

Simultaneous specification of several properties



We postulated that if

$$\hat{A}\Psi = s\Psi$$

then a measurement of the physical property \boldsymbol{A} is certain to yield the result \boldsymbol{s}

if:

$$\hat{A}\Psi=s\Psi$$
 and $\hat{B}\Psi=t\Psi$

then we can simultaneously assign definite values to the physical properties \boldsymbol{A} and \boldsymbol{B}



When
$$\hat{A}\Psi=s\Psi$$
 and $\hat{B}\Psi=t\Psi$?

Simultaneous specification of several properties

THE PARTY OF THE P

Theorems:

A necessary condition for the existence of a complete set of simultaneous eigenfunctions of two operators is that the operators commute with each other.

If A and B are two commuting operators that correspond to physical quantities, then there exists a complete set of functions that are eigenfunctions of both A and B



$$\text{if} \quad [\hat{A},\hat{B}] = 0. \quad \longrightarrow \quad \hat{A}\Psi = s\Psi \qquad \text{and} \quad \hat{B}\Psi = t\Psi$$

Simultaneous specification of several properties



Some important commutator identities

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$[\hat{A},\hat{B}]=-[\hat{B},\hat{A}]$$

$$[\hat{A}, \hat{A}^n] = 0, \quad n = 1, 2, 3, \dots$$

$$[k\hat{A},\hat{B}]=[\hat{A},k\hat{B}]=k[\hat{A},\hat{B}]$$

$$[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}], \quad [\hat{A} + \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}], \quad [\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$



Simultaneous specification of several properties

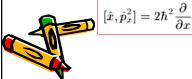
Example:

Starting from [d/dx, x] = 1, use the commutator identities to find (a) $[x, p_x]$; (b) $[x, p_x^2]$; (c) [x, H] for a one-particle, threedimensional system

a)
$$[\hat{x}, \hat{p}_x] = \left[x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right] = \frac{\hbar}{i} \left[x, \frac{\partial}{\partial x} \right] = -\frac{\hbar}{i} \left[\frac{\partial}{\partial x}, x \right] = -\frac{\hbar}{i}$$

$$[\hat{x}, \hat{p}_x] = i\hbar$$

b)
$$[\hat{x}, \hat{p}_x^2] = [\hat{x}, \hat{p}_x]\hat{p}_x + \hat{p}_x[\hat{x}, \hat{p}_x] = i\hbar \cdot \frac{\hbar}{i} \frac{\partial}{\partial x} + \frac{\hbar}{i} \frac{\partial}{\partial x} \cdot i\hbar$$



Simultaneous specification of several properties

$$\begin{split} \textbf{c)} & \quad [\hat{x}, \hat{H}] = [\hat{x}, , \hat{T} + \hat{V}] = [\hat{x}, \hat{T}] + [\hat{x}, \hat{V}(x, y, z)] = [\hat{x}, \hat{T}] \\ & \quad = [\hat{x}, (1/2m)(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2)] \\ & \quad = (1/2m)[\hat{x}, \hat{p}_x^2] + (1/2m)[\hat{x}, \hat{p}_y^2] + (1/2m)[\hat{x}, \hat{p}_z^2] \\ & \quad = \frac{1}{2m} \cdot 2\hbar^2 \frac{\partial}{\partial x} + 0 + 0 \\ & \quad [\hat{x}, \hat{H}] = \frac{\hbar^2}{m} \frac{\partial}{\partial x} = \frac{i\hbar}{m} \hat{p}_x \end{split}$$



Simultaneous specification of several properties



We can not expected the state function to be simultaneously an eigenfunction of \hat{x} and \hat{p}_{x}

$$\left[\hat{x}, \hat{H}\right] \neq 0$$
 \longrightarrow ?

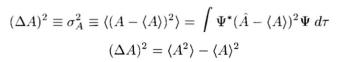
 $\hat{A}\Psi \neq cte\Psi$



$$\langle A \rangle$$
 $A_i - \langle A \rangle$ $\sigma_A^2 \equiv (\Delta A)^2$

variance

Simultaneous specification of several properties



Standard deviation $\sigma_A \equiv \Delta A$

$$\Delta A \Delta B \ge \frac{1}{2} \left| \int \Psi^*[\hat{A}, \hat{B}] \Psi \ d\tau \right|$$

$$\Delta x \Delta p_x \geq rac{1}{2} \left| \int \Psi^*[\hat{x}, \hat{p}_x] \Psi \ d au
ight| = rac{1}{2} \left| \int \Psi^* i \hbar \Psi \ d au
ight| = rac{1}{2} \hbar |i| \left| \int \Psi^* \Psi \ d au
ight|$$



 $\Delta x \Delta p_x \geq rac{1}{2} \hbar$ Heisenberg uncertainty principle

example

For the ground state of the particle in a three-dimensional box, use the $\ensuremath{\,^{\text{results}}}$

$$\langle x \rangle = a/2, \ \langle x^2 \rangle = a^2 (1/3 - 1/2\pi^2), \ \langle p_x \rangle = 0, \ \langle p_x^2 \rangle = h^2/4a^2$$

to check that the uncertainty principle is obeyed.

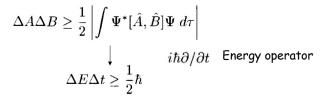
$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = a^2 (1/3 - 1/2\pi^2) - a^2/4 = a^2 (\pi^2 - 6)/(12)\pi^2$$

$$\Delta x = a(\pi^2 - 6)^{1/2}/12^{1/2}\pi$$

$$(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 = h^2/4a^2, \quad \Delta p_x = h/2a$$

$$\Delta x \Delta p_x = \frac{h}{2\pi} \left(\frac{\pi^2 - 6}{12} \right)^{1/2} = 0.568\hbar > \frac{1}{2}\hbar$$

Simultaneous specification of several properties



$$[\hat{A}, \hat{B}] = 0$$
 $[\hat{A}, \hat{C}] = 0$

Is not enough to ensure that there exist simultaneous eigenfunctions



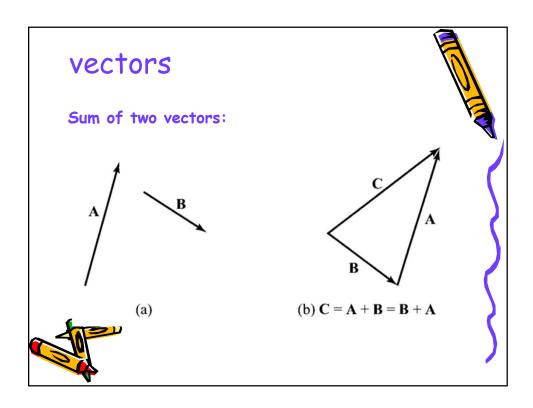
$$[\hat{A}, \hat{B}] = 0$$
 $[\hat{A}, \hat{C}] = 0$ $[\hat{B}, \hat{C}] = 0$

Is required

Scalars: physical properties that are specified by their magnitude (mass, length, energy)

Vectors: physical properties that require specification of both magnitude and direction (force, velocity, momentum)





The product of a scalar (c) and a vector A

с**А**

Is defined as a vector of length |c| times the length of $\bf A$ with the same direction of $\bf A$ if c is positive, or the opposite direction to $\bf A$ if c is negative.





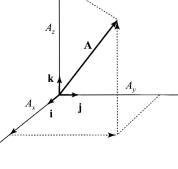
vectors

Algebraic way of representing vectors:

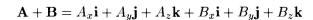
$$\mathbf{A} = A_x \mathbf{i} + A_y \mathbf{j} + A_z \mathbf{k}$$

 $\text{if} \quad A_x = B_x, \, A_y = B_y \, \text{and} A_z = B_z$









$$\mathbf{A} + \mathbf{B} = (A_x + B_x)\mathbf{i} + (A_y + B_y)\mathbf{j} + (A_z + B_z)\mathbf{k}$$

$$c\mathbf{A} = cA_x\mathbf{i} + cA_y\mathbf{j} + cA_z\mathbf{k}$$

The magnitude of a vector \mathbf{A} $A = |\mathbf{A}|$



vectors

Dot product or scalar product A.B:

$$\mathbf{A} \cdot \mathbf{B} = |\mathbf{A}| |\mathbf{B}| \cos \theta = \mathbf{B} \cdot \mathbf{A}$$

$$(\mathbf{A} + \mathbf{B}) \cdot \mathbf{C} = \mathbf{A} \cdot \mathbf{C} + \mathbf{B} \cdot \mathbf{C}$$
$$\mathbf{i} \cdot \mathbf{i} = \mathbf{j} \cdot \mathbf{j} = \mathbf{k} \cdot \mathbf{k} = \cos 0 = 1, \quad \mathbf{i} \cdot \mathbf{j} = \mathbf{j} \cdot \mathbf{k} = \mathbf{k} \cdot \mathbf{i} = \cos (\pi/2) = 0$$

$$\mathbf{A} \cdot \mathbf{B} = (A_x \mathbf{i} + A_y \mathbf{j} + A_z \mathbf{k}) \cdot (B_x \mathbf{i} + B_y \mathbf{j} + B_z \mathbf{k})$$

$$\mathbf{A} \cdot \mathbf{B} = A_x B_x + A_y B_y + A_z B_z$$



$$\mathbf{A} \cdot \mathbf{A} = |\mathbf{A}|^2$$

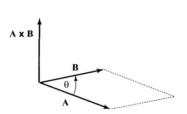
$$|\mathbf{A}| = (A_x^2 + A_y^2 + A_z^2)^{1/2}$$



$$|\mathbf{A} \times \mathbf{B}| = |\mathbf{A}||\mathbf{B}|\sin\theta$$

$$\mathbf{B} \times \mathbf{A} = -\mathbf{A} \times \mathbf{B}$$

$$\mathbf{A} \times (\mathbf{B} + \mathbf{C}) = \mathbf{A} \times \mathbf{B} + \mathbf{A} \times \mathbf{C}$$





vectors

$$\mathbf{i} \times \mathbf{i} = \mathbf{j} \times \mathbf{j} = \mathbf{k} \times \mathbf{k} = \sin 0 = 0$$

$$\mathbf{i}\times\mathbf{j}=\mathbf{k},\ \mathbf{j}\times\mathbf{i}=-\mathbf{k},\ \mathbf{j}\times\mathbf{k}=\mathbf{i},\ \mathbf{k}\times\mathbf{j}=-\mathbf{i},\ \mathbf{k}\times\mathbf{i}=\mathbf{j},\ \mathbf{i}\times\mathbf{k}=-\mathbf{j}$$

$$\mathbf{A} \times \mathbf{B} = (A_x \mathbf{i} + A_y \mathbf{j} + A_z \mathbf{k}) \times (B_x \mathbf{i} + B_y \mathbf{j} + B_z \mathbf{k})$$

$$\mathbf{A} \times \mathbf{B} = (A_y B_z - A_z B_y)\mathbf{i} + (A_z B_x - A_x B_z)\mathbf{j} + (A_x B_y - A_y B_x)\mathbf{k}$$

$$\mathbf{A} \times \mathbf{B} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix} = \mathbf{i} \begin{vmatrix} A_y & A_z \\ B_y & B_z \end{vmatrix} - \mathbf{j} \begin{vmatrix} A_x & A_z \\ B_x & B_z \end{vmatrix} + \mathbf{k} \begin{vmatrix} A_x & A_y \\ B_x & B_y \end{vmatrix}$$



$$\nabla \equiv \mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z}$$

$$\hat{p}_x = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \hat{p}_y = \frac{\hbar}{i} \frac{\partial}{\partial y}, \quad \hat{p}_z = \frac{\hbar}{i} \frac{\partial}{\partial z}$$

$$\hat{\mathbf{p}} = -i\hbar \nabla.$$

$$\mathbf{grad}\ g(x,y,z) \equiv \mathbf{\nabla} g(x,y,z) \equiv \mathbf{i}\,\frac{\partial g}{\partial x} + \mathbf{j}\,\frac{\partial g}{\partial y} + \mathbf{k}\,\frac{\partial g}{\partial z}$$

$$\mathbf{F} = -\nabla V(x, y, z) = -\mathbf{i} \frac{\partial V}{\partial x} - \mathbf{j} \frac{\partial V}{\partial y} - \mathbf{k} \frac{\partial V}{\partial z}$$



$$\begin{split} A_x &= A_x(t), \, A_y = A_y(t) \, \text{and} A_z = A_z(t) \\ \frac{d\mathbf{A}}{dt} &= \mathbf{i} \, \frac{dA_x}{dt} + \mathbf{j} \, \frac{dA_y}{dt} + \mathbf{k} \, \frac{dA_z}{dt} \end{split}$$

Vectors in n-dimentional space

A vector A is an n-dimentional real vector space (called hyperspace); is specified with n numbers

Components of **B** B_1, B_2, \cdots, B_n

$$B_1, B_2, \cdots, B_n$$

$$\psi(\mathbf{r}_1,\mathbf{r}_2)$$

$$q_1 = x_1, \ q_2 = y_1, \ q_3 = z_1, \ q_4 = x_2, \ q_5 = y_2, \ q_6 = z_2$$

 $\psi(\mathbf{q})$

$$\int |\psi(\mathbf{q})|^2 d\mathbf{q}$$



Vectors in n-dimentional space



$$\mathbf{B} = \mathbf{C}$$

$$B_1 = C_1, B_2 = C_2, \cdots, B_n = C_n$$

The sum of two n-dimentional vector $\mathbf{B} + \mathbf{D}$:

$$(B_1 + D_1, B_2 + D_2, \cdots, B_n + D_n)$$



$$k\mathbf{B}$$
 $(kB_1, kB_2, \cdots, kB_n)$

Vectors in n-dimentional space



 (A_x,A_y,A_z) Define a point in three-dimensional space

$$(B_1,B_2,\cdots,B_n)$$

The length of an n-dimentional real vector:

$$|\mathbf{B}| = (\mathbf{B} \cdot \mathbf{B})^{1/2} = (B_1^2 + B_2^2 + \dots + B_n^2)^{1/2}$$



$$\mathbf{B} \cdot \mathbf{G} \equiv B_1 G_1 + B_2 G_2 + \dots + B_n G_n$$
$$\cos \theta \equiv \mathbf{B} \cdot \mathbf{C} / |\mathbf{B}| |\mathbf{C}|$$

Vectors in n-dimentional space



In three-dimentional space:

$$\mathbf{i} = (1,0,0), \, \mathbf{j} = (0,1,0), \, \mathbf{k} = (0,0,1)$$

In n-dimentional space:

$$\mathbf{e}_1 \equiv (1,0,0,\cdots,0), \, \mathbf{e}_2 \equiv (0,1,0,\cdots,0),\cdots, \, \mathbf{e}_n \equiv (0,0,0,\cdots,1)$$
 :

$$\mathbf{B} = B_1 \mathbf{e}_1 + B_2 \mathbf{e}_2 + \cdots + B_n \mathbf{e}_n$$

 e_1, e_2, \dots, e_n A basis for the n-dimentional real space

Orthogonal and normalized

 $\mathbf{B} \cdot \mathbf{e}_i$ = the component of B in the direction of basis vector $\mathbf{e}_{\scriptscriptstyle i}$

Vectors in n-dimentional space



A three-dimensional vector can be specified with:

a) Three components or b) its length and its direction

The angles the vector makes with the positive halves of x, y, and z axes \equiv direction angles (are between 0 and 180 degrees)

There are two direction angles.

In three-dimensional space: the length and two direction angles

In n-dimensional space: the length and n-1 direction angles



$$f(q_1,q_2,\cdots,q_n)$$

$$\nabla f = (\partial f/\partial q_1)\mathbf{e}_1 + (\partial f/\partial q_2)\mathbf{e}_2 + \dots + (\partial f/\partial q_n)\mathbf{e}_n$$

In classical mechanics:

a particle of mass m moving according to the laws of classical mechanics

$$\mathbf{r} = \mathbf{i} \, x + \mathbf{j} \, y + \mathbf{k} \, z$$

r is the position vector

$$\mathbf{v} \equiv \frac{d\mathbf{r}}{dt} = \mathbf{i} \frac{dx}{dt} + \mathbf{j} \frac{dy}{dt} + \mathbf{k} \frac{dz}{dt}$$

$$v_x = dx/dt$$
, $v_u = dy/dt$, $v_z = dz/dt$

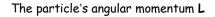
The particle's linear momentum P

$$\mathbf{p} \equiv m\mathbf{v}$$

$$p_x = mv_x, \quad p_y = mv_y, \quad p_z = mv_z$$



Angular momentum of a one-particle system



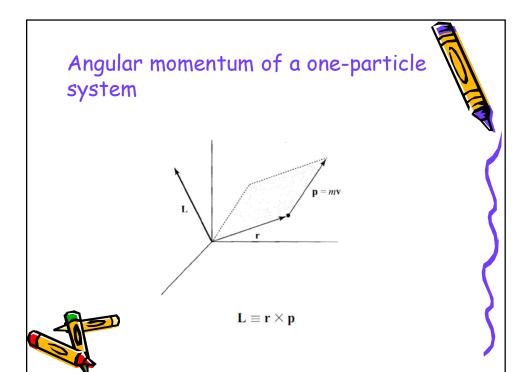
$$L \equiv r \times p$$

$$\mathbf{L} = egin{bmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \ x & y & z \ p_x & p_y & p_z \ \end{pmatrix}$$

$$L_x = yp_z - zp_y,$$
 $L_y = zp_x - xp_z,$ $L_z = xp_y - yp_x$

$$L^2 = \mathbf{L} \cdot \mathbf{L} = L_x^2 + L_y^2 + L_z^2$$





If a force F acts on the particle, then the torque T on the particle is defined as

$$\mathbf{T} = \mathbf{r} \times \mathbf{F} = \mathbf{r} \times \frac{d\mathbf{p}}{dt}$$
 $\mathbf{F} = d\mathbf{p}/dt$

$$\frac{d\mathbf{L}}{dt} = \left(\frac{d\mathbf{r}}{dt} \times \mathbf{p}\right) + \left(\mathbf{r} \times \frac{d\mathbf{p}}{dt}\right)$$

$$\frac{d\mathbf{r}}{dt} \times \mathbf{p} = \frac{d\mathbf{r}}{dt} \times m\frac{d\mathbf{r}}{dt} = 0$$

$$T = \frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t}$$

$$\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = \mathbf{r} \times \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t}$$

If there is no force acting on the particle, the torque is zero. Consequently, the rate of change of the angular momentum is zero and the angular momentum is conserved.

In quantum mechanics:

In quantum mechanics, there are two angular momenta:

- 1) orbital angular momentum
- 2) spin angular momentum

orbital angular momentum result from motion of a particle through the space and is the analogue of classical-mechanical quantity.

spin angular momentum is an intrinsic property of many microscopic particles and has no classical-mechanical analogue.



Angular momentum of a one-particle system

The quantum-mechanical operators for the components of the orbital angular momentum are obtained by replacing p_x , p_v , p_z in the classical expressions by their corresponding quantum operators

$$\hat{L}_x = y\hat{p}_z - z\hat{p}_y = \frac{\hbar}{i} \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$\hat{L}_{y} = z\hat{p}_{x} - x\hat{p}_{z} = \frac{\hbar}{i} \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

$$\hat{L}_z = x\hat{p}_y - y\hat{p}_x = \frac{\hbar}{i} \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

$$\hat{y}\hat{p}_z = \hat{p}_z\hat{y}$$
, etc.



$$\hat{\mathbf{L}} = \mathbf{i} \hat{L}_x + \mathbf{j} \hat{L}_y + \mathbf{k} \hat{L}_z$$
 operator for **L**

$$\hat{L}^2 = \hat{\mathbf{L}} \cdot \hat{\mathbf{L}} = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$
 operator for \mathbf{L}^2



Commutation relations

The commutator $[\hat{L}_x, \hat{L}_y]$

$$\begin{aligned} [\hat{L}_x, \, \hat{L}_y] &= [y \, \hat{p}_z - z \, \hat{p}_y, \, z \, \hat{p}_x - x \, \hat{p}_z] \\ &= [y \, \hat{p}_z, \, z \, \hat{p}_x] + [z \, \hat{p}_y, \, x \, \hat{p}_z] - [y \, \hat{p}_z, \, x \, \hat{p}_z] - [z \, \hat{p}_y, \, z \, \hat{p}_x] \\ &\underbrace{0} \quad \underbrace{0} \quad \underbrace{0} \quad \end{aligned}$$

$$[\hat{L}_x, \hat{L}_y] = y\hat{p}_x\hat{p}_zz - y\hat{p}_xz\hat{p}_z + x\hat{p}_yz\hat{p}_z - x\hat{p}_y\hat{p}_zz$$
$$= (x\hat{p}_y - y\hat{p}_x)[z, \hat{p}_z]$$



$$[\hat{L}_x,\,\hat{L}_y]=\mathrm{i}\hbar\hat{L}_z$$

Angular momentum of a one-particle system

$$\hat{L}_{y}f = -i\hbar \left(z \frac{\partial f}{\partial x} - x \frac{\partial f}{\partial z} \right)$$

$$\hat{L}_{x}\hat{L}_{y}f = -\hbar^{2} \left(y \frac{\partial f}{\partial x} + yz \frac{\partial^{2} f}{\partial z \partial x} - yx \frac{\partial^{2} f}{\partial z^{2}} - z^{2} \frac{\partial^{2} f}{\partial y \partial x} + zx \frac{\partial^{2} f}{\partial y \partial z} \right)$$

$$\hat{L}_{x}f = -i\hbar \left(y \frac{\partial f}{\partial z} - z \frac{\partial f}{\partial y} \right)$$

$$\hat{L}_{y}\hat{L}_{x}f = -\hbar^{2} \left(zy \frac{\partial^{2} f}{\partial x \partial z} - z^{2} \frac{\partial^{2} f}{\partial x \partial y} - xy \frac{\partial^{2} f}{\partial z^{2}} + x \frac{\partial f}{\partial y} + xz \frac{\partial^{2} f}{\partial z \partial y} \right)$$

$$\hat{L}_{x}\hat{L}_{y}f - \hat{L}_{y}\hat{L}_{x}f = -\hbar^{2} \left(y \frac{\partial f}{\partial x} - x \frac{\partial f}{\partial y} \right)$$



$$[\hat{L}_x,\,\hat{L}_y]=\mathrm{i}\hbar\hat{L}_z \qquad \qquad [\hat{L}_y,\,\hat{L}_z]=\mathrm{i}\hbar\hat{L}_x \qquad [\hat{L}_z,\,\hat{L}_x]=\mathrm{i}\hbar\hat{L}_y$$

$$\hat{\mathbf{L}} \times \hat{\mathbf{L}} = i\hbar \hat{\mathbf{L}}$$

$$\begin{split} [\hat{L}^2,\hat{L}_x] &= [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2,\hat{L}_x] \\ &= [\hat{L}_x^2,\hat{L}_x] + [\hat{L}_y^2,\hat{L}_x] + [\hat{L}_z^2,\hat{L}_x] \\ &= [\hat{L}_y^2,\hat{L}_x] + [\hat{L}_z^2,\hat{L}_x] \\ &= [\hat{L}_y,\hat{L}_x]\hat{L}_y + [\hat{L}_y(\hat{L}_y,\hat{L}_x)] + [\hat{L}_z,\hat{L}_x]\hat{L}_z + \hat{L}_z[\hat{L}_z,\hat{L}_x] \\ &= -i\hbar\hat{L}_z\hat{L}_y - i\hbar\hat{L}_y\hat{L}_z + i\hbar\hat{L}_y\hat{L}_z + i\hbar\hat{L}_z\hat{L}_y \end{split}$$

Angular momentum of a one-particle system

 $x = r\sin\theta\cos\varphi$

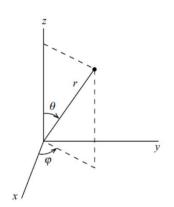
 $y = r\sin\theta\sin\varphi$

 $z = r \cos \theta$

 $r = (x^2 + y^2 + z^2)^{1/2}$

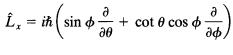
 $\theta = \cos^{-1}(z/(x^2 + y^2 + z^2)^{1/2})$

 $\varphi = \tan^{-1}(y/x)$





Spherical polar coordinate system.



$$\hat{L}_{y} = -i\hbar \left(\cos\phi \, \frac{\partial}{\partial\theta} - \cot\theta \sin\phi \, \frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

$$\hat{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \, \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \, \frac{\partial^2}{\partial \phi^2} \right)$$



One-particle orbital-angular-momentum eigenfunctions and eigenvalues

The common eigenfunctions of \hat{L}^2 and \hat{L}_z

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

$$\hat{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right)$$

Variables $\equiv \theta$ and Φ $Y = Y(\theta, \phi)$

We must

$$\begin{cases} \hat{L}_z Y(\theta, \phi) = b Y(\theta, \phi) \\ \hat{L}^2 Y(\theta, \phi) = c Y(\theta, \phi) \end{cases}$$

Eigenvalues: b and c



$$\begin{split} -i\hbar\frac{\partial}{\partial\phi}Y(\theta,\phi) &= bY(\theta,\phi) \\ &\qquad \qquad \qquad \qquad Y(\theta,\phi) = S(\theta)T(\phi) \\ -i\hbar\frac{\partial}{\partial\phi}\left[S(\theta)T(\phi)\right] &= bS(\theta)T(\phi) \\ -i\hbar S(\theta)\frac{dT(\phi)}{d\phi} &= bS(\theta)T(\phi) \\ \frac{dT(\phi)}{T(\phi)} &= \frac{ib}{\hbar}d\phi \end{split}$$



$$T(\phi) = Ae^{ib\phi/\hbar}$$

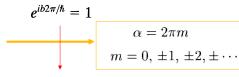
One-particle orbital-angular-momentum eigenfunctions and eigenvalues

For T to be single-valued: $T(\phi + 2\pi) = T(\phi)$

$$T(\phi) = Ae^{ib\phi/\hbar}$$

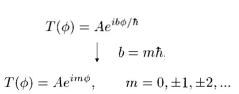
$$Ae^{ib\phi/\hbar}e^{ib2\pi/\hbar} = Ae^{ib\phi/\hbar}$$

 $e^{i\alpha}=\cos\alpha+i\sin\alpha=1$



$$2\pi b/\hbar = 2\pi m$$



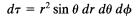


Normalizing: $F = f(r, \theta, \Phi)$

$$0 \leq r \leq \infty, \qquad 0 \leq \theta \leq \pi, \qquad 0 \leq \phi \leq 2\pi$$



One-particle orbital-angular-momentum eigenfunctions and eigenvalues



r to
$$r + dr$$
, θ to $\theta + d\theta$, and ϕ to $\phi + d\phi$

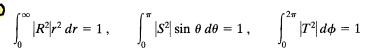
Normalization condition

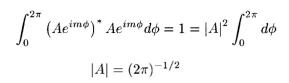
$$\int_0^\infty \left[\int_0^\pi \left[\int_0^{2\pi} \left| F^2(r, \theta, \phi) \right| d\phi \right] \sin \theta d\theta \right] r^2 dr = 1$$

$$F(r, \theta, \phi) = R(r)S(\theta)T(\phi)$$

$$\int_0^\infty |R^2(r)| r^2 dr \int_0^\pi |S^2(\theta)| \sin \theta d\theta \int_0^{2\pi} |T^2(\phi)| d\phi = 1$$

It is convenient to normalize each factor



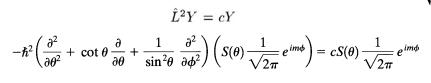


$$T(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}, \qquad m = 0, \pm 1, \pm 2, \pm \dots$$





One-particle orbital-angular-momentum eigenfunctions and eigenvalues



$$\frac{d^2S}{d\theta^2} + \cot\theta \frac{dS}{d\theta} - \frac{m^2}{\sin^2\theta} S = -\frac{c}{\hbar^2} S$$

$$w = \cos \theta$$

$$S(\theta) = G(w)$$



$$\frac{dS}{d\theta} = \frac{dG}{dw} \frac{dw}{d\theta} = -\sin\theta \frac{dG}{dw} = -(1 - w^2)^{1/2} \frac{dG}{dw}$$



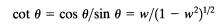
$$d^2S/d\theta^2 = ?$$

$$\frac{d}{d\theta} = -(1 - w^2)^{1/2} \frac{d}{dw}$$

$$\frac{d^2}{d\theta^2} = (1 - w^2)^{1/2} \frac{d}{dw} (1 - w^2)^{1/2} \frac{d}{dw}$$

$$\frac{d^2}{d\theta^2} = (1 - w^2) \frac{d^2}{dw^2} + (1 - w^2)^{1/2} (\frac{1}{2}) (1 - w^2)^{-1/2} (-2w) \frac{d}{dw}$$

$$\frac{d^2S}{d\theta^2} = (1 - w^2) \frac{d^2G}{dw^2} - w \frac{dG}{dw}$$





One-particle orbital-angular-momentum eigenfunctions and eigenvalues

$$\frac{d^2S}{d\theta^2} + \cot\theta \frac{dS}{d\theta} - \frac{m^2}{\sin^2\theta} S = -\frac{c}{\hbar^2} S$$

$$(1 - w^2)\frac{d^2G}{dw^2} - 2w\frac{dG}{dw} + \left[\frac{c}{\hbar^2} - \frac{m^2}{1 - w^2}\right]G(w) = 0$$

$$-1 \leq w \leq 1$$

To get a two term recursion relation G^{\prime} , $G^{\prime\prime}$

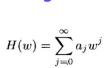
$$G^\prime$$
 , G^\prime

$$G(w)=(1-w^2)^{|m|/2}H(w)$$
 Divide by $(1-w^2)^{|m|/2}$

Divide by
$$(1-w^2)^{|m|/2}$$



$$(1-w^2)H''-2(|m|+1)wH'+[c\hbar^{-2}-|m|(|m|+1)]H=0$$



$$H'(w) = \sum_{j=0}^{\infty} j a_j w^{j-1}$$

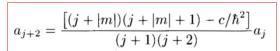
$$H''(w) = \sum_{j=0}^{\infty} j(j-1)a_j w^{j-2} = \sum_{j=0}^{\infty} (j+2)(j+1)a_{j+2} w^j$$

$$\sum_{j=0}^{\infty} \left[(j+2)(j+1)a_{j+2} + \left(-j^2 - j - 2|m|j + \frac{c}{\hbar^2} - |m|^2 - |m| \right) a_j \right] w^j = 0$$



$$a_{j+2} = \frac{\left[(j+|m|)(j+|m|+1) - c/\hbar^2 \right]}{(j+1)(j+2)} a_j$$

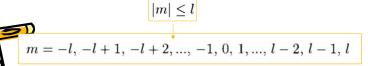
One-particle orbital-angular-momentum eigenfunctions and eigenvalues



Setting the coefficient of ak equal to zero:

$$c = \hbar^2(k + |m|)(k + |m| + 1),$$
 $k = 0, 1, 2, ...$

$$|\mathbf{m}|$$
 = 0, 1, 2, ... $l \equiv k + |m|$ $c = l(l+1)\hbar^2$, $l = 0, 1, 2, ...$ $|\mathbf{L}| = [l(l+1)]^{1/2}\hbar$



$$w = \cos \theta$$
 $S(\theta) = G(w)$ $G(w) = (1 - w^2)^{|m|/2} H(w)$ $l \equiv k + |m|$ $H(w) = \sum_{j=0}^{\infty} a_j w^j$

is even or odd

Whether
$$l-|m|$$
 is even or odd
$$S_{l,m}(\theta)=\sin^{-|m|}\theta\sum_{\substack{j=1,3,\dots\\j=0,2,\dots}}^{l-|m|}a_j\cos^j\theta$$

$$a_{j+2} = \frac{[(j+|m|)(j+|m|+1) - l(l+1)}{(j+1)(j+2)}a_j$$



$$Y_l^m(\theta,\phi) = S_{l,m}(\theta)T(\phi) = \frac{1}{\sqrt{2\pi}}S_{l,m}(\theta)e^{im\phi}$$

One-particle orbital-angular-momentum eigenfunctions and eigenvalues

Find $Y_l^m(\theta, \phi)$ and the \hat{L}^2 and \hat{L}_z eigenvalues for (a) l=0; (b) l=1.

a) $S_{0,0}(\theta) = a_0$ $\int_0^\pi \left|a_0^2\right| \sin\,\theta d\theta = 1 = 2\left|a_0^2\right|$ $\left|a_0\right| = 2^{-1/2}$

$$|a_0| = 2^{-1/2}$$

$$Y_0^0(\theta,\phi) = \frac{1}{\sqrt{4\pi}} \hspace{1cm} \text{No angular dependence} \\ \text{Spherically symmetric}$$







b) I = 1, m = -1, 0, 1
$$S_{1,\pm 1}(\theta) = a_0 \sin \theta$$

$$1=|a_0^2|\int_0^\infty \sin^2\theta \sin\theta d\theta=|a_0^2|\int_{-1}^1 (1-w^2)dw \qquad \overline{w=\cos\theta}.$$

$$|a_0|=\sqrt{3}/2$$

$$S_{1,\pm 1} = (3^{1/2}/2) \sin \theta$$

$$Y_1^1 = (3/8\pi)^{1/2} \sin \, \theta \, e^{i\phi}, \qquad Y_1^{-1} = (3/8\pi)^{1/2} \sin \, \theta \, e^{-i\phi}$$



One-particle orbital-angular-momentum eigenfunctions and eigenvalues



$$S_{1,0} = a_1 \cos \theta$$

$$S_{1,0} = (3/2)^{1/2} \cos \theta.$$

$$Y_1^0 = (3/4\pi)^{1/2} \cos \theta$$

$$I = 1, m = -1, 0, 1$$

$$\begin{cases}
C = \hbar^2 \\
B = -\hbar, 0, \hbar
\end{cases}$$





$$S_{l,m}(\theta)=\sin^{-|m|}\theta\sum_{\substack{j=1,3,\dots\\j=0,2,\dots}}^{l-|m|}a_j\cos^j\theta$$
 Associated Legendre functions multiplied by a normalization

Associated Legendre functions

$$P_l^{|m|}(w) \equiv \frac{1}{2^l l!} (1 - w^2)^{|m|/2} \frac{d^{l+|m|}}{dw^{l+|m|}} (w^2 - 1)^l, \qquad l = 0, 1, 2, \dots$$



$$P_0^0(w) = 1$$
 $P_2^0(w) = \frac{1}{2}(3w^2 - 1)$
 $P_1^0(w) = w$ $P_2^1(w) = 3w(1 - w^2)^{1/2}$
 $P_1^1(w) = (1 - w^2)^{1/2}$ $P_2^2(w) = 3 - 3w^2$

One-particle orbital-angular-momentum eigenfunctions and eigenvalues

It can be shown:

$$S_{l,m}(\theta) = \left[\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\theta)$$

Spherical harmonics:

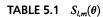
$$Y_{l}^{m}(\theta,\phi) = \left[\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_{l}^{|m|}(\cos\theta) e^{im\phi}$$

In summary:



$$\hat{L}^{2}Y_{l}^{m}(\theta,\phi) = l(l+1)\hbar^{2}Y_{l}^{m}(\theta,\phi), \qquad l = 0, 1, 2, ...$$

$$\hat{L}_{z}Y_{l}^{m}(\theta,\phi) = m\hbar Y_{l}^{m}(\theta,\phi), \qquad m = -l, -l+1, ..., l-1, l$$



l=0:	$S_{0,0}$	=	$\frac{1}{2}\sqrt{2}$

$$l = 1$$
: $S_{1,0} = \frac{1}{2}\sqrt{6}\cos\theta$

$$S_{1,\pm 1} = \frac{1}{2}\sqrt{3}\sin\theta$$

$$l=2$$
: $S_{2,0} = \frac{1}{4}\sqrt{10}(3\cos^2\theta - 1)$

$$S_{2, \pm 1} = \frac{1}{2}\sqrt{15} \sin \theta \cos \theta$$

 $S_{2, \pm 2} = \frac{1}{4}\sqrt{15} \sin^2 \theta$

$$S_{2,\pm 2} = \frac{3}{4} \sqrt{15} \sin^{2}\theta$$

$$l = 3: \qquad S_{3,0} = \frac{3}{4} \sqrt{14} \left(\frac{5}{3} \cos^{3}\theta - \cos\theta \right)$$

$$S_{3,\pm 1} = \frac{1}{8}\sqrt{42}\sin\theta (5\cos^2\theta - 1)$$

$$S_{3,\pm 2} = \frac{1}{4}\sqrt{105}\sin^2\theta\cos\theta$$

$$S_{3,\pm 3} = \frac{1}{8}\sqrt{70} \sin^3 \theta$$



One-particle orbital-angular-momentum eigenfunctions and eigenvalues



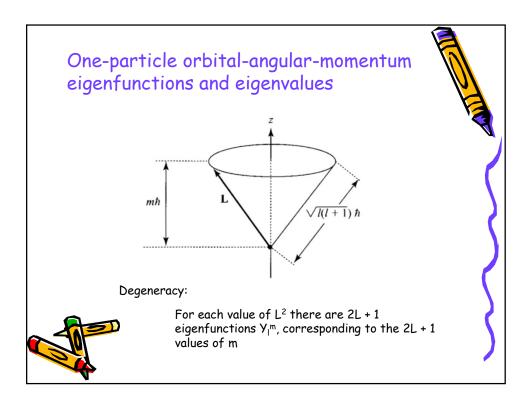
$$l \ge |m| \longrightarrow [l(l+1)]^{1/2}\hbar \le |m|\hbar$$

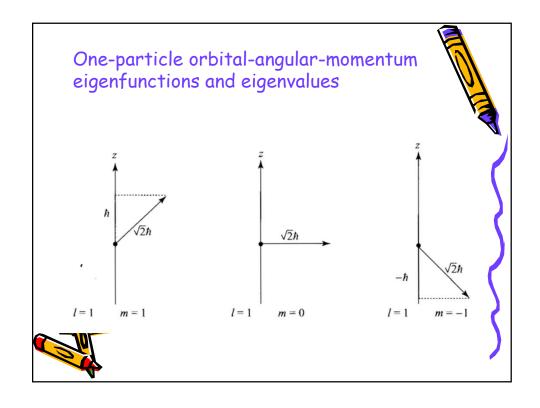
The magnitude of ${\bf L}$

The magnitude of Lz

$$\Delta L_x \Delta L_y \ge \frac{1}{2} \left| \int \Psi^* [\hat{L}_x, \hat{L}_y] \Psi \ d\tau \right| = \frac{\hbar}{2} \left| \int \Psi^* \hat{L}_z \Psi \ d\tau \right|$$

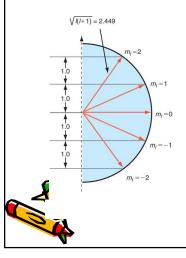






Spatial quantization

First, we see the semiclassical description

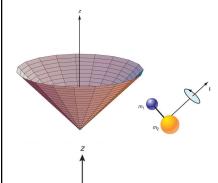


angular momentum cannot lie on the z-axis. Why? $| \mathbf{m_l} | \le \mathbf{l}$ is condition of $\mathbf{m_l}$ and magnitude of \mathbf{l} is given by $\sqrt{l(l+1)}$

Therefore, if the case of $m_L = I$ (extreme case) $\sqrt{m_I(m_I+1)} > m_I$ \rightarrow z-component cannot be same as the magnitude of angular momentum.

Angular momentum lie on the z-axis : x, y component = 0

→ know 3 component simultaneously But it cannot be possible because commutator is not zero!



If we know the total angular momentum and z-component, then we cannot know the x and y component and only we know the

$$l^2 - l_z^2 = l_x^2 + l_y^2 = [l(l+1) - m_l^2]\hbar^2$$

 \rightarrow cone has an open end

Finally, we can see the I=2 case(d orbital, too), vector model of angular momentum

Vector of angular momentum only have certain orientation in space.

→ spatial quantization

c.f) classical case : possible I values make the surface of sphere, not a cone

The ladder operator method for angular momentum

It is possible to find the eigenvalues of L^2 and L_z using only operator commutation relations

Any kind of angular momentum: M

Linear operators

$$\hat{M}_x,~\hat{M}_y$$
 , \hat{M}_z

All we know about them:

$$[\hat{M}_x,\hat{M}_y]=i\hbar\hat{M}_z, \quad [\hat{M}_y,\hat{M}_z]=i\hbar\hat{M}_x, \quad [\hat{M}_z,\hat{M}_x]=i\hbar\hat{M}_y$$

We define:

$$\hat{M}^2 = \hat{M}_x^2 + \hat{M}_y^2 + \hat{M}_z^2$$



 $oldsymbol{ ilde{1}}$ Our problem is to find the eigenvalues of $\,\hat{M}^2\,$ and $\,\hat{M}_z$

The ladder operator method for angular momentum

We can evaluate:

$$[\hat{M}^2, \hat{M}_x] = [\hat{M}^2, \hat{M}_y] = [\hat{M}^2, \hat{M}_z] = 0$$

We define:

Raising operator
$$\hat{M}_+ \equiv \hat{M}_x + i\hat{M}_y$$
 lowering operator $\hat{M}_- \equiv \hat{M}_x - i\hat{M}_y$ Ladder operators

The properties of ladder operators:

$$\hat{M}_{+}\hat{M}_{-} = (\hat{M}_{x} + i\hat{M}_{y})(\hat{M}_{x} - i\hat{M}_{y})$$

$$= \hat{M}_{x}(\hat{M}_{x} - i\hat{M}_{y}) + i\hat{M}_{y}(\hat{M}_{x} - i\hat{M}_{y})$$

$$= \hat{M}_{x}^{2} - i\hat{M}_{x}\hat{M}_{y} + i\hat{M}_{y}\hat{M}_{x} + \hat{M}_{y}^{2}$$

$$= \hat{M}^{2} - \hat{M}_{z}^{2} + i[\hat{M}_{y}, \hat{M}_{x}]$$



The ladder operator method for angular momentum



$$\hat{M}_{+}\hat{M}_{-}=\hat{M}^{2}-\hat{M}_{z}^{2}+\hbar\hat{M}_{z}$$

$$\hat{M}_{-}\hat{M}_{+} = \hat{M}^{2} - \hat{M}_{z}^{2} - \hbar \hat{M}_{z}$$

$$\begin{split} [\hat{M}_{+}, \hat{M}_{z}] &= [\hat{M}_{x} + i\hat{M}_{y}, \hat{M}_{z}] \\ &= [\hat{M}_{x}, \hat{M}_{z}] + i[\hat{M}_{y}, \hat{M}_{z}] = -i\hbar\hat{M}_{y} - \hbar\hat{M}_{x} \\ [\hat{M}_{+}, \hat{M}_{z}] &= -\hbar\hat{M}_{+} \end{split}$$



$$\hat{M}_+ \hat{M}_z = \hat{M}_z \hat{M}_+ - \hbar \hat{M}_+$$

$$\hat{M}_-\hat{M}_z=\hat{M}_z\hat{M}_-+\hbar\hat{M}_-$$

The ladder operator method for angular momentum

 $\hat{M}^2Y=cY$ \qquad Y: Common eigenfunctions of ${\rm M^2}$ and ${\rm M_z}$ $\hat{M}_zY=bY$

b: $\hat{M}_{+}\hat{M}_{z}Y = \hat{M}_{+}bY \\ \hat{M}_{+}\hat{M}_{z} = \hat{M}_{z}\hat{M}_{+} - \hbar\hat{M}_{+} \\ (\hat{M}_{z}\hat{M}_{+} - \hbar\hat{M}_{+})Y = b\hat{M}_{+}Y \\ \hat{M}_{z}(\hat{M}_{+}Y) = (b + \hbar)(\hat{M}_{+}Y) \\ \hat{M}_{z}(\hat{M}_{+}^{2}Y) = (b + 2\hbar)(\hat{M}_{+}^{2}Y)$



$$\hat{M}_z(\hat{M}_+^k Y) = (b + k\hbar)(\hat{M}_+^k Y) \qquad k = 0, \, 1, \, 2, \dots$$

The ladder operator method for angular momentum



If we operat with $M_{\scriptscriptstyle \perp}$:

$$\hat{M}_z(\hat{M}_-Y) = (b - \hbar)(\hat{M}_-Y)$$

$$\hat{M}_z(\hat{M}_-^kY) = (b - k\hbar)(\hat{M}_-^kY)$$

With raising and lowering operators we generate a ladder of eigenvalues

$$\cdots b-2\hbar, b-\hbar, b+\hbar, b+2\hbar, \cdots$$

Eigenfunctions and

Eigenfunctions and eigenvalues of
$$\mathbf{M}^2$$
 and $\mathbf{M}_z \hat{M}_\pm^k Y = (b \pm k\hbar) \hat{M}_\pm^k Y$ $k=0,1,2,\dots$



The ladder operator method for angular momentum



$$\hat{M}^2 \hat{M}_{\pm}^k Y = c \hat{M}_{\pm}^k Y, \qquad k = 0, 1, 2, \dots$$

We first show:

$$[\hat{M}^2, \hat{M}_{\pm}] = [\hat{M}^2, \hat{M}_x \pm i\hat{M}_y] = [\hat{M}^2, \hat{M}_x] \pm i[\hat{M}^2, \hat{M}_y] = 0 \pm 0 = 0$$

$$[\hat{M}^2, \hat{M}_{\pm}^2] = [\hat{M}^2, \hat{M}_{\pm}] \hat{M}_{\pm} + \hat{M}_{\pm} [\hat{M}^2, \hat{M}_{\pm}] = 0 + 0 = 0$$

Thus:

$$[\hat{M}^2, \hat{M}_{\pm}^k] = 0$$
 or $\hat{M}^2 \hat{M}_{\pm}^k = \hat{M}_{\pm}^k \hat{M}^2$, $k = 0, 1, 2, ...$



The ladder operator method for angular momentum



$$\begin{split} \hat{M}^2Y &= cY \\ \hat{M}_\pm^k \hat{M}^2Y &= \hat{M}_\pm^k cY \\ &\qquad \qquad \downarrow \qquad \hat{M}^2 \hat{M}_\pm^k = \hat{M}_\pm^k \hat{M}^2 \\ \hat{M}^2 (\hat{M}_+^k Y) &= c(\hat{M}_+^k Y) \end{split}$$

The set of M_z eigenvalues must be bounded:

$$\hat{M}_z Y = b Y$$
 $\hat{M}_z Y_k = b_k Y_k$
 $Y_k = \hat{M}_{\pm}^k Y$
 $b_k = b \pm k \hbar$



The ladder operator method for angular momentum



$$\hat{M}_z Y_k = b_k Y_k \longrightarrow \hat{M}_z^2 Y_k = b_k \hat{M}_z Y_k$$
$$\hat{M}_z^2 Y_k = b_k^2 Y_k$$

$$\begin{array}{c} \hat{M}^2(\hat{M}_{\pm}^kY) = c(\hat{M}_{\pm}^kY) \\ \hat{M}_z^2Y_k = b_k^2Y_k \end{array} \right] \qquad \hat{M}^2Y_k - \hat{M}_z^2Y_k = cY_k - b_k^2Y_k \\ \downarrow \qquad \qquad \qquad \hat{M}^2 = \hat{M}_x^2 + \hat{M}_y^2 + \hat{M}_z^2 \\ (\hat{M}_x^2 + \hat{M}_y^2)Y_k = (c - b_k^2)Y_k \end{array}$$

$$\hat{M}_x^2 + \hat{M}_y^2$$
 Corresponds to a nonnegative physical quantity



$$c-b_k^2\geqslant 0$$
 and $c^{1/2}\geqslant |b_k|$
$$c^{1/2}\geqslant b_k\geqslant -c^{1/2}\,,\qquad k=0,\ \pm 1,\ \pm 2,\ldots$$

The ladder operator method for angular momentum

Let b_{max} and b_{min} denotes the maximum and minimum values od b_k corresponding to Y_{max} and Y_{min}

$$\hat{M}_z Y_{\text{max}} = b_{\text{max}} Y_{\text{max}}$$
$$\hat{M}_z Y_{\text{min}} = b_{\text{min}} Y_{\text{min}}$$

$$\hat{M}_{+}\hat{M}_{z}Y_{\text{max}} = b_{\text{max}}\hat{M}_{+}Y_{\text{max}}$$
$$\hat{M}_{z}(\hat{M}_{+}Y_{\text{max}}) = (b_{\text{max}} + \hbar)(\hat{M}_{+}Y_{\text{max}})$$

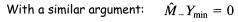
$$\hat{M}_+ Y_{\text{max}} = 0$$

$$0 = \hat{M}_{-}\hat{M}_{+}Y_{\text{max}} = (\hat{M}^{2} - \hat{M}_{z}^{2} - \hbar\hat{M}_{z})Y_{\text{max}} = (c - b_{\text{max}}^{2} - \hbar b_{\text{max}})Y_{\text{max}}$$



$$c - b_{\text{max}}^2 - \hbar b_{\text{max}} = 0$$
$$c = b_{\text{max}}^2 + \hbar b_{\text{max}}$$

The ladder operator method for angular momentum



$$c = b_{\min}^2 - \hbar b_{\min}$$

$$c = b_{\max}^2 + \hbar b_{\max}$$

$$c = b_{\min}^2 - \hbar b_{\min}$$

$$b_{\text{max}}^2 + \hbar b_{\text{max}} + (\hbar b_{\text{min}} - b_{\text{min}}^2) = 0$$

$$b_{\max} = -b_{\min}$$
, $b_{\max} = b_{\min} - \hbar$

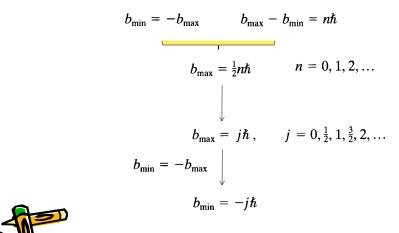


$$b_k = b \pm k\hbar$$

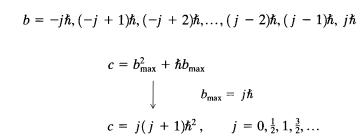
$$b_{\text{max}} - b_{\text{min}} = n\hbar$$
, $n = 0, 1, 2, ...$

$$n = 0, 1, 2, \dots$$

The ladder operator method for angular momentum



The ladder operator method for angular momentum





$$\hat{M}^{2}Y = j(j+1)\hbar^{2}Y, \qquad j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, ...$$

$$\hat{M}_{z}Y = m_{j}\hbar Y, \qquad m_{j} = -j, -j+1, ..., j-1, j$$