Lecture #2

Symmetries & Conservation Laws

Orbital angular momentum & spin

Quantum mechanics of angular momentum

Chapter 1, pages 1-10 of the Lectures on Atomic Physics

Chapter 6, pages 207-223 of QM by Jasprit Singh

Chapters 6.1-6.3, 6.7 pages 266-288, 299-302, Bransden & Joachain, Quantum Mechanics

Symmetries and conservation laws

If Hamiltonian H has a symmetry defined by the operator Õ

↓

This operation (Õ) leaves Hamiltonian H unchanged

$$\psi(\mathbf{r}_i') = \tilde{O}\psi(\mathbf{r}_i)$$

$$\tilde{O}(H\psi) = H(\tilde{O}\psi)$$

$$\Downarrow$$

$$\tilde{O}H - H\tilde{O} = 0$$

+

Quantum equation of motion

$$\frac{d\tilde{O}}{dt} = \frac{\partial\tilde{O}}{\partial t} + \frac{1}{i\hbar}\left[\tilde{O}, H\right]$$

$$\frac{d\tilde{O}}{dt} = 0$$

← The physical observable corresponding to operator Õ is conserved

Example: Spatial translation and momentum conservation

System of particles not in external field

$$\mathbf{r}_a \to \mathbf{r}_a + \delta\mathbf{r}$$

small spatial displacement

$$\left(\frac{\partial}{\partial x_a}, \frac{\partial}{\partial y_a}, \frac{\partial}{\partial z_a}\right)$$

$$\psi(\mathbf{r}_1 + \delta\mathbf{r}, \mathbf{r}_2 + \delta\mathbf{r}, \ldots) \to \psi(\mathbf{r}_1, \mathbf{r}_2, \ldots) + \delta\mathbf{r} \cdot \sum_a \nabla_a \psi$$

$$= \underbrace{\left(1 + \delta\mathbf{r} \cdot \sum_a \nabla_a\right)}_{\text{Operator of a small translation}} \psi(\mathbf{r}_1, \mathbf{r}_2, \ldots)$$

Operator of a small translation

$$\left(\sum_a \nabla_a H - H \sum_a \nabla_a\right) = 0, \quad p = -i\hbar\nabla \Rightarrow \textit{Conservation of momentum}$$

Symmetries	Conservation Laws
Translation in space	Conservation of momentum
Translation in time	Conservation of energy
Rotational invariance	Conservation of angular momentum
Symmetry under a phase change of the electron wave function	Conservation of charge
Symmetry under reflection	Conservation of parity

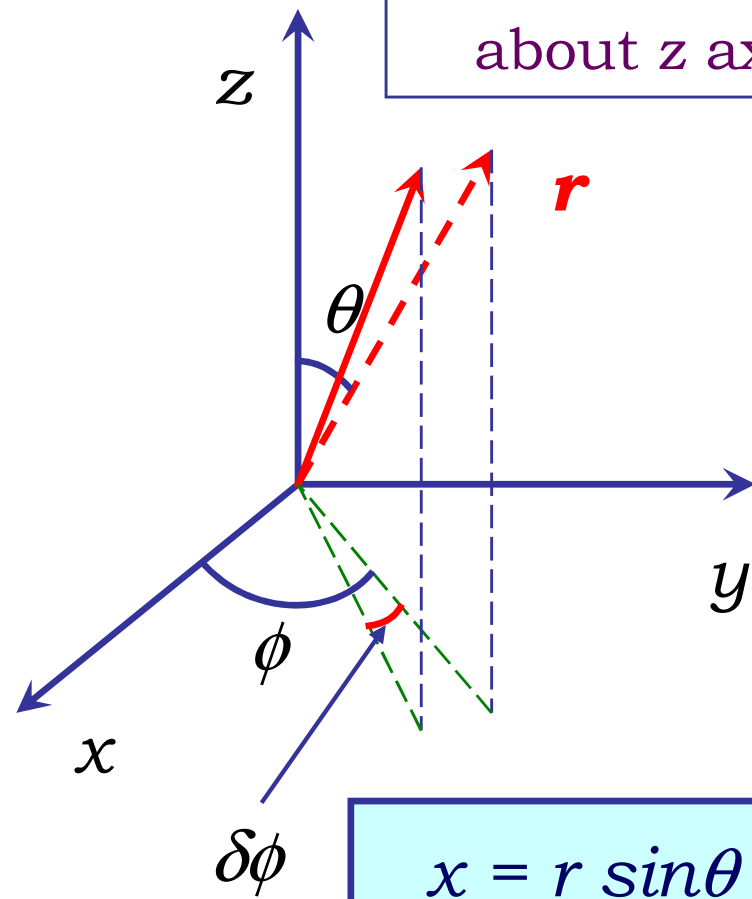
Infinitesimal rotation

Small rotation $\delta\phi$ about z axis

$$x' = r\sin\theta\cos(\phi-\delta\phi)$$
$$\approx r\sin\theta\,(\cos\phi+\delta\phi\,\sin\phi)$$
$$= x + \delta\phi\, y$$

$$y' = r\sin\theta\sin(\phi-\delta\phi)$$
$$\approx r\sin\theta\,(\sin\phi-\delta\phi\,\cos\phi)$$
$$= -\delta\phi\, x + y$$

$$z' = z$$



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

Infinitesimal rotation

Small rotation $\delta\phi$ about z axis

$\delta\mathbf{r}\cdot\nabla$

$x' = x + \delta\phi\, y$
$y' = y - \delta\phi\, x$
$z' = z$

$$\delta\psi(x,y,z) = \psi(x',y',z') - \psi(x,y,z)$$

$$= \left(\underbrace{\delta\phi\, y}_{\delta x} \frac{\partial}{\partial x} \underbrace{-\delta\phi\, x}_{\delta y} \frac{\partial}{\partial y} \right) \psi(x,y,z)$$

$$= -\delta\phi \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right) \psi(x,y,z)$$

L=r×p

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

$$\delta\psi(x,y,z) = -\frac{i}{\hbar} L_z \psi(x,y,z)$$

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

Operator L_z generates an infinitesimal rotation about Z axis

$$[p_i, x_i] = -i\hbar$$

Orbital angular momentum L

$$L_x = -ih\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$L_y = -ih\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$L_z = -ih\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$[L_x, L_y] = i\hbar L_z$$
$$[L_y, L_z] = i\hbar L_x$$
$$[L_z, L_x] = i\hbar L_y$$

→

$$[L_i, L_j] = i\hbar\varepsilon_{ijk} L_k$$

$$\varepsilon_{ijk} = \begin{cases} 1 \text{ for } \textit{cyclic permutations} \text{ from } 123: 231, 312 \\ -1 \text{ for } \textit{non-cyclic permutations} \text{ from } 123: 213, 132, 321 \\ 0 \text{ for all other cases} \end{cases}$$

$$[L_i, x_j] = i\hbar\varepsilon_{ijk} x_k$$

$$[L_i, p_j] = i\hbar\varepsilon_{ijk} p_k$$

$$[L^2, L_i] = 0$$ → It is possible to find simultaneous eigenstates of L^2 and any one component of **L.**

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

Quantum mechanics of the angular momentum

$\hbar = 1$

$$\left[J_i, J_j\right] = i\varepsilon_{ijk} J_k$$

$$\left[J^2, J_z\right] = 0$$

$$J^2 = J_x^2 + J_y^2 + J_z^2$$

J^2, J_z: Commuting hermitian operators so they have a complete set of simultaneous eigenvalues.

$$J^2 \left|\gamma\lambda m\right\rangle = \lambda \left|\gamma\lambda m\right\rangle$$

$$J_z \left|\gamma\lambda m\right\rangle = m \left|\gamma\lambda m\right\rangle$$

Our mission: find λ and m

Quantum mechanics of the angular momentum

$\hbar = 1$

$$\left[J_i, J_j\right] = i\varepsilon_{ijk} J_k$$

$$J_+ = J_x + iJ_y$$

$$J_- = J_x - iJ_y$$

$$J_z J_\pm |\lambda m\rangle = ?$$

$$J^2 J_\pm |\lambda m\rangle = ?$$

$$\left[J_z, J_+\right] = \left[J_z, J_x + iJ_y\right] = iJ_y + J_x = J_+$$

$$J^2 |\lambda m\rangle = \lambda |\lambda m\rangle$$

$$\left[J_z, J_-\right] = -J_-$$

$$J_z |\lambda m\rangle = m |\lambda m\rangle$$

$$\left[J^2, J_\pm\right] = 0$$

$$J_+ J^2 |\lambda m\rangle = \lambda J_+ |\lambda m\rangle$$

$$J^2 J_+ |\lambda m\rangle = \lambda J_+ |\lambda m\rangle$$

$$J_+ J_z |\lambda m\rangle = \left(J_z J_+ - [J_z, J_+]\right) |\lambda m\rangle$$

$$= J_z J_+ |\lambda m\rangle - J_+ |\lambda m\rangle = m J_+ |\lambda m\rangle$$

$$J_z J_+ |\lambda m\rangle = (m+1) J_+ |\lambda m\rangle$$

Quantum mechanics of the angular momentum

$\hbar = 1$

$$J^2 J_+ |\lambda m\rangle = \lambda J_+ |\lambda m\rangle$$
$$J_z J_+ |\lambda m\rangle = (m+1) J_+ |\lambda m\rangle$$

So $J_+ |\lambda m\rangle$ is a new eigenfunction belonging to the same eigenvalue of J^2 but to eigenvalue (m+1) of J_z.

$$J^2 J_- |\lambda m\rangle = \lambda J_- |\lambda m\rangle$$
$$J_z J_- |\lambda m\rangle = (m-1) J_- |\lambda m\rangle$$

$$J_+ \text{ and } J_- : \text{step-up(down) operators}$$
$$\text{ladder operators}$$

Quantum mechanics of the angular momentum

$$J^2 = J_x^2 + J_y^2 + J_z^2$$

$$J_x^2 + J_y^2 \; is\ a\ positive\ hermitian\ operator : \lambda \geq m^2$$

↓

For a definite value of λ m must have upper and lower bounds

j ≡ maximum value of m for a given λ

↓

$$J_+ |\lambda j\rangle = 0$$

$$J_- J_+ |\lambda j\rangle = 0$$

$$J_- J_+ = J^2 - J_z^2 - J_z$$

$$\left(\lambda - j^2 - j\right)|\lambda j\rangle = 0$$

→

$$Since\ |\lambda j\rangle \neq 0$$

$$\lambda - j^2 - j = 0 \Rightarrow \lambda = j(j+1)$$

Quantum mechanics of the angular momentum

$$J^2 = J_x^2 + J_y^2 + J_z^2$$

For a definite value of λ m must have upper and lower bounds

j-r ≡ minimum value of m for a given λ

$$J_-\left|\lambda, j-r\right\rangle = 0$$

$$J_+J_-\left|\lambda, j-r\right\rangle = 0$$

$$J_+J_- = J^2 - J_z^2 + J_z$$

$$\left(\lambda - (j-r)^2 + j - r\right)\left|\lambda, j-r\right\rangle = 0$$

$$Since \left|\lambda j\right\rangle \neq 0$$

$$j(j+1) - (j-r)^2 + j - r = 0$$

$$r = 2j$$

$$m_{\min} = -j$$

Quantum mechanics of the angular momentum: SUMMARY

$$J^2 | jm\rangle = j(j+1) | jm\rangle$$
$$J_z | jm\rangle = m | jm\rangle$$

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

$$m = -j, -j+1, \ldots, j-1, j : \; (2j+1) \; \textit{eigenfunctions for each value of } j$$

2j is an integer

$$j : 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$$

Ladder operators

$\hbar = 1$

$$J^2 J_+ |jm\rangle = j(j+1) J_+ |jm\rangle$$

$$J_z J_+ |jm\rangle = (m+1) J_+ |jm\rangle$$

So $J_+ |jm\rangle$ is a new eigenfunction belonging to the same eigenvalue of J^2 but to eigenvalue (m+1) of J_z.

$$J^2 J_- |jm\rangle = j(j+1) J_- |jm\rangle$$

$$J_z J_- |jm\rangle = (m-1) J_- |jm\rangle$$

$$J_\pm |jm\rangle = ?$$

Ladder operators

$$J_{\pm}\,|\,jm\rangle = ?$$

$$J_+^\dagger = J_-$$

$$J_+\,|\,j,m\rangle = \alpha_{jm}\,|\,j,m+1\rangle$$

$$\left(J_+\,|\,j,m\rangle\right)^* = \langle j,m|\,J_+^\dagger = \langle j,m|\,J_- = \alpha^*_{jm}\,\langle j,m+1|$$

$$\langle j,m|\,J_-J_+\,|\,j,m\rangle = \left|\alpha_{jm}\right|^2 \langle j,m+1|\,j,m+1\rangle$$

$$J_-J_+ = J^2 - J_z^2 - J_z$$

$$\langle j,m|\,j,m\rangle\left(j(j+1) - m^2 - m\right) = \left|\alpha_{jm}\right|^2 \langle j,m+1|\,j,m+1\rangle$$

$$\left|\alpha_{jm}\right|^2 = j(j+1) - m(m+1)$$

$$\alpha_{jm} = \sqrt{j(j+1) - m(m+1)}$$

Ladder operators

$$J_+ \left| j, m \right\rangle = \sqrt{j(j+1) - m(m+1)} \left| j, m+1 \right\rangle$$

$$J_- \left| j, m \right\rangle = \sqrt{j(j+1) - m(m-1)} \left| j, m-1 \right\rangle$$

Why orbital angular momentum can not have half integer values?

In spherical coordinates

$$L_z = -i\frac{\partial}{\partial\phi}$$

$$L_z\psi = m\psi$$

$$-i\frac{\partial\psi}{\partial\phi} = m\psi$$

$$\psi = f(r,\theta)e^{im\phi}$$

$$\Phi(\phi) = e^{im\phi}$$

$$\Phi(0) = \Phi(2\pi)$$

$$e^{i2\pi m} = 1 \Rightarrow m\ must\ be\ integer$$

l must be integer

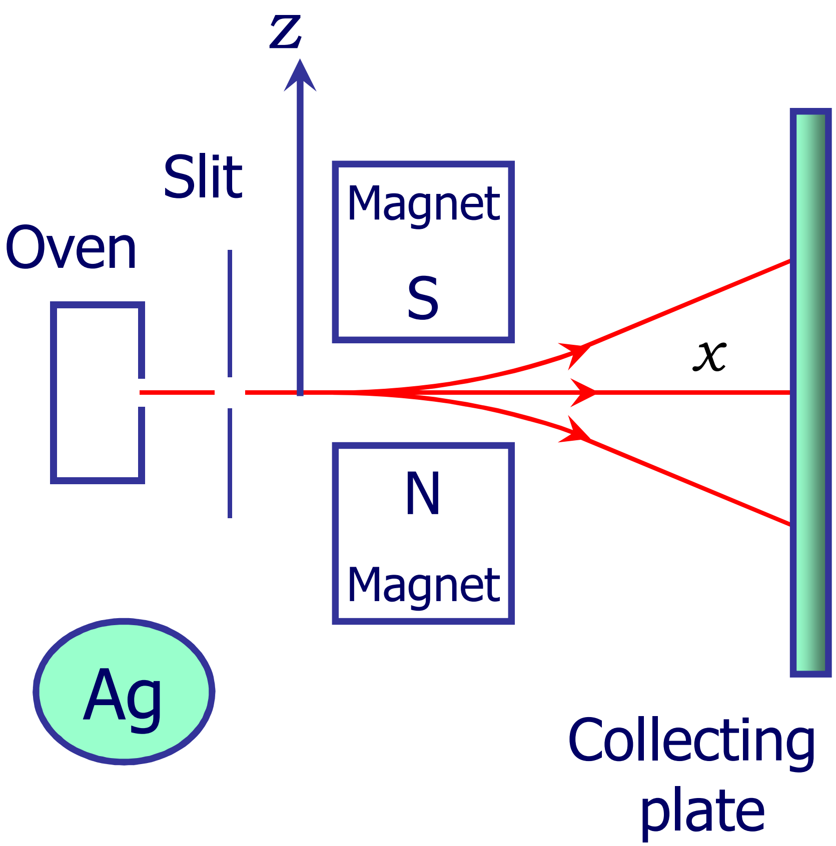
Spin: internal angular momentum

The Stern-Gerlach experiment

measuring magnetic moments of atoms

$$\mathcal{M} = -\frac{e}{2m}\mathbf{L}$$

$$F_i = \mathcal{M} \cdot \frac{\partial \mathbf{B}}{\partial x_i}$$



Expected: uniform distribution deflections as the direction of the atomic magnetic moment $\mathcal{M}$ is at random and every value of the $\mathcal{M}_z$ ($\mathcal{M} \leq \mathcal{M}_z \leq \mathcal{M}$) can occur in z direction

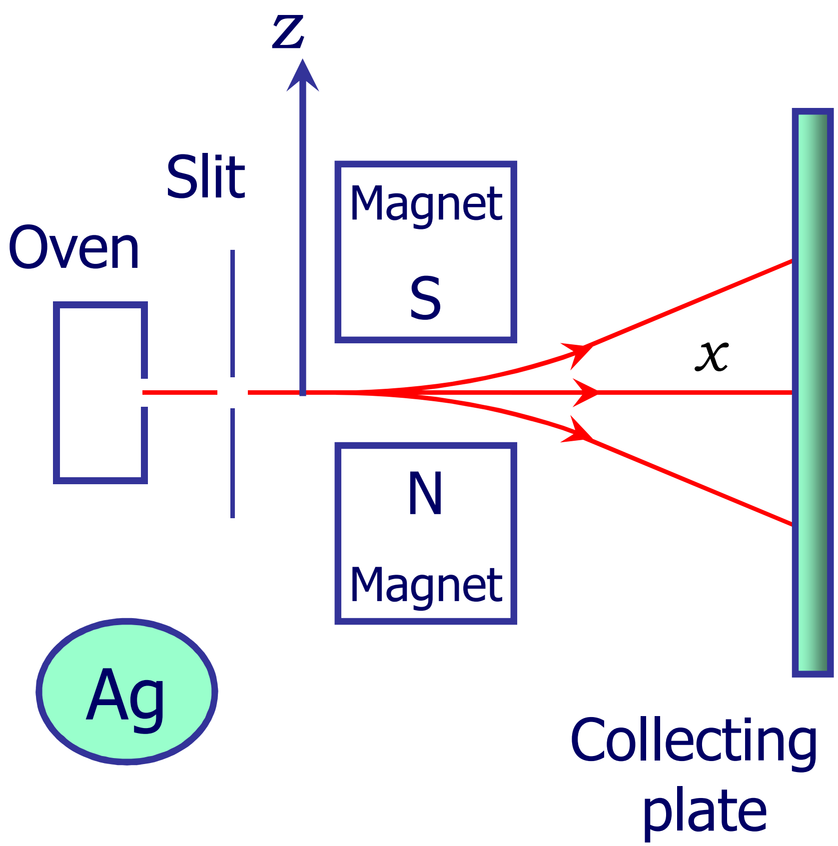
Spin: internal angular momentum

$$\mathcal{M} = -\frac{e}{2m}\mathbf{L}$$

$$F_i = \mathcal{M} \cdot \frac{\partial \mathbf{B}}{\partial x_i}$$

The Stern-Gerlach experiment

measuring magnetic moments of atoms



Found: two distinct traces
(beam was split to two components)
So multiplicity $\alpha = 2l+1 = 2! \Rightarrow l = 1/2?$
Ag, Au, Cu, Na, K, Cs, H

Spin: internal angular momentum

$$\mathcal{M} = -\frac{e}{2m}\mathbf{L}$$

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The Stern-Gerlach experiment

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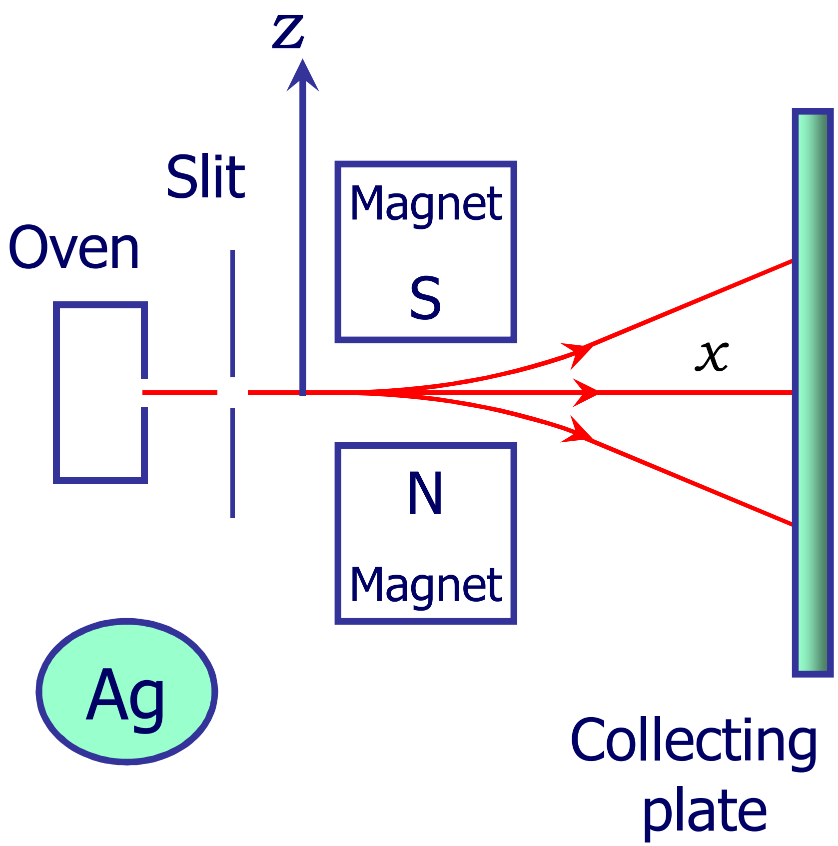

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H	1s
Na	$\{1s^2 2s^2 2p^6\} 3s^1$
K	$\{1s^2 2s^2 2p^6 3s^2 3p^6\} 4s^1$
Cu	$\{1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}\} 4s^1$
Ag	$\{1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10}\} 5s^1$
Cs	$\{[Ag] 5s^2 5p^6\} 6s^1$
Au	$\{[Cs] 5d^{10} 4f^{14}\} 6s^1$

l=0, s=1/2