992

[5] J.S. Townsend, “A Modern Approach to Quantum Mechanics”, ed. University Science Books, 2000

[6] R. Eisberg and R. Resnick, “Física cuántica”, Ed. Limusa, 2004

[7] C. Sánchez del Río, “Física cuántica”, Ed. Pirámide, 2003