1 Angular momentum algebra

1.1 The algebra

The commutation relations are

$$[L_x, L_y] = i\hbar L_z \tag{1}$$

and others obtained from cycling

$$x \to y \to z \to x \tag{2}$$

We also have

$$[L_x, L^2] = 0 \tag{3}$$

We write

$$L_z|\beta, \alpha\rangle = \alpha|\beta, \alpha\rangle, \quad L^2|\beta, \alpha\rangle = \beta|\beta, \alpha\rangle \tag{4}$$

Thus L^2, L_z will be simple in our representation. We define

$$L_+ = L_x + iL_y \tag{5}$$

$$L_- = L_x - iL_y \tag{6}$$

Then we find

$$L_+L_- = L_x^2 + L_y^2 - i[L_x, L_y] = L_x^2 + L_y^2 + \hbar L_z \tag{7}$$

$$L_-L_+ = L_x^2 + L_y^2 + i[L_x, L_y] = L_x^2 + L_y^2 - \hbar L_z \tag{8}$$

This gives

$$L^2 = L_+L_- - \hbar L_z + L_z^2 \tag{9}$$

$$L^2 = L_-L_+ + \hbar L_z + L_z^2 \tag{10}$$

Thus

$$L_+L_- = L^2 + \hbar L_z - L_z^2 \tag{11}$$

$$L_-L_+ = L^2 - \hbar L_z - L_z^2 \tag{12}$$

1.2 Raising and lowering

Now we see that

$$L_zL_+|\alpha, \beta\rangle = (\alpha + \hbar)L_+|\beta, \alpha\rangle \tag{13}$$

$$L_zL_-|\alpha, \beta\rangle = (\alpha - \hbar)L_z|\beta, \alpha\rangle \tag{14}$$

$$L^2L_\pm|\alpha, \beta\rangle = \beta L_\pm|\beta, \alpha\rangle \tag{15}$$

Positivity shows that

$$\alpha^2 \le \beta \tag{16}$$

So there is a maximum value for α. We call this α_{max}. Since we cannot raise α any higher than this, we have

$$L_+|\alpha_{max}, \beta\rangle = 0 \tag{17}$$

Then we have

$$L^2|\alpha_{max}, \beta\rangle = (L_-L_+ + \hbar L_z + L_z^2)|\alpha_{max}, \beta\rangle = \alpha_{max}^2 + \hbar\alpha_{max} \tag{18}$$

Thus

$$\beta = \alpha_{max}(\alpha_{max} + \hbar) \tag{19}$$

1.3   Coefficients

We assume normalized states $|\beta, \alpha\rangle$ so that

$$\langle\beta, \alpha|\beta, \alpha\rangle = 1 \tag{20}$$

Let us define

$$L_-|\beta, \alpha\rangle = C_-(\beta, \alpha) \tag{21}$$

$$L_+|\beta, \alpha\rangle = C_+(\beta, \alpha) \tag{22}$$

We have

$$L_+L_- = L^2 + \hbar L_z - L_z^2 \tag{23}$$

We have

$$\langle\beta, \alpha|L_+L_-|\beta, \alpha\rangle = |C_-(\beta, \alpha)|^2 \tag{24}$$

The LHS can be written as

$$\langle\beta, \alpha|L_+L_-|\beta, \alpha\rangle = \langle\beta, \alpha|(L^2 + \hbar L_z - L_z^2)|\beta, \alpha\rangle \tag{25}$$

This is

$$\langle\beta, \alpha|(\beta + \hbar\alpha - \alpha^2)|\beta, \alpha\rangle = (\beta + \hbar\alpha - \alpha^2) \tag{26}$$

Using the value of β, we find

$$C_-(\beta, \alpha) = [\alpha_{max}(\alpha_{max} + \hbar) + \hbar\alpha - \alpha^2]^{\frac{1}{2}} \tag{27}$$

Similarly we find

$$C_+(\beta, \alpha) = [\alpha_{max}(\alpha_{max} + \hbar) - \hbar\alpha - \alpha^2]^{\frac{1}{2}} \tag{28}$$

1.4 Multiplets

For the lowest state in the multiplet, we must have

$$C_-(\beta, \alpha) = 0 \qquad (29)$$

This gives a quadratic equation for α, with the solutions

$$\alpha = \alpha_{max} + \hbar \qquad (30)$$

and

$$\alpha = -\alpha_{max} \qquad (31)$$

The first is not an allowed value of α, so we take the second value. The change in α from the highest to the lowest value is

$$\Delta\alpha = \alpha_{max} - (-\alpha_{max}) = 2\alpha_{max} \qquad (32)$$

This must be an integer number N times the step size $\hbar$. Thus

$$2\alpha_{max} = N\hbar \qquad (33)$$

$$\alpha_{max} = \frac{N}{2}\hbar \qquad (34)$$

We write

$$l = \frac{N}{2} \qquad (35)$$

and get the allowed values

$$l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots \qquad (36)$$

2 The coordinate representation of the $\hat{L}_i$

2.1 The 2-d case

Consider the plane x, y with

$$x = r\cos\theta, \quad y = r\sin\theta \qquad (37)$$

Perform a rotation so that the function value at the point θ gets carried to the point $\theta + \delta\alpha$. We write this as

$$\theta \to \theta + \delta\alpha \qquad (38)$$

The new function is

$$\tilde{f}(\theta) = f(\theta - \delta\alpha) = f(\theta) + \delta\alpha(-\frac{\partial}{\partial\theta})f(\theta) + \ldots \qquad (39)$$

The angular momentum generator is

$$\hat{L} = -i\hbar\frac{\partial}{\partial\theta} \qquad (40)$$

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2.2 The 3-d case

Now we have two coordinates θ, ϕ. Under a rotation, we will have

$$\theta \to \theta + c_1 \delta\alpha \tag{41}$$

$$\phi \to \phi + c_2 \delta\alpha \tag{42}$$

$$\tilde{f}(\theta, \phi) = f(\theta - c_1 \delta\alpha, \phi - c_2 \delta\alpha) = f(\theta, \phi) + \delta\alpha(-c_1 \frac{\partial}{\partial\theta} - c_2 \frac{\partial}{\partial\phi})f(\theta, \phi) + \dots \tag{43}$$

Thus we should write

$$\hat{L} = -i\hbar(c_1 \frac{\partial}{\partial\theta} + c_2 \frac{\partial}{\partial\phi}) \tag{44}$$

Now we look at each case.

2.3 $\hat{L}_z$

We have

$$x = r \sin\theta \cos\phi, \quad y = r \sin\theta \sin\phi, \quad z = r \cos\theta \tag{45}$$

We need

$$\delta z = 0, \quad \delta y = x\delta\alpha, \quad \delta x = -y\delta\alpha \tag{46}$$

Since we will remain on the sphere, we set $r = 1$ so that

$$\delta r = 0 \tag{47}$$

Then

$$\delta z = -r \sin\theta\delta\theta = 0 \tag{48}$$

which gives

$$\delta\theta = 0 \tag{49}$$

We also have

$$\delta x = r \cos\theta\delta\theta \cos\phi - r \sin\theta \sin\phi\delta\phi \tag{50}$$

We set this equal to $-y\delta\alpha$ getting

$$r \cos\theta\delta\theta \cos\phi - r \sin\theta \sin\phi\delta\phi = -r \sin\theta \sin\phi\delta\alpha \tag{51}$$

which gives

$$\delta\phi = \delta\alpha \tag{52}$$

Thus we get

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\phi} \tag{53}$$

as expected.

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2.4 $\hat{L}_x$

We need
$$\delta x = 0, \quad \delta z = y\delta\alpha, \quad \delta y = -z\delta\alpha \tag{54}$$

From $\delta x = 0$ we get
$$r\cos\theta\delta\theta\cos\phi - r\sin\theta\sin\phi\delta\phi \tag{55}$$

which gives
$$\delta\phi = \cot\theta\cot\phi\delta\theta \tag{56}$$

From $\delta z = y\delta\alpha$ we get
$$-r\sin\theta\delta\theta = r\sin\theta\sin\phi\delta\alpha \tag{57}$$

which gives
$$\delta\theta = -\sin\phi\delta\alpha \tag{58}$$

Then we get
$$\delta\phi = \cot\theta\cot\phi\delta\theta = -\cot\theta\cos\phi\delta\alpha \tag{59}$$

Thus
$$\hat{L}_x = -i\hbar(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}) \tag{60}$$

2.5 $\hat{L}_y$

We need
$$\delta y = 0, \quad \delta x = z\delta\alpha, \quad \delta z = -x\delta\alpha \tag{61}$$

From $\delta y = 0$ we get
$$r\cos\theta\delta\theta\sin\phi + r\sin\theta\cos\phi\delta\phi \tag{62}$$

which gives
$$\delta\phi = -\cot\theta\tan\phi\delta\theta \tag{63}$$

From $\delta z = -x\delta\alpha$ we get
$$-r\sin\theta\delta\theta = -r\sin\theta\cos\phi\delta\alpha \tag{64}$$

which gives
$$\delta\theta = \cos\phi\delta\alpha \tag{65}$$

Then we get
$$\delta\phi = -\cot\theta\tan\phi\delta\theta = -\cot\theta\sin\phi\delta\alpha \tag{66}$$

Thus
$$\hat{L}_y = -i\hbar(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}) \tag{67}$$

2.6 Computing $\hat{L}_\pm$

We have

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y = -i\hbar \left((-\sin\phi + i\cos\phi)\frac{\partial}{\partial\theta} - \cot\theta(\cos\phi + i\sin\phi)\frac{\partial}{\partial\phi} \right) = -i\hbar \left(ie^{i\phi}\frac{\partial}{\partial\theta} - \cot\theta e^{i\phi}\frac{\partial}{\partial\phi} \right)$$
(68)

This gives

$$\hat{L}_+ = \hbar e^{i\phi} \left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi} \right)$$
(69)

Similarly, we have

$$\hat{L}_- = \hat{L}_x + i\hat{L}_y = -i\hbar \left((-\sin\phi - i\cos\phi)\frac{\partial}{\partial\theta} - \cot\theta(\cos\phi - i\sin\phi)\frac{\partial}{\partial\phi} \right) = -i\hbar \left(-ie^{-i\phi}\frac{\partial}{\partial\theta} - \cot\theta e^{-i\phi}\frac{\partial}{\partial\phi} \right)$$
(70)

This gives

$$\hat{L}_- = \hbar e^{-i\phi} \left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi} \right)$$
(71)

3 Spin

3.1 The problem with spin

We have, under a rotation about the z axis by angle $\delta\alpha$

$$\phi \to \phi + \delta\alpha$$
(72)

We get the change of functions

$$f(\phi) \to \tilde{f}(\phi)$$
(73)

where

$$\tilde{f}(\phi) = f(\phi - \delta\alpha) \approx f(\phi) - \delta\alpha\frac{\partial}{\partial\phi}f(\phi)$$
(74)

We get this from

$$f \to (1 - i\delta\alpha\frac{\hat{L}_z}{\hbar})f = (1 - i\delta\alpha\frac{1}{\hbar}(-i\hbar\frac{\partial}{\partial\phi}))f = (1 - \delta\alpha\frac{\partial}{\partial\phi})f$$
(75)

For finite rotations, we get

$$f \to \tilde{f} = e^{-i\alpha\frac{\hat{L}_z}{\hbar}}f$$
(76)

Suppose that

$$\hat{L}_z f = \hbar m f$$
(77)

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Then we get

$$f \to \tilde{f} = e^{-i\alpha \frac{\hat{L}_z}{\hbar}} f = e^{-i\alpha \frac{m}{\hbar}} f = e^{-i\alpha m} f \tag{78}$$

If m is an integer then $\alpha = 2\pi$ gives

$$e^{-i\alpha m} = e^{2\pi mi} = 1 \tag{79}$$

But if α is a half integer, then $\alpha = 2\pi$ gives

$$e^{-i\alpha m} = e^{2\pi mi} = -1 \tag{80}$$

3.2 Making a matrix representation of the $\hat{L}_i$

We start with the normalized basis

$$|l, m\rangle \tag{81}$$

Thus

$$\langle l', m' | l, m \rangle = \delta_{l,l'} \delta_{m,m'} \tag{82}$$

Then we have

$$\hat{L}_z | l, m \rangle = \hbar m | l, m \rangle \tag{83}$$

$$\hat{L}_+ | l, m \rangle = \hbar \sqrt{(l-m)(l+m+1)} | l, m+1 \rangle \tag{84}$$

$$\hat{L}_- | l, m \rangle = \hbar \sqrt{(l+m)(l-m+1)} | l, m-1 \rangle \tag{85}$$

3.3 The matrices for $l = \frac{1}{2}$

We write

$$| \frac{1}{2}, \frac{1}{2} \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{86}$$

$$| \frac{1}{2}, -\frac{1}{2} \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{87}$$

Thus

$$|\psi\rangle = \alpha | \frac{1}{2}, \frac{1}{2} \rangle + \beta | \frac{1}{2}, -\frac{1}{2} \rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{88}$$

We have

$$\langle \psi | \psi \rangle = |\alpha|^2 + |\beta|^2 \tag{89}$$

If the state is normalized, then

$$\langle \psi | \psi \rangle = |\alpha|^2 + |\beta|^2 = 1 \tag{90}$$

Then

$$\hat{L}_z \equiv \hat{s}_z = \begin{pmatrix} \frac{1}{2}\hbar & 0 \\ 0 & -\frac{1}{2}\hbar \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \equiv \frac{1}{2}\hbar \sigma_z \tag{91}$$

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$$\hat{L}_+ \equiv \hat{s}_+ = \begin{pmatrix} 0 & \hbar \\ 0 & 0 \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} \equiv \frac{1}{2}\hbar\sigma_+ \tag{92}$$

$$\hat{L}_- \equiv \hat{s}_- = \begin{pmatrix} 0 & 0 \\ \hbar & 0 \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix} \equiv \frac{1}{2}\hbar\sigma_- \tag{93}$$

We can also define

$$\sigma_+ = \sigma_x + i\sigma_y, \quad \sigma_- = \sigma_x - i\sigma_y \tag{94}$$

which gives

$$\sigma_x = \frac{1}{2}(\sigma_+ + \sigma_-) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{95}$$

$$\sigma_y = \frac{1}{2i}(\sigma_+ - \sigma_-) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{96}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{97}$$

In short,

$$\hat{s}_i = \frac{1}{2}\hbar\sigma_i, \quad i = x, y, z \tag{98}$$

3.4   The algebra of Pauli matrices

We have

$$\sigma_x^2 = 1, \quad \sigma_y^2 = 1, \quad \sigma_z^2 = 1 \tag{99}$$

$$\sigma_x\sigma_y = i\sigma_z, \quad \sigma_y\sigma_z = i\sigma_x, \quad \sigma_z\sigma_x = i\sigma_y \tag{100}$$

Thus

$$[\sigma_x, \sigma_y] = 2i\sigma_z, \quad [\sigma_y, \sigma_z] = 2i\sigma_x, \quad [\sigma_z, \sigma_x] = 2i\sigma_y \tag{101}$$

Now we compute

$$e^{i(\alpha_x\sigma_x + \alpha_y\sigma_y + \alpha_z\sigma_z)} \equiv e^{i\vec{\alpha}\cdot\vec{\sigma}} \tag{102}$$

We can also write this as

$$(\alpha_x, \alpha_y, \alpha_z) = \alpha(n_x, n_y, n_z), \quad \vec{\alpha} = \alpha\hat{n} \tag{103}$$

where $\hat{n}$ is a unit vector. We note that

$$(n_x\sigma_x + n_y\sigma_y + n_z\sigma_z)^2 = n_x^2 + n_y^2 + n_z^2 = 1 \tag{104}$$

Thus we get

$$e^{i\vec{\alpha}\cdot\vec{\sigma}} = e^{i\alpha\hat{n}\cdot\vec{\sigma}} = 1 + i\alpha\hat{n}\cdot\vec{\sigma} - \frac{\alpha^2}{2!} - i\frac{\alpha^3}{3!}\hat{n}\cdot\vec{\sigma} + \ldots = \cos\alpha + i(\hat{n}\cdot\vec{\sigma})\sin\alpha \tag{105}$$

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3.5 Rotations

For rotations about the z axis we have

$$|\psi\rangle \rightarrow |\psi\rangle = e^{-i\alpha \frac{\hat{s}_z}{\hbar}} |\psi\rangle \tag{106}$$

For rotations about the x axis we have

$$|\psi\rangle \rightarrow |\psi\rangle = e^{-i\frac{1}{2}\alpha \frac{\hat{s}_x}{\hbar}} |\psi\rangle = (\cos\frac{\alpha}{2} - i\sin\frac{\alpha}{2}\sigma_x)|\psi\rangle = \begin{pmatrix} \cos\frac{\alpha}{2} & -i\sin\frac{\alpha}{2} \\ -i\sin\frac{\alpha}{2} & \cos\frac{\alpha}{2} \end{pmatrix} |\psi\rangle \tag{107}$$

3.6 Measurements

We write

$$|\frac{1}{2},\frac{1}{2}\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{108}$$

$$|\frac{1}{2},-\frac{1}{2}\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{109}$$

In general we have

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \tag{110}$$

If the wavefunction (spinor) is normalized, we have

$$|\alpha|^2 + |\beta|^2 = 1 \tag{111}$$

We can write

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = c_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + c_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{112}$$

If we measure $\hat{s}_z$ we will get $\frac{1}{2}\hbar$ with probability $|c_1|^2$ and $-\hbar$ with probability $|c_2|^2$.

If we measure $\hat{s}_x$, we will again get two possibilities $\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$. But we need the eigenfunctions:

$$\hat{s}_x = \frac{1}{2}\hbar\sigma_x \tag{113}$$

$$\lambda = \frac{1}{2}\hbar: \quad |\psi_+\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \tag{114}$$

$$\lambda = -\frac{1}{2}\hbar: \quad |\psi_-\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \tag{115}$$

Suppose we are given

$$|\psi\rangle = \begin{pmatrix} \frac{3}{5} \\ \frac{4}{5} \end{pmatrix} \tag{116}$$

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Then we should write this as

$$\begin{pmatrix} \frac{3}{5} \\ \frac{4}{5} \end{pmatrix} = c_1 \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} + c_2 \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \tag{117}$$

If we measure $\hat{s}_x$ we will get $\frac{1}{2}\hbar$ with probability $|c_1|^2$ and $-\hbar$ with probability $|c_2|^2$.

An easy way to compute c_i, c_2 is to note that the eigenvectors are orthonormal. Thus wee have

$$|\psi\rangle = c_1|\psi_+\rangle_x + c_2|\psi_-\rangle_x \tag{118}$$

where $|\psi_\pm\rangle_x$ are the eigenstates of s_x with eigenvalues $\pm\frac{1}{2}\hbar$. Then we have

$$_x\langle\psi_+|\psi\rangle = c_1 \ _x\langle\psi_+|\psi_+\rangle_x + c_2 \ _x\langle\psi_+|\psi_-\rangle_x = c_1 \tag{119}$$

$$_x\langle\psi_-|\psi\rangle = c_1 \ _x\langle\psi_-|\psi_+\rangle_x + c_2 \ _x\langle\psi_-|\psi_-\rangle_x = c_2 \tag{120}$$

Thus we will get

$$c_1 = \left((\tfrac{1}{\sqrt{2}})^*, (\tfrac{1}{\sqrt{2}})^* \right) \begin{pmatrix} \frac{3}{5} \\ \frac{4}{5} \end{pmatrix} = \frac{7}{5\sqrt{2}} \tag{121}$$

Similarly,

$$c_2 = \left((\tfrac{1}{\sqrt{2}})^*, -(\tfrac{1}{\sqrt{2}})^* \right) \begin{pmatrix} \frac{3}{5} \\ \frac{4}{5} \end{pmatrix} = -\frac{1}{5\sqrt{2}} \tag{122}$$

As a check, we see that the probabilities add up to unity

$$|c_1|^2 + |c_2|^2 = 1 \tag{123}$$

4 Hamiltonians

The Schrodinger equation is

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \tag{124}$$

This gives

$$\psi = e^{-i\frac{1}{\hbar}\hat{H}t}\psi_0, \quad \psi_0 = \psi(t=0) \tag{125}$$

For spin systems, we have a 2-dimensional Hilbert space, and so we can write

$$\hat{H} = AI + B\sigma_1 + C\sigma_2 + D\sigma_3 \tag{126}$$

We need

$$\hat{H} = \hat{H}^\dagger \tag{127}$$

We have

$$I^\dagger = I, \quad \sigma_i^\dagger = \sigma_i \tag{128}$$

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Thus A, B, C, D are real.

In particular for a spin placed in a magnetic field, we have

$$\hat{H} = -\vec{\mu} \cdot \vec{B} \tag{129}$$

We have

$$\vec{\mu} = -\nu \vec{S} \tag{130}$$

But

$$\vec{S} = \frac{1}{2}\hbar\vec{\sigma} \tag{131}$$

Thus

$$\hat{H} = \nu\frac{1}{2}\hbar\vec{B} \cdot \vec{\sigma} \tag{132}$$

4.1   Problem 10-8

We start with the spin in the state

$$\psi_0 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \tag{133}$$

The first evolution gives

$$\psi_1 = e^{-\frac{i}{\hbar}\hat{H}_1 T}\psi_0 = e^{-i\frac{1}{2}\nu B\sigma_z T}\psi_0 = \left(\cos(\frac{1}{2}\nu BT) - i\sin(\frac{1}{2}\nu BT)\sigma_z\right)\psi_0 \tag{134}$$

$$= \begin{pmatrix} \cos(\frac{1}{2}BT) - i\sin(\frac{1}{2}\nu BT) & 0 \\ 0 & \cos(\frac{1}{2}\nu BT) + i\sin(\frac{1}{2}\nu BT) \end{pmatrix}\psi_0 \tag{135}$$

The second evolution gives

$$\psi_2 = e^{-\frac{i}{\hbar}\hat{H}_2 T}\psi_1 = e^{-i\frac{1}{2}\nu B\sigma_y T}\psi_1 = \left(\cos(\frac{1}{2}\nu BT) - i\sin(\frac{1}{2}\nu BT)\sigma_y\right)\psi_1 \tag{136}$$

$$= \begin{pmatrix} \cos(\frac{1}{2}BT) & -\sin(\frac{1}{2}\nu BT) \\ \sin(\frac{1}{2}\nu BT) & \cos(\frac{1}{2}\nu BT) \end{pmatrix}\psi_1 \tag{137}$$

Thus the final wavefunction is

$$\psi_f = \begin{pmatrix} \cos(\frac{1}{2}BT) & -\sin(\frac{1}{2}\nu BT) \\ \sin(\frac{1}{2}\nu BT) & \cos(\frac{1}{2}\nu BT) \end{pmatrix} \begin{pmatrix} \cos(\frac{1}{2}BT) - i\sin(\frac{1}{2}\nu BT) & 0 \\ 0 & \cos(\frac{1}{2}\nu BT) + i\sin(\frac{1}{2}\nu BT) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\tag{138}$$

The probability amplitude to get $\sigma_x = \frac{1}{2}\hbar$ is

$$
\begin{aligned}
A &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} \cos(\frac{1}{2}BT) & -\sin(\frac{1}{2}\nu BT) \\ \sin(\frac{1}{2}\nu BT) & \cos(\frac{1}{2}\nu BT) \end{pmatrix} \\
&\begin{pmatrix} \cos(\frac{1}{2}BT) - i\sin(\frac{1}{2}\nu BT) & 0 \\ 0 & \cos(\frac{1}{2}\nu BT) + i\sin(\frac{1}{2}\nu BT) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}
\end{aligned}
\tag{139}
$$

$$
= \cos^2(\frac{1}{2}\nu BT) - i\sin^2(\frac{1}{2}\nu BT) \tag{140}
$$

and the probability is

$$
P = |A|^2 = \cos^4(\frac{1}{2}BT) + \sin^4(\frac{1}{2}BT) \tag{141}
$$

We can simplify this further by using the identities

$$
\cos^2\theta = \frac{1}{2}(1 + \cos(2\theta)), \quad \sin^2\theta = \frac{1}{2}(1 - \cos(2\theta)) \tag{142}
$$

which give

$$
\cos^4\theta + \sin^4\theta = \frac{1}{4}(1 + \cos(2\theta))^2 + \frac{1}{4}(1 - \cos(2\theta))^2 = \frac{1}{2}(1 + \cos^2(2\theta)) \tag{143}
$$

Thus we get

$$
P = \frac{1}{2}(1 + \cos^2(\nu BT)) \tag{144}
$$

This can b mapped to the text through

$$
\nu = \frac{eg}{2m} \tag{145}
$$

5   The Hydrogen atom

In 3-d we have

$$
i\hbar\frac{\partial}{\partial t}\psi(x, y, z, t) = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi(x, y, , t) + V(x, y, z, t)\psi(x, y, z, t) \tag{146}
$$

We wish to write this in polar coordinates:

$$
x = r\sin\theta\cos\phi, \quad y = r\sin\theta\sin\phi, \quad z = r\cos\theta \tag{147}
$$

We can write

$$
\psi(x, y, z, t) \to \tilde{\psi}(r, \theta, \phi, t) \tag{148}
$$

(We will write the $\tilde{\psi} \to \psi$ from now on.) Similarly, we can write

$$
V(x, y, z, t) \to \tilde{V}(r, \theta, \phi, t) \tag{149}
$$

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and write $\tilde{V} \to V$ from now on. But we have

$$\frac{\partial \psi}{\partial x} = \frac{\partial \psi}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial \psi}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial \psi}{\partial \phi}\frac{\partial \phi}{\partial x} \tag{150}$$

Thus we need the inverse relations

$$r = (x^2 + y^2 + z^2)^{\frac{1}{2}}, \quad \theta = \tan^{-1}\frac{\sqrt{x^2 + y^2}}{z}, \quad \phi = \tan^{-1}\frac{y}{x} \tag{151}$$

For the second derivative

$$\begin{aligned}\frac{\partial^2 \psi}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial \psi}{\partial x} \quad &= \quad \frac{\partial}{\partial r}[\frac{\partial \psi}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial \psi}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial \psi}{\partial \phi}\frac{\partial \phi}{\partial x}]\frac{\partial r}{\partial x} \\ &+ \quad \frac{\partial}{\partial \theta}[\frac{\partial \psi}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial \psi}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial \psi}{\partial \phi}\frac{\partial \phi}{\partial x}]\frac{\partial \theta}{\partial x} \\ &+ \quad \frac{\partial}{\partial \phi}[\frac{\partial \psi}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial \psi}{\partial \theta}\frac{\partial \theta}{\partial x} + \frac{\partial \psi}{\partial \phi}\frac{\partial \phi}{\partial x}]\frac{\partial \phi}{\partial x}\end{aligned} \tag{152}$$

For this we will need to write

$$\frac{\partial r}{\partial x}, \quad \frac{\partial \theta}{\partial x}, \quad \frac{\partial \phi}{\partial x} \tag{153}$$

in terms of r, θ, ϕ.

We can simplify this by computing

$$M = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial y}{\partial r} & \frac{\partial z}{\partial r} \\ \frac{\partial x}{\partial \theta} & \frac{\partial y}{\partial \theta} & \frac{\partial z}{\partial \theta} \\ \frac{\partial x}{\partial \phi} & \frac{\partial y}{\partial \phi} & \frac{\partial z}{\partial \phi} \end{pmatrix} \tag{154}$$

Then

$$M^{-1} = \begin{pmatrix} \frac{\partial r}{\partial x} & \frac{\partial r}{\partial y} & \frac{\partial r}{\partial z} \\ \frac{\partial \theta}{\partial x} & \frac{\partial \theta}{\partial y} & \frac{\partial \theta}{\partial z} \\ \frac{\partial \phi}{\partial x} & \frac{\partial \phi}{\partial y} & \frac{\partial \phi}{\partial z} \end{pmatrix} \tag{155}$$

and now the derivatives will automatically be in terms of r, θ, ϕ.

With all this we find (using the Mathematica file)

$$(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2})\psi = (\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}[\frac{\partial^2}{\partial \theta^2} + \cot\theta\frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2}])\psi \tag{156}$$

6 Solving the Hydrogen atom

We have

$$V = -\frac{1}{4\pi\epsilon_0}\frac{e^2}{r} = -\frac{k}{r} \tag{157}$$

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where
$$k = \frac{e^2}{4\pi\epsilon_0} \tag{158}$$

Then
$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right)\psi - \frac{k}{r}\psi \tag{159}$$

There is no explicit t dependence anywhere. Just as in an algebraic equation
$$\frac{d^2y}{\partial t^2} = \alpha y \tag{160}$$

we can write $y = e^{at}$, getting $a^2 = \alpha$, we can try an exponential ansatz. Thus we write
$$\psi = \chi(r,\theta,\phi)e^{-i\frac{E}{\hbar}t} \tag{161}$$

getting
$$E\chi(r,\theta,\phi)e^{-i\frac{E}{\hbar}t} = \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right) - \frac{k}{r}\right]\chi(r,\theta,\phi)e^{-i\frac{E}{\hbar}t} \tag{162}$$

Now the t dependence drops out
$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right)\chi(r,\theta,\phi) - \frac{k}{r}\chi(r,\theta,\phi) = E\chi(r,\theta,\phi) \tag{163}$$

If we solve this, we will get an energy eigenstate with energy E. But not all E values may be allowed; thus we have to find the spectrum.

No we notice that the terms with derivatives in r separate out from terms with derivatives in θ, ϕ. Thus we try
$$\chi(r,\theta,\phi) = A(r)B(\theta,\phi) \tag{164}$$

$$-\frac{\hbar^2}{2m}\left(B(\theta,\phi)\frac{\partial^2 A(r)}{\partial r^2} + B(\theta,\phi)\frac{2}{r}\frac{\partial A(r)}{\partial r} + A(r)\frac{1}{r^2}\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]B(\theta,\phi)\right) \tag{165}$$

$$-\frac{k}{r}A(r)B(\theta,\phi) = EA(r)B(\theta,\phi) \tag{166}$$

We divide both sides by $A(r)B(\theta,\phi)$ and multiply by r^2
$$-\frac{\hbar^2}{2m}\frac{r^2}{A(r)}\left[\frac{\partial^2 A(r)}{\partial r^2} + \frac{2}{r}\frac{\partial A(r)}{\partial r} + \frac{2m}{\hbar^2}\frac{k}{r}A(r)\right] \tag{167}$$

$$= \frac{1}{B(\theta,\phi)}\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]B(\theta,\phi)) + Er^2 \tag{168}$$

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7 The angular Laplacian

We had

$$L^2 = L_x^2 + L_y^2 + L_z^2 \tag{169}$$

This is

$$L^2 = L_+L_- - \hbar L_z + L_z^2 \tag{170}$$

$$\hat{L}_+ = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right) \tag{171}$$

$$\hat{L}_- = \hbar e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right) \tag{172}$$

Thus

$$L_+L_- = \hbar^2[e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)][e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)] \tag{173}$$

$$= \hbar^2[-\frac{\partial^2}{\partial\theta^2} + i\cot\theta\frac{\partial^2}{\partial\theta\partial\phi} - i\csc^2\theta\frac{\partial}{\partial\phi} - i\cot\theta\frac{\partial^2}{\partial\phi\partial\theta} - \cot\theta\frac{\partial}{\partial\theta} - \cot^2\theta\frac{\partial^2}{\partial\phi^2} + i\cot^2\theta\frac{\partial}{\partial\phi}] \tag{174}$$

$$= -\hbar^2[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + i\frac{\partial}{\partial\phi}] \tag{175}$$

$$-\hbar L_z + L_z^2 = \hbar^2 i\frac{\partial}{\partial\phi} - \hbar^2\frac{\partial^2}{\partial\phi^2} \tag{176}$$

Therefore

$$L^2 = L_+L_- - \hbar L_z + L_z^2 = -\hbar^2[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + i\frac{\partial}{\partial\phi} + -i\frac{\partial}{\partial\phi} + \frac{\partial^2}{\partial\phi^2}] \tag{177}$$

$$= -\hbar^2[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}] \tag{178}$$

Thus this operator should take the eigenvalues

$$\hbar^2 l(l+1) \tag{179}$$

8 The radial equation

We had

$$-\frac{\hbar^2}{2m}\frac{r^2}{A(r)}[\frac{\partial^2 A(r)}{\partial r^2} + \frac{2}{r}\frac{\partial A(r)}{\partial r} + \frac{2m}{\hbar^2}\frac{k}{r}A(r)] \tag{180}$$

$$= \frac{1}{B(\theta,\phi)}\frac{\hbar^2}{2m}[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]B(\theta,\phi)) + Er^2 \tag{181}$$

We write

$$\frac{1}{B(\theta,\phi)}\frac{\hbar^2}{2m}[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]B(\theta,\phi)) = -C \tag{182}$$

$$-\hbar^2[\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}]B(\theta,\phi)) = 2mCB(\theta,\phi) \tag{183}$$

Thus

$$2mC = \hbar^2 l(l+1), \quad C = \frac{\hbar^2 l(l+1)}{2m} \tag{184}$$

Thus we get

$$-\frac{\hbar^2}{2m}\frac{r^2}{A(r)}[\frac{\partial^2 A(r)}{\partial r^2} + \frac{2}{r}\frac{\partial A(r)}{\partial r} + \frac{2m}{\hbar^2}\frac{k}{r}A(r)] = Er^2 - C = Er^2 - \frac{\hbar^2 l(l+1)}{2m} \tag{185}$$

This is

$$[\frac{\partial^2 A(r)}{\partial r^2} + \frac{2}{r}\frac{\partial A(r)}{\partial r} + \frac{2m}{\hbar^2}\frac{k}{r}A(r)] + [\frac{2mE}{\hbar^2} - \frac{l(l+1)}{r^2}]A(r) = 0 \tag{186}$$

This is

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{2m}{\hbar^2}\left(\frac{k}{r} + E - \frac{\hbar^2 l(l+1)}{2mr^2}\right)\right]A(r) = 0 \tag{187}$$

9 Long distance limit

We have

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{2m}{\hbar^2}\left(\frac{k}{r} + E - \frac{\hbar^2 l(l+1)}{2mr^2}\right)\right]A(r) = 0 \tag{188}$$

In the limit $r \to \infty$ we get

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2mE}{\hbar^2}\right]A(r) = 0 \tag{189}$$

Since we have $E < 0$ for a bound state, we write this as

$$\frac{\partial^2 A(r)}{\partial r^2} = \left(-\frac{2mE}{\hbar^2}\right)A(r) \tag{190}$$

which gives

$$A(r) = Ce^{-\sqrt{-\frac{2mE}{\hbar^2}}r} \tag{191}$$

10 Short distance limit

For $r \sim 0$ we have

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2} \right] A(r) = 0 \tag{192}$$

We try $A \sim r^a$. This gives

$$a(a-1) + 2a - l(l+1) = 0 \tag{193}$$

$$a^2 + a - l(l+1) = 0 \tag{194}$$

$$a = \frac{1}{2}[-1 \pm \sqrt{1 + 4l^2 + 4l}] = \frac{1}{2}[-1 \pm (2l+1)] = l, -l-1 \tag{195}$$

Thus we get

$$A(r) \sim r^l \tag{196}$$

11 Simplifying the equation

We have

$$\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{2m}{\hbar^2}\left(\frac{k}{r} + E - \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] A(r) = 0 \tag{197}$$

The constant term is, noting that $E < 0$

$$-\left(\frac{2m(-E)}{\hbar^2} \right) \equiv -C \tag{198}$$

We write

$$r = \alpha \rho \tag{199}$$

$$\left[\frac{1}{\alpha^2}\frac{\partial^2}{\partial \rho^2} + \frac{1}{\alpha^2}\frac{2}{\rho}\frac{\partial}{\partial \rho} + \frac{2m}{\hbar^2}\left(\frac{1}{\alpha}\frac{k}{\rho} - \frac{1}{\alpha^2}\frac{\hbar^2 l(l+1)}{2m\rho^2} \right) - C \right] A(\rho) = 0 \tag{200}$$

We multiply through by α^2

$$\left[\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} + \frac{2m}{\hbar^2}\left(\frac{\alpha k}{\rho} - \frac{\hbar^2 l(l+1)}{2m\rho^2} \right) - \alpha^2 C \right] A(\rho) = 0 \tag{201}$$

We set

$$\alpha^2 C = \frac{1}{4}, \quad \alpha = \sqrt{\frac{1}{4C}} = \sqrt{\frac{\hbar^2}{8m(-E)}} \tag{202}$$

The equation is

$$\left[\frac{\partial^2}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} + \left(\frac{\sqrt{\frac{\hbar^2}{8m(-E)}}2mk}{\hbar^2 \rho} - \frac{l(l+1)}{\rho^2} \right) - \frac{1}{4} \right] A(\rho) = 0 \tag{203}$$

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$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{2}{\rho}\frac{\partial}{\partial\rho} + \left(\sqrt{\frac{2m}{(-E)}}\frac{k}{2\hbar}\frac{1}{\rho} - \frac{l(l+1)}{\rho^2}\right) - \frac{1}{4}\right]A(\rho) = 0 \tag{204}$$

Writing

$$\lambda = \sqrt{\frac{2m}{(-E)}}\frac{k}{2\hbar} \tag{205}$$

this is

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{2}{\rho}\frac{\partial}{\partial\rho} + \left(\frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2}\right) - \frac{1}{4}\right]A(\rho) = 0 \tag{206}$$

In this notation, the behavior at infinity is

$$A \sim e^{-\sqrt{-\frac{2mE}{\hbar^2}}r} \sim e^{-\sqrt{-\frac{2mE}{\hbar^2}}\sqrt{\frac{\hbar^2}{8m(-E)}}\rho} \sim e^{-\frac{1}{2}\rho} \tag{207}$$

The behavior near the origin is

$$A \sim \rho^l \tag{208}$$

12 Separating out the behavior at infinity

We write

$$A = e^{-\frac{1}{2}\rho}G \tag{209}$$

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{2}{\rho}\frac{\partial}{\partial\rho} + \left(\frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2}\right) - \frac{1}{4}\right]e^{-\frac{1}{2}\rho}G(\rho) = 0 \tag{210}$$

$$\frac{1}{4}e^{-\frac{1}{2}\rho}G(\rho) - e^{-\frac{1}{2}\rho}G'(\rho) + e^{-\frac{1}{2}\rho}G''(\rho) + \frac{2}{\rho}(-\frac{1}{2}e^{-\frac{1}{2}\rho}G(\rho) + e^{-\frac{1}{2}\rho}G'(\rho)) + \left[\left(\frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2}\right) - \frac{1}{4}\right]e^{-\frac{1}{2}\rho}G(\rho) = 0 \tag{211}$$

$$-G'(\rho) + G''(\rho) + \frac{2}{\rho}(-\frac{1}{2}G(\rho) + G'(\rho)) + \left[\left(\frac{\lambda}{\rho} - \frac{l(l+1)}{\rho^2}\right)\right]G(\rho) = 0 \tag{212}$$

$$G''(\rho) + [\frac{2}{\rho} - 1]G'(\rho) + \left[\left(\frac{(\lambda-1)}{\rho} - \frac{l(l+1)}{\rho^2}\right)\right]G(\rho) = 0 \tag{213}$$

13 Separating out the behavior at the origin

We write

$$G = \rho^l H \tag{214}$$

$$G''(\rho) + [\frac{2}{\rho} - 1]G'(\rho) + \left[\left(\frac{(\lambda-1)}{\rho} - \frac{l(l+1)}{\rho^2}\right)\right]G(\rho) = 0 \tag{215}$$

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$$\rho^l H'' + l(l-1)\rho^{l-2}H + 2l\rho^{l-1}H' + [\frac{2}{\rho} - 1](l\rho^{l-1}H + \rho^l H') + \left[\left(\frac{(\lambda-1)}{\rho} - \frac{l(l+1)}{\rho^2}\right)\right]\rho^l H = 0 \tag{216}$$

$$\rho^l H'' + 2l\rho^{l-1}H' + \frac{2}{\rho}\rho^l H' - (l\rho^{l-1}H + \rho^l H') + \left[\left(\frac{(\lambda-1)}{\rho}\right)\right]\rho^l H = 0 \tag{217}$$

$$H'' + 2l\frac{1}{\rho}H' + \frac{2}{\rho}H' - (l\frac{1}{\rho}H + H') + \left[\left(\frac{(\lambda-1)}{\rho}\right)\right]H = 0 \tag{218}$$

$$H'' + (\frac{2l+2}{\rho} - 1)H' + [\frac{(\lambda-1-l)}{\rho}]H = 0 \tag{219}$$

14   Getting the lowest levels for each l

We can set $H = const.$ if

$$\lambda = l + 1 \tag{220}$$

Thus

$$\sqrt{\frac{2m}{(-E)}}\frac{k}{2\hbar} = l + 1 \tag{221}$$

$$\frac{2m}{(-E)}(\frac{k}{2\hbar})^2 = (l+1)^2 \tag{222}$$

$$E = -\frac{mk^2}{2\hbar^2(l+1)^2} = -\frac{mZ^2 e^4}{2(4\pi\epsilon_0)^2\hbar^2(l+1)^2} \tag{223}$$

The wavefunctions are

$$\psi_l \sim r^l e^{-\sqrt{-\frac{2mE}{\hbar^2}}r} \tag{224}$$

15   Series solution for H

We write

$$H = \sum_{k\geq 0} a_k \rho^k \tag{225}$$

$$H'' + (\frac{2l+2}{\rho} - 1)H' + [\frac{(\lambda-1-l)}{\rho}]H = 0 \tag{226}$$

$$k(k-1)a_k\rho^{k-2} + (\frac{2l+2}{\rho} - 1)ka_k\rho^{k-1} + [\frac{(\lambda-1-l)}{\rho}]a_k\rho^k = 0 \tag{227}$$

We look at the coefficient of ρ^{k-1}

$$(k+1)ka_{k+1} + (2l+2)(k+1)a_{k+1} - ka_k + [(\lambda-1-l)]a_k = 0 \tag{228}$$

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$$(k+1)(k+2l+2)a_{k+1} = (k-\lambda+1+l)a_k \tag{229}$$

$$a_{k+1} = \frac{(k-\lambda+1+l)}{(k+1)(k+2l+2)}a_k \tag{230}$$

Thus we get

$$\lambda = l+1+k, \quad k = 0,1,2,\dots \tag{231}$$

We define

$$n = l+1+k \tag{232}$$

Then

$$\sqrt{\frac{2m}{(-E)}}\frac{k}{2\hbar} = n \tag{233}$$

$$\frac{2m}{(-E)}\frac{k^2}{4\hbar^2} = n^2 \tag{234}$$

$$E = -\frac{mk^2}{2\hbar^2 n^2} = -\frac{mZ^2 e^4}{2(4\pi\epsilon_0)^2\hbar^2}\frac{1}{n^2} \tag{235}$$

16 Perturbation theory

We begin by recalling the perturbation theory for a general Hamiltonian. The details of the perturbation expansion depends on the level of degeneracy that exists in the problem. Consider a Hamiltonian

$$H = H^{(0)} + \lambda H^{(1)} \tag{236}$$

The eigenvalue condition is

$$H\psi = E\psi \tag{237}$$

This condition will be solved by a state of the form

$$\psi = \psi^{(0)} + \lambda\psi^{(1)} + \lambda^2\psi^{(2)} + \dots \tag{238}$$

and the eigenvalue will be given by an expression of the form

$$E = E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \dots \tag{239}$$

Now consider different levels of degeneracy:

(i) The unperturbed Hamiltonian $H^{(0)}$ is nondegenerate for the energy level $E^{(0)}$ that we are seeking to perturb.

(ii) The unperturbed Hamiltonian $H^{(0)}$ is degenerate for the energy level $E^{(0)}$, but the perturbing Hamiltonian $H^{(1)}$ lifts this degeneracy at first order in the perturbation.

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(iii) The unperturbed Hamiltonian $H^{(0)}$ is degenerate for the energy level $E^{(0)}$, and the perturbing Hamiltonian $H^{(1)}$ fails to lift the degeneracy to first order in the perturbation. The degeneracy is however lifted to second order.

We can continue in this fashion to more complicated situations. The standard text-book treatment of perturbation theory terms (i) as the nondegenerate case and (ii) as the degenerate case. In our problem however we will find that we are in case (iii). While perturbation theory for all kinds of degeneracy is of course fully understood, we will review in this section the theory for case (iii). This will help set notation, as well as remind us of the expressions for lifting when we are not in either of cases (i) or (ii).

16.1 Zeroth order

The eigenstates of $H^{(0)}$ yield a complete orthonormal basis $|\psi_k^{(0)}\rangle$

$$\langle \psi_{k_i} | \psi_{k_j} \rangle = \delta_{ij} \tag{240}$$

We will let the starting eigenvector for our perturbation theory have the index k_0. At the zeroth order in λ we have

$$H^{(0)} |\psi_{k_0}^{(0)}\rangle = E_{k_0}^{(0)} |\psi_{k_0}^{(0)}\rangle \tag{241}$$

16.2 First order

At the first order we get

$$(H^{(0)} - E^{(0)}) |\psi^{(1)}\rangle = -H^{(1)} |\psi_{k_0}^{(0)}\rangle + E^{(1)} |\psi_{k_0}^{(0)}\rangle \tag{242}$$

We write

$$|\psi^{(1)}\rangle = \sum_{k \neq k_0} C_k |\psi_k^{(0)}\rangle \tag{243}$$

where we have choosen to not include the $k = k_0$ term since that is already present in the zeroth order wavefunction.

Substituting this in (242) gives

$$\sum_{k \neq k_0} C_k (E_k^{(0)} - E_{k_0}^{(0)}) \psi_k^{(0)} = -H^{(1)} \psi_{k_0}^{(0)} + E^{(1)} |\psi_{k_0}^{(0)}\rangle \tag{244}$$

Taking the inner product of both sides with $\langle \psi_{k_0}^{(0)} |$ we find

$$E^{(1)} = \langle \psi_{k_0}^{(0)} | H^{(1)} | \psi_{k_0}^{(0)} \rangle \tag{245}$$

Now we ask for the expansion coefficients C_k. To get these, we return to (244) and take the inner product of both sides with $\langle \psi_{k'}^{(0)}|$ with $k' \neq k_0$. This gives

$$\sum_{k \neq k_0} C_k (E_k^{(0)} - E_{k_0}^{(0)}) \delta_{k,k'} = -\langle \psi_{k'}^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle \tag{246}$$

Now we have two cases:

16.2.1   Nondegenerate level $E_{k_0}^{(0)}$

Suppose that the energy level $E_{k_0}^{(0)}$ is nondegenerate for the Hamiltonian $H^{(0)}$. Then (246) gives

$$C_k = \frac{\langle \psi_k^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle}{(E_{k_0}^{(0)} - E_k^{(0)})}, \qquad k \neq k_0 \tag{247}$$

16.2.2   Degenerate level $E_{k_0}^{(0)}$

Suppose that the eigenvalue $E_{k_0}^{(0)}$ is degenerate; then $|\psi_{k_0}^{(0)}\rangle$ is one vector in a subspace corresponding to this eigenvalue. We decompose this subspace into the vector $|\psi_{k_0}^{(0)}\rangle$ and the vectors $|\psi_{\bar{k}_i}^{(0)}\rangle$ orthogonal to $|\psi_{k_0}^{(0)}\rangle$. Then (246) gives a contradiction for the values $k' = \bar{k}_i$, unless

$$\langle \psi_{\bar{k}_i}^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle = 0 \tag{248}$$

To resolve this difficulty we note that since the energy level $E_{k_0}^{(0)}$ is degenerate, there is no unique choice of the starting eigenvector $|\psi_{k_0}^{(0)}\rangle$. Thus we first diagonalize $H^{(1)}$ in the subspace formed by these degenerate states with eigenvalue $E_{k_0}^{(0)}$, and let the starting state $|\psi_{k_0}^{(0)}\rangle$ be one of these eigenstates. Then (248) is true. For $k \neq k_0, \bar{k}_i$ we get

$$C_k = \frac{\langle \psi_k^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle}{(E_{k_0}^{(0)} - E_k^{(0)})}, \qquad k \neq k_0, \bar{k}_i \tag{249}$$

while for the coefficients $C_{\bar{k}_i}$ are undetermined at this stage.

16.3   Second order

At second order in λ we have

$$(H^{(0)} - E_{k_0}^{(0)})|\psi^{(2)}\rangle = -H^{(1)}|\psi^{(1)}\rangle + E^{(1)}|\psi^{(1)}\rangle + E^{(2)}|\psi_{k_0}^{(0)}\rangle \tag{250}$$

We can expand as before

$$|\psi^{(2)}\rangle = \sum_{k \neq k_0} D_k |\psi_k^{(0)}\rangle \tag{251}$$

getting

$$\sum_{k' \neq k_0} D_{k'}(E_{k'}^{(0)} - E_{k_0}^{(0)})|\psi_{k'}^{(0)}\rangle = -H^{(1)}|\psi^{(1)}\rangle + E^{(1)}|\psi^{(1)}\rangle + E^{(2)}|\psi_{k_0}^{(0)}\rangle \tag{252}$$

We take the inner product of each side with $|\psi_{k_0}^{(0)}\rangle$, getting

$$E^{(2)} = \langle \psi_{k_0}^{(0)}|H^{(1)}|\psi^{(1)}\rangle = \sum_{k \neq k_0} C_k \langle \psi_{k_0}^{(0)}|H^{(1)}|\psi_k^{(0)}\rangle \tag{253}$$

To find the D_k we take the inner product of both sides of (252) with $\langle \psi_k^{(0)}|$ with $k \neq k_0$. Note that $\langle \psi_k^{(0)}|\psi^{(1)}\rangle = 0$ due to the expansion (243). We find

$$D_k(E_k^{(0)} - E_{k_0}^{(0)}) = -\sum_{k'' \neq k_0} C_{k''}\langle \psi_k^{(0)}|H^{(1)}|\psi_{k''}^{(0)}\rangle + E^{(1)}C_k \tag{254}$$

Now we consider different cases.

16.3.1 Nondegenerate level $E_{k_0}^{(0)}$

Suppose that the energy level $E_{k_0}^{(0)}$ is nondegenerate for the Hamiltonian $H^{(0)}$. Then using (247) we can write

$$E^{(2)} = \sum_{k \neq k_0} \frac{|\langle \psi_k^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle|^2}{(E_{k_0}^{(0)} - E_k^{(0)})} \tag{255}$$

**This is the point till which you need to know for this course **

Now we find the D_k. Substituting the value of C_k from (247) into (254) we get

$$D_k = \sum_{k'' \neq k_0} \frac{\langle \psi_k^{(0)}|H^{(1)}|\psi_{k''}^{(0)}\rangle \langle \psi_{k''}^{(0)}|H^{(1)}\psi_{k_0}^{(0)}\rangle}{(E_{k_0}^{(0)} - E_k^{(0)})(E_{k_0}^{(0)} - E_{k''}^{(0)})} - \frac{\langle \psi_k^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle \langle \psi_{k_0}^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle}{(E_{k_0}^{(0)} - E_k^{(0)})^2}, \quad k \neq k_0 \tag{256}$$

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16.3.2 Degenerate level $E_{k_0}^{(0)}$, degeneracy lifted at first order

First consider the relation (253) for the perturbed energy. The coefficients $C_{\bar{k}_i}$ appearing on the RHS are undetermined. But these coefficients multiply the factor $\langle \psi_{k_0}^{(0)}|H^{(1)}|\psi_{\bar{k}_i}^{(0)}\rangle$ which vanishes due to the choice (248). Thus we can write

$$E^{(2)} = \sum_{k \neq \{k_0, \bar{k}_i\}} \frac{|\langle \psi_k^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle|^2}{(E_{k_0}^{(0)} - E_k^{(0)})} \tag{257}$$

Now let us come to the determination of the wavefunction. Let us set $k = \bar{k}_i$. Then the LHS of (254) vanishes, and we get

$$-\sum_{k'' \neq \{k_0, \bar{k}_i\}} C_{k''}\langle \psi_{\bar{k}_i}^{(0)}|H^{(1)}|\psi_{k''}^{(0)}\rangle - \sum_{\bar{k}_j} C_{\bar{k}_j}\langle \psi_{\bar{k}_i}^{(0)}|H^{(1)}|\psi_{\bar{k}_j}^{(0)}\rangle + E^{(1)}C_{\bar{k}_i} = 0 \tag{258}$$

where we have separated the contribution of the $\bar{k}_i$ from the other states. Note that $H^{(1)}$ has already been diagonalized on the space $k = \bar{k}_i$, and its eigenvalues are real. Thus we have

$$\langle \psi_{\bar{k}_j}^{(0)}|H^{(1)}|\psi_{\bar{k}_i}^{(0)}\rangle = E^{(1,i)}\delta_{ij} \tag{259}$$

Thus

$$\sum_{\bar{k}_j} C_{\bar{k}_j}\langle \psi_{\bar{k}_i}^{(0)}|H^{(1)}|\psi_{\bar{k}_j}^{(0)}\rangle = E^{(1,i)}C_{\bar{k}_i}\delta_{ij} \tag{260}$$

The relation (258) then gives

$$(E^{(1)} - E^{(1,i)})C_{\bar{k}_i} = \sum_{k'' \neq \{k_0, \bar{k}_i\}} C_{k''}\langle \psi_{\bar{k}_i}^{(0)}|H^{(1)}|\psi_{k''}^{(0)}\rangle \tag{261}$$

Suppose that the degeneracy of the level $E_{k_0}^{(0)}$ at leading order is lifted completely at first order; i.e.,

$$E^{(1)} - E^{(1,i)} \neq 0 \tag{262}$$

for all i. Then (261) gives

$$C_{\bar{k}_i} = \frac{1}{(E^{(1)} - E^{(1,i)})} \sum_{k'' \neq \{k_0, \bar{k}_i\}} \frac{\langle \psi_{\bar{k}_i}^{(0)}|H^{(1)}|\psi_{k''}^{(0)}\rangle\langle \psi_{k''}^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle}{(E_{k_0}^{(0)} - E_{k''}^{(0)})} \tag{263}$$

Now consider the D_k given through (254). Using the $C_k, k \neq k_0, \bar{k}_i$ from (607), the $C_{\bar{k}_i}$ from (263) and the E^1 from (245) we get

$$D_k = \frac{1}{(E_{k_0}^{(0)} - E_k^{(0)})} \times \Bigg[$$

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$$\sum_{\bar{k}_i} \frac{1}{(E^{(1)} - E^{(1,i)})} \sum_{k'' \neq \{k_0, \bar{k}_i\}} \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_{\bar{k}_i}^{(0)} \rangle \langle \psi_{\bar{k}_i}^{(0)} | H^{(1)} | \psi_{k''}^{(0)} \rangle \langle \psi_{k''}^{(0)} | H^{(1)} | \psi_{k_0}^{(0)} \rangle}{(E_{k_0}^{(0)} - E_{k''}^{(0)})}$$

$$+ \sum_{k'' \neq k_0, \bar{k}_i} \frac{\langle \psi_k^{(0)} | H^{(1)} \psi_{k''}^{(0)} \rangle \langle \psi_{k''}^{(0)} | H^{(1)} | \psi_{k_0}^{(0)} \rangle}{(E_{k_0}^{(0)} - E_{k''}^{(0)})} - \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_{k_0}^{(0)} \rangle \langle \psi_{k_0}^{(0)} | H^{(1)} | \psi_{k_0}^{(0)} \rangle}{(E_{k_0}^{(0)} - E_k^{(0)})} \Bigg]$$

$$(264)$$

16.3.3 Degenerate level $E_{k_0}^{(0)}$, degeneracy not lifted at first order

Now we assume that the energy level $E_{k_0}^{(0)}$ is degenerate for the Hamiltonian $H^{(0)}$, and further, that $H^{(1)}$ does not lift this degeneracy at first order. Let the indices $\bar{k}_a, \bar{k}_b, \ldots$ run over the entire degenerate subspace of $H^{(0)}$ with energy $E_{k_0}^{(0)}$; i.e., these indices run over k_0 as well as the $\bar{k}_i$. Thus in place of (259) we have

$$\langle \psi_{\bar{k}_b}^{(0)} | H^{(1)} | \psi_{\bar{k}_a}^{(0)} \rangle = E^{(1)} \delta_{ab} \tag{265}$$

The difficulty this leads to can be seen as follows. Consider the relation (258). From (265) we have $\langle \psi_{\bar{k}_i}^{(0)} | H^{(1)} | \psi_{\bar{k}_j}^{(0)} \rangle = E^{(1)} \delta_{ij}$, and we find that the last two terms cancel. Substituting the value of the C_k from (607), we get

$$\sum_{k'' \neq \{k_0, \bar{k}_i\}} \frac{\langle \psi_{\bar{k}_i}^{(0)} | H^{(1)} | \psi_{k''}^{(0)} \rangle \langle \psi_{k''}^{(0)} | H^{(1)} | \psi_{k_0}^{(0)} \rangle}{(E_{k_0}^{(0)} - E_{k''}^{(0)})} = 0 \tag{266}$$

But there is no reason for this relation to be true in general. Thus we have a contradiction, and need to find a different way to proceed.

The essential point is that if $H^{(1)}$ fails to lift the degeneracy of the level $E_{k_0}^{(0)}$ at first order, then we have no way of selecting the starting vector $|\psi_{k_0}\rangle$ from the degenerate subspace at the present stage. Thus we must postpone the selection of the eventual eigenvector to the time when we have solved the perturbation to second order. Let us carry out this step.

We define

$$\sum_{k'' \neq \{k_c\}} \frac{\langle \psi_{\bar{k}_b}^{(0)} | H^{(1)} | \psi_{k''}^{(0)} \rangle \langle \psi_{k''}^{(0)} | H^{(1)} | \psi_{\bar{k}_a}^{(0)} \rangle}{(E_{k_0}^{(0)} - E_{k''}^{(0)})} \equiv M_{ba} \tag{267}$$

So far we have no particular reason to choose any preferred orthonormal basis in the space of the $\bar{k}_a$, but now we choose one that diagonalizes M_{ba}. Thus we have

$$M_{ba} = E^{(2),a} \delta_{ba} \tag{268}$$

and the $|\psi_{\bar{k}_a}^{(0)}\rangle$ are the eigenvectors of M_{ba}. Let us focus on one of the $\bar{k}_a$, and this will be our starting vector $\bar{k}_0$ in what follows. The $\bar{k}_a$ orthogonal to $\bar{k}_0$ will be termed $\bar{k}_i$ as before.

Let us return to the relation (253). We have

$$\sum_{k\neq k_0} C_k\langle\psi_{k_0}^{(0)}|H^{(1)}|\psi_k^{(0)}\rangle = \sum_{k\neq\{k_0,\bar{k}_i\}} C_k\langle\psi_{k_0}^{(0)}|H^{(1)}|\psi_k^{(0)}\rangle + \sum_{k=\bar{k}_i} C_k\langle\psi_{k_0}^{(0)}|H^{(1)}|\psi_k^{(0)}\rangle \quad (269)$$

The last term on the RHS vanishes because of (265), and we get

$$E^{(2)} = \sum_{k\neq\{k_0,\bar{k}_i\}} C_k\langle\psi_{k_0}^{(0)}|H^{(1)}|\psi_k^{(0)}\rangle = \sum_{k\neq\{k_0,\bar{k}_i\}} \frac{|\langle\psi_k^{(0)}|H^{(1)}|\psi_{k_0}^{(0)}\rangle|^2}{(E_{k_0}^{(0)} - E_k^{(0)})} \quad (270)$$

just as in (257). But note that we had to first compute and diagonalize the matrix M_{ba} to find the vectors $|\psi_{k_0}^{(0)}\rangle, |\psi_{\bar{k}_i}^{(0)}\rangle$ before the above relation could be written down for the case where $H^{(1)}$ fails to lift the degeneracy at first order.

Let us now consider the wavefunction. In place of (243) we write the more general relation

$$|\psi^{(1),a}\rangle = \sum_{k\neq k_a} C_k^a|\psi_k^{(0)}\rangle \quad (271)$$

Following the steps leading to (247) we get

$$C_k^a = \frac{\langle\psi_k^{(0)}|H^{(1)}|\psi_{\bar{k}_a}^{(0)}\rangle}{(E_{\bar{k}_a}^{(0)} - E_k^{(0)})}, \qquad k \neq \bar{k}_c \quad (272)$$

while the $C_{\bar{k}_b}^a$ remain undetermined at this stage. These undetermined coefficients will be determined at the next order in perturbation theory if the degeneracy is lifted at that level, and at a later order still if the degeneracy persists at the next level. The undetermined $C_{\bar{k}_b}^a$ lead to indeterminate coefficients D_k^a at second order so the D_k^a will have to be determined at a later stage as well.

17   The Stark effect

17.1   Dipole moments

Suppose we have charges $q, -q$ separated by a distance d. Then the dipole moment is

$$|\vec{p}| = qd \quad (273)$$

with direction that points from the negative to the positive charge The electric field is

$$\vec{\mathcal{E}} = -\vec{\nabla}\Phi \quad (274)$$

where Φ is the electric potential. For $\vec{\mathcal{E}} = \mathcal{E}\hat{z}$, we have $\Phi = -Ez$. For the dipole centered at $z = 0$, aligned along $\hat{z}$, we have charge q at $(0, 0, \frac{d}{2})$ and charge $-q$ at $(0, 0, -\frac{d}{2})$. The energy is

$$E = q\Phi(\frac{d}{2}) - q\Phi(-\frac{d}{2}) = -qd\mathcal{E} \tag{275}$$

More generally,

$$E = -\vec{p} \cdot \vec{\mathcal{E}} \tag{276}$$

Energy eigenstates of the Hydrogen atom do not have dipole moments if we take definite n, l, m. But we can make states with nonzero dipole moments if we take linear combinations of degenerate states with the same n but different l, m. For example, note that

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \tag{277}$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta \tag{278}$$

While $Y_{0,0}$ is invariant under $z \to -z$, we find that $Y_{1,0}$ changes sign. Thus in a sum like $Y_{0,0} + Y_{1,0}$ the amplitudes will add for $z > 0$ and partially cancel for $z < 0$. Of course in our actual problem these spherical harmonics will be multiplied by functions of r, but we see that in general the probability for the electron to be at $z > 0$ need not be the same as the probability for the electron to be at $z < 0$. This gives the atom a dipolee moment in such states.

17.2 The matrix of $\hat{H}^{(1)}$

We have

$$\hat{H}^{(1)} = q\Phi = e\mathcal{E}z = e\mathcal{E}r\cos\theta \tag{279}$$

We find

$$[\hat{L}_z, \hat{H}^{(1)}] = 0 \tag{280}$$

Thus $\hat{H}^{(1)}$ can only connect states with the same m. Since the ground state has $m = 0$, we look at the matrix

$$\begin{pmatrix} \langle 2, 0, 0|\hat{H}^{(1)}|2, 0, 0\rangle & \langle 2, 0, 0|\hat{H}^{(1)}|2, 1, 0\rangle \\ \langle 2, 1, 0|\hat{H}^{(1)}|2, 0, 0\rangle & \langle 2, 1, 0|\hat{H}^{(1)}|2, 1, 0\rangle \end{pmatrix} \tag{281}$$

17.3 The wavefunctions

We have a form

$$\psi = C\rho^l e^{-\frac{1}{2}\rho} A(\rho) \tag{282}$$

Recall that

$$a_{k+1} = \frac{(k - \lambda + 1 + l)}{(k + 1)(k + 2l + 2)} a_k \tag{283}$$

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$$\lambda = l + 1 + k = n \tag{284}$$

To compute $A(\rho)$, we note that with $n = 2, l = 1$

$$a_0 = 1, \quad a_1 = \frac{0 - 2 + 1 + 1}{1 \times 4} = 0 \tag{285}$$

giving $A(\rho) = 1$.

With $n = 2, l = 0$

$$a_0 = 1, \quad a_1 = \frac{0 - 2 + 1 + 0}{1 \times 2} = 0 \tag{286}$$

giving $A(\rho) = 1 - \frac{1}{2}\rho$.

We have

$$r = \alpha\rho, \quad \alpha = \sqrt{\frac{\hbar^2}{8m(-E)}} \tag{287}$$

$$E = -\frac{mZ^2e^4}{2(4\pi\epsilon_0)^2\hbar^2}\frac{1}{n^2} \tag{288}$$

Thus

$$\alpha = \sqrt{\frac{\hbar^2 2(4\pi\epsilon_0)^2\hbar^2 n^2}{8mmZ^2e^4}} = \frac{\hbar^2(4\pi\epsilon_0)n}{2mZe^2} \tag{289}$$

$$\alpha^{-1} = \frac{2mZe^2}{\hbar^2(4\pi\epsilon_0)n} \tag{290}$$

Thus we have

$$\rho = \alpha^{-1}r = \frac{2mZe^2}{\hbar^2(4\pi\epsilon_0)n}r \tag{291}$$

We define

$$a_0 = \frac{\hbar^2(4\pi\epsilon_0)}{me^2} \tag{292}$$

Then we have as the falloff

$$e^{-\frac{1}{2}\rho} = e^{-\frac{1}{2}\alpha^{-1}r} = e^{-\frac{Zr}{na_0}} \tag{293}$$

We also have, for $n = 2$

$$(1 - \frac{1}{2}\rho) = 1 - \frac{Zr}{2a_0} \tag{294}$$

Let us now compute the wavefunctions. We have

$$A(10) = Ce^{-\frac{Zr}{a_0}} \tag{295}$$

We have

$$\int_0^\infty dr\, r^2 e^{-br} = \frac{d^2}{db^2}\int_0^\infty dr\, e^{-br} = \frac{d^2}{db^2}\frac{1}{b} = \frac{2}{b^3} \tag{296}$$

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Thus

$$|C|^2 \int_0^\infty dr r^2 e^{-2\frac{Zr}{a_0}} = |C|^2 2(\frac{a_0}{2Z})^3 = 1, \quad C = 2(\frac{Z}{a_0})^{\frac{3}{2}} \tag{297}$$

Thus the wavefunction is

$$\psi_{100} = 2(\frac{Z}{a_0})^{\frac{3}{2}} e^{-\frac{Zr}{a_0}} \tag{298}$$

We find

$$A_{20} = C(1 - \frac{Zr}{2a_0})e^{-\frac{Zr}{2a_0}}, \quad C = 2(\frac{Z}{2a_0})^{\frac{3}{2}} \tag{299}$$

Thus the wavefunction is

$$\psi_{200} = 2(\frac{Z}{2a_0})^{\frac{3}{2}}(1 - \frac{Zr}{2a_0})e^{-\frac{Zr}{2a_0}} \tag{300}$$

We have

$$A_{21} = Cre^{-\frac{Zr}{2a_0}}, \quad C = \frac{1}{2\sqrt{6}}(\frac{Z}{a_0})^{\frac{5}{2}} \tag{301}$$

Thus the wavefunction is

$$\psi_{21m} = \frac{1}{\sqrt{3}}(\frac{Z}{2a_0})^{\frac{3}{2}}\frac{Zr}{a_0}e^{-\frac{Zr}{2a_0}}Y_{1m}(\theta, \phi) \tag{302}$$

The spherical harmonics are

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}} \tag{303}$$

$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi} \tag{304}$$

$$Y_{1,-1} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\phi} \tag{305}$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta \tag{306}$$

17.4   Elements of the $\hat{H}^{(1)}$ matrix

We have

$$\langle 2,0,0|\hat{H}^{(1)}|2,0,0\rangle = \int_0^\infty dr r^2 \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\phi$$
$$[2(\frac{Z}{2a_0})^{\frac{3}{2}}(1 - \frac{Zr}{2a_0})e^{-\frac{Zr}{2a_0}}\frac{1}{\sqrt{4\pi}}][e\mathcal{E}r\cos\theta][2(\frac{Z}{2a_0})^{\frac{3}{2}}(1 - \frac{Zr}{2a_0})e^{-\frac{Zr}{2a_0}}\frac{1}{\sqrt{4\pi}}] \tag{307}$$

We have

$$\int_0^{2\pi} d\phi = 2\pi \tag{308}$$

$$\int_0^{\pi} d\theta \sin\theta \cos\theta = 0 \tag{309}$$

Thus we get

$$\langle 2,0,0|\hat{H}^{(1)}|2,0,0\rangle = 0 \tag{310}$$

We have

$$\langle 2,0,0|\hat{H}^{(1)}|2,1,0\rangle = \int_0^{\infty} dr r^2 \int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\phi$$

$$[2(\frac{Z}{2a_0})^{\frac{3}{2}}(1-\frac{Zr}{2a_0})e^{-\frac{Zr}{2a_0}}\frac{1}{\sqrt{4\pi}}][e\mathcal{E}r\cos\theta][\frac{1}{\sqrt{3}}(\frac{Z}{2a_0})^{\frac{3}{2}}\frac{Zr}{a_0}e^{-\frac{Zr}{2a_0}}\sqrt{\frac{3}{4\pi}}\cos\theta] \tag{311}$$

We have

$$\int_0^{2\pi} d\phi = 2\pi \tag{312}$$

$$\int_0^{\pi} d\theta \sin\theta \cos^2\theta = \frac{2}{3} \tag{313}$$

$$\int_0^{\infty} dr r^2 (1-\frac{Zr}{2a_0})e^{-\frac{Zr}{2a_0}}r\frac{Zr}{a_0}e^{-\frac{Zr}{2a_0}} = -36\frac{a_0^4}{Z^4} \tag{314}$$

$$\langle 2,0,0|\hat{H}^{(1)}|2,1,0\rangle = [2(\frac{Z}{2a_0})^{\frac{3}{2}}\frac{1}{\sqrt{4\pi}}][e\mathcal{E}][\frac{1}{\sqrt{3}}(\frac{Z}{2a_0})^{\frac{3}{2}}\sqrt{\frac{3}{4\pi}}](2\pi)(\frac{2}{3})(-36\frac{a_0^4}{Z^4}) = -3\frac{a_0}{Z}e\mathcal{E} \tag{315}$$

We have

$$\langle 2,1,0|\hat{H}^{(1)}|2,1,0\rangle = \int_0^{\infty} dr r^2 \int_0^{\pi} d\theta \sin\theta \int_0^{2\pi} d\phi$$

$$[\frac{1}{\sqrt{3}}(\frac{Z}{2a_0})^{\frac{3}{2}}\frac{Zr}{a_0}e^{-\frac{Zr}{2a_0}}\sqrt{\frac{3}{4\pi}}\cos\theta][e\mathcal{E}r\cos\theta][\frac{1}{\sqrt{3}}(\frac{Z}{2a_0})^{\frac{3}{2}}\frac{Zr}{a_0}e^{-\frac{Zr}{2a_0}}\sqrt{\frac{3}{4\pi}}\cos\theta] \tag{316}$$

$$\int_0^{2\pi} d\phi = 2\pi \tag{317}$$

$$\int_0^{\pi} d\theta \sin\theta \cos^3\theta = 0 \tag{318}$$

Thus we get

$$\langle 2,1,0|\hat{H}^{(1)}|2,1,0\rangle = 0 \tag{319}$$

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17.5 The matrix

Thus we have

$$\begin{pmatrix} \langle 2,0,0|\hat{H}^{(1)}|2,0,0\rangle & \langle 2,0,0|\hat{H}^{(1)}|2,1,0\rangle \\ \langle 2,1,0|\hat{H}^{(1)}|2,0,0\rangle & \langle 2,1,0|\hat{H}^{(1)}|2,1,0\rangle \end{pmatrix} = -\frac{3a_0 e\mathcal{E}}{Z}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{320}$$

The eigenvalues and eigenvectors of

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{321}$$

are

$$\lambda = 1 \;:\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \qquad \lambda = -1 \;:\; \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{322}$$

Thus the energies are

$$E = E_2^{(0)} - \frac{3a_0 e\mathcal{E}}{Z}, \quad |\psi\rangle = \frac{1}{\sqrt{2}}(|2,0,0\rangle + |2,1,0\rangle) \tag{323}$$

$$E = E_2^{(0)} + \frac{3a_0 e\mathcal{E}}{Z}, \quad |\psi\rangle = \frac{1}{\sqrt{2}}(|2,0,0\rangle - |2,1,0\rangle) \tag{324}$$

18 Two particles

Consider two particles that can move on a circle parametrized by the coordinate θ. Let the coordinate of the first particle be θ_1 and of the second particle be θ_2. The general wavefunction will then have the form $\Psi(\theta_1, \theta_2)$.

We can however start with simpler wavefunctions of the form

$$\Psi = \psi_1(\theta_1)\psi_2(\theta_2) \tag{325}$$

The reason is that we can then take a superposition of such product wavefunctions

$$\Psi = \psi_1(\theta_1)\psi_2(\theta_2) + \psi_3(\theta_1)\psi_4(\theta_2) + \dots \tag{326}$$

and thereby get any arbitrary function $\Psi(\theta_1, \theta_2)$.

18.1 The effect of rotations

Let us recall how we expressed the effect of rotations on functions. Consider the 2-d plane, and a particle that lives on the unit circle parametrized by $0 \leq \theta < 2\pi$.

Suppose we perform a rotation so that the function value at the point θ gets carried to the point $\theta + \delta\alpha$. We write this as

$$\theta \to \theta + \delta\alpha \tag{327}$$

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For any function $f(\theta)$, the new function is

$$\tilde{f}(\theta) = f(\theta - \delta\alpha) = f(\theta) + \delta\alpha(-\frac{\partial}{\partial\theta})f(\theta) + \dots \tag{328}$$

We define the angular momentum generator is

$$\hat{L} = -i\hbar\frac{\partial}{\partial\theta} \tag{329}$$

Now let us consider the effect of rotations on a function $\Psi = \psi_1(\theta_1)\psi_2(\theta_2)$. We have

$$\Psi \to \tilde{\Psi} = \psi_1(\theta_1 - \delta\alpha)\psi_2(\theta_2 - \delta\alpha) \tag{330}$$

We assume that $\delta\alpha$ is small. Then $\psi_1(\theta_1)$ changes as

$$\psi_1(\theta_1) \to \tilde{\psi}_1(\theta_1) = \psi_1(\theta_1 - \delta\alpha) = \psi_1(\theta_1) + \delta\alpha(-\frac{\partial}{\partial\theta_1})\psi_1(\theta_1) + \dots \tag{331}$$

Similarly, $\psi_2(\theta_2)$ changes as

$$\psi_2(\theta_2) \to \tilde{\psi}_2(\theta_2) = \psi_2(\theta_2 - \delta\alpha) = \psi_2(\theta_2) + \delta\alpha(-\frac{\partial}{\partial\theta_2})\psi_2(\theta_2) + \dots \tag{332}$$

Thus Ψ changes as

$$\begin{aligned}
\Psi \to \tilde{\Psi} &= \tilde{\psi}_1(\theta_1)\tilde{\psi}_2(\theta_2) = \psi_1(\theta_1 - \delta\alpha)\psi_2(\theta_2 - \delta\alpha) \\
&= \left(\psi_1(\theta_1) + \delta\alpha(-\frac{\partial}{\partial\theta_1})\psi_1(\theta_1) + \dots\right)\left(\psi_2(\theta_2) + \delta\alpha(-\frac{\partial}{\partial\theta_2})\psi_2(\theta_2) + \dots\right) \\
&\approx \psi_1(\theta_1)\psi_2(\theta_2) + \delta\alpha(-\frac{\partial}{\partial\theta_1})\psi_1(\theta_1)\ \psi_2(\theta_2) + \psi_1(\theta_1)\ \delta\alpha(-\frac{\partial}{\partial\theta_2})\psi_2(\theta_2) \quad (333)
\end{aligned}$$

Let us now write these relations in terms of infinitesimal changes. The change in $\psi_1(\theta_1)$ is

$$\delta\psi_1(\theta_1) = \tilde{\psi}_1(\theta_1) - \psi_1(\theta_1) = \delta\alpha(-\frac{\partial}{\partial\theta_1})\psi_1(\theta_1) + \dots \tag{334}$$

Similarly, the change in $\psi_2(\theta_2)$ is

$$\delta\psi_2(\theta_2) = \tilde{\psi}_2(\theta_2) - \psi_2(\theta_2) = \delta\alpha(-\frac{\partial}{\partial\theta_2})\psi_2(\theta_2) + \dots \tag{335}$$

The change in Ψ is

$$\begin{aligned}
\delta\Psi &= \tilde{\Psi} - \Psi \\
&\approx \delta\alpha(-\frac{\partial}{\partial\theta_1})\psi_1(\theta_1)\ \psi_2(\theta_2) + \psi_1(\theta_1)\ \delta\alpha(-\frac{\partial}{\partial\theta_2})\psi_2(\theta_2)
\end{aligned}$$

$$\tag{336}$$

We see that in the first term we have a derivative acting on $\psi_1(\theta_1)$, but we leave $\psi_2(\theta_2)$ untouched, while in the second term we have a derivative acting on $\psi_2(\theta_2)$, but we leave $\psi_1(\theta_1)$ untouched. When we leave a function untouched we say that we acted on the function with the identity operator I. Thus we would write

$$\delta\alpha(-\frac{\partial}{\partial\theta_1})\psi_1(\theta_1)\ \psi_2(\theta_2) \ = \ \left(\delta\alpha(-\frac{\partial}{\partial\theta_1})\otimes I\right)\ \psi_1(\theta_1)\ \psi_2(\theta_2) \tag{337}$$

Here the operator is in the brackets (...). The full wavefunction $\psi_1(\theta_1)\ \psi_2(\theta_2)$ is placed on the right, and the symbol $\otimes$ separates the two parts of the operator so that we know that the part of the left of this symbol will act on $\psi_1(\theta_1)$ and the part on the right of this symbol will act on $\psi_2(\theta_2)$.

Finally we can write all this with a small change of notation where we define

$$\hat{L} = -i\hbar\frac{\partial}{\partial\theta} \tag{338}$$

Then we get for any wavefunction, under an infinitesimal rotation $\delta\alpha$

$$\delta\psi = -\frac{i}{\hbar}\delta\alpha\hat{L}\psi \tag{339}$$

We then find that

$$\hat{L}^{(T)}\Psi = \left(\hat{L}^{(1)}\otimes 1\right)\psi_1(\theta_1)\psi_2(\theta_2) + \left(1\otimes\hat{L}^{(2)}\right)\psi_1(\theta_1)\psi_2(\theta_2) \tag{340}$$

19 Decomposing the product of two spin $\frac{1}{2}$ representations

Suppose we have two systems each with spin $\frac{1}{2}$. Thus the states are

$$|\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2$$
$$|\frac{1}{2},-\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2$$
$$|\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},-\frac{1}{2}\rangle_2$$
$$|\frac{1}{2},-\frac{1}{2}\rangle_1|\frac{1}{2},-\frac{1}{2}\rangle_2$$

$$\tag{341}$$

where $|\frac{1}{2},\frac{1}{2}\rangle_1$ means the state of system 1, with $l=\frac{1}{2}$ and $m=\frac{1}{2}$ etc.

How do these four states respond to rotations? Do they fom a single representation $l,m\rangle$ with $l=\frac{3}{2}$, and $m=\frac{3}{2}, m=\frac{1}{2}, m=-\frac{1}{2}, m=-\frac{3}{2}$? Or perhaps a representation $|l,m\rangle$ with $l=1$ and $m=1,0,-1$ and another representation with $|l,m\rangle$ with $l=0, m=0$?

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The total $\vec{L}^{(T)}$ operator is given by

$$\vec{L}^{(T)} = \vec{L}^{(1)} + \vec{L}^{(2)} \tag{342}$$

This is equivalent to the three relations

$$\begin{aligned}
L_x^{(T)} &= L_x^{(1)} + L_x^{(2)} \\
L_y^{(T)} &= L_y^{(1)} + L_y^{(2)} \\
L_z^{(T)} &= L_z^{(1)} + L_z^{(2)}
\end{aligned} \tag{343}$$

We can define, as before

$$\begin{aligned}
L_\pm^{(1)} &= L_x^{(1)} \pm i L_y^{(1)} \\
L_\pm^{(2)} &= L_x^{(2)} \pm i L_y^{(2)}
\end{aligned} \tag{344}$$

Note that

$$\frac{1}{2}\left(L_+^{(1)} \otimes L_-^{(2)} + L_-^{(1)} \otimes L_+^{(2)}\right) = L_x^{(1)} \otimes L_x^{(2)} + L_y^{(1)} \otimes L_y^{(2)} \tag{345}$$

Thus

$$\begin{aligned}
L_z^{(1)} \otimes L_z^{(2)} + \frac{1}{2}\left(L_+^{(1)} \otimes L_-^{(2)} + L_-^{(1)} \otimes L_+^{(2)}\right) &= L_x^{(1)} \otimes L_x^{(2)} + L_y^{(1)} \otimes L_y^{(2)} + L_z^{(1)} \otimes L_z^{(2)} \\
&\equiv \vec{L}^{(1)} \cdot \vec{L}^{(2)}
\end{aligned} \tag{346}$$

Note that to avoid complicated notation, we sometimes omit the $\otimes$ symbol.

19.1   Examining the states

Let us look at the state

$$|\frac{1}{2}, \frac{1}{2}\rangle_1 |\frac{1}{2}, \frac{1}{2}\rangle_2 \tag{347}$$

The total angular momentum operator has the components

$$L_x^{(T)}, \quad L_y^{(T)}, \quad L_z^{(T)} \tag{348}$$

We define

$$L_\pm^{(T)} = L_x^{(T)} \pm i L_y^{(T)} \tag{349}$$

Let us compute

$$L_+^{(T)} |\frac{1}{2}, \frac{1}{2}\rangle_1 |\frac{1}{2}, \frac{1}{2}\rangle_2 = \left(L_+^{(1)} \otimes I + I \otimes L_+^{(2)}\right) |\frac{1}{2}, \frac{1}{2}\rangle_1 |\frac{1}{2}, \frac{1}{2}\rangle_2 \tag{350}$$

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Recall that

$$
\begin{aligned}
L_+^{(1)} |\frac{1}{2}, \frac{1}{2}\rangle_1 &= 0 \\
L_+^{(1)} |\frac{1}{2}, -\frac{1}{2}\rangle_1 &= |\frac{1}{2}, \frac{1}{2}\rangle_1 \\
L_-^{(1)} |\frac{1}{2}, \frac{1}{2}\rangle_1 &= |\frac{1}{2}, -\frac{1}{2}\rangle_1 \\
L_-^{(1)} |\frac{1}{2}, -\frac{1}{2}\rangle_1 &= 0
\end{aligned}
\tag{351}
$$

Similarly

$$
\begin{aligned}
L_+^{(2)} |\frac{1}{2}, \frac{1}{2}\rangle_2 &= 0 \\
L_+^{(2)} |\frac{1}{2}, -\frac{1}{2}\rangle_2 &= |\frac{1}{2}, \frac{1}{2}\rangle_2 \\
L_-^{(2)} |\frac{1}{2}, \frac{1}{2}\rangle_2 &= |\frac{1}{2}, -\frac{1}{2}\rangle_2 \\
L_-^{(2)} |\frac{1}{2}, -\frac{1}{2}\rangle_2 &= 0
\end{aligned}
\tag{352}
$$

20   Decomposing a product of representations

We have two spin half particles. The states are

$$
\begin{aligned}
&|\frac{1}{2}, \frac{1}{2}\rangle_1 |\frac{1}{2}, \frac{1}{2}\rangle_2 \\
&|\frac{1}{2}, -\frac{1}{2}\rangle_1 |\frac{1}{2}, \frac{1}{2}\rangle_2 \\
&|\frac{1}{2}, \frac{1}{2}\rangle_1 |\frac{1}{2}, -\frac{1}{2}\rangle_2 \\
&|\frac{1}{2}, -\frac{1}{2}\rangle_1 |\frac{1}{2}, -\frac{1}{2}\rangle_2
\end{aligned}
\tag{353}
$$

20.1   The spin 1 (triplet) representation

Let us start with

$$
\Psi = |\frac{1}{2}, \frac{1}{2}\rangle_1 |\frac{1}{2}, \frac{1}{2}\rangle_2
\tag{354}
$$

We see that

$$
\begin{aligned}
\hat{L}_z^{(T)}\Psi &= \left(\hat{L}_z^{(1)}\otimes I + I \otimes \hat{L}_z^{(2)}\right)|\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2 \\
&= \frac{1}{2}\hbar|\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2 + \frac{1}{2}\hbar|\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2 \\
&= \hbar|\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2
\end{aligned}
\tag{355}
$$

Thus we see that $m_T = 1$. More generally, we see that

$$
m_T = m_1 + m_2
\tag{356}
$$

Now let us check

$$
\begin{aligned}
\hat{L}_+^{(T)}\Psi &= \left(\hat{L}_+^{(1)}\otimes 1 + 1 \otimes \hat{L}_+^{(2)}\right)|\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2 \\
&= 0 + 0 = 0
\end{aligned}
\tag{357}
$$

Thus we see that $\hat{L}_+^{(T)}\Psi = 0$, so that it would be a $m_t = 1$ member of a multiplet with $l_T = 1$. Thus we write

$$
|l_T, m_T\rangle = |1,1\rangle = |\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2
\tag{358}
$$

Now let us compute

$$
\begin{aligned}
\hat{L}_-^{(T)}\Psi &= \left(\hat{L}_-^{(1)}\otimes 1 + 1 \otimes \hat{L}_-^{(2)}\right)|\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2 \\
&= |\frac{1}{2},-\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2 + |\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},-\frac{1}{2}\rangle_2
\end{aligned}
\tag{359}
$$

We see that this is a state with $m_T = 0$. Thus we expect this to be a $l_T = 1, m_T = 0$. It is not normalized however, and we find its norm is $1 + 1 = 2$. Thus we define the normalized state

$$
|l_T, m_T\rangle = |1,0\rangle = \frac{1}{\sqrt{2}}\left(|\frac{1}{2},-\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2 + |\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},-\frac{1}{2}\rangle_2\right)
\tag{360}
$$

From the above we see that

$$
\hat{L}_-^{(T)}|1,1\rangle = \sqrt{2}|1,0\rangle
\tag{361}
$$

which agrees with the algebra of the $\hat{L}_i$.

Now let us compute

$$
\begin{aligned}
\hat{L}_-^{(T)}|1,0\rangle &= \left(\hat{L}_-^{(1)}\otimes 1 + 1 \otimes \hat{L}_-^{(2)}\right)\frac{1}{\sqrt{2}}\left(|\frac{1}{2},-\frac{1}{2}\rangle_1|\frac{1}{2},\frac{1}{2}\rangle_2 + |\frac{1}{2},\frac{1}{2}\rangle_1|\frac{1}{2},-\frac{1}{2}\rangle_2\right) \\
&= \frac{1}{\sqrt{2}}|\frac{1}{2},-\frac{1}{2}\rangle_1|\frac{1}{2},-\frac{1}{2}\rangle_2 + \frac{1}{\sqrt{2}}|\frac{1}{2},-\frac{1}{2}\rangle_1|\frac{1}{2},-\frac{1}{2}\rangle_2 \\
&= \sqrt{2}\frac{1}{\sqrt{2}}|\frac{1}{2},-\frac{1}{2}\rangle_1|\frac{1}{2},-\frac{1}{2}\rangle_2
\end{aligned}
\tag{362}
$$

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We define
$$|l_T, m_T\rangle = |1, -1\rangle = \frac{1}{\sqrt{2}}|\frac{1}{2}, -\frac{1}{2}\rangle_1|\frac{1}{2}, -\frac{1}{2}\rangle_2 \tag{363}$$

20.2   The spin 0 (singlet) representation

It is a general rule that states of different representation are orthogonal to each other. We need to have $m_T = 0$. Thus we are looking for states in the subspace
$$c_1|\frac{1}{2}, -\frac{1}{2}\rangle_1|\frac{1}{2}, \frac{1}{2}\rangle_2 + c_2|\frac{1}{2}, \frac{1}{2}\rangle_1|\frac{1}{2}, -\frac{1}{2}\rangle_2 \tag{364}$$

We already have the state
$$|1, 0\rangle = \frac{1}{\sqrt{2}}\left(|\frac{1}{2}, -\frac{1}{2}\rangle_1|\frac{1}{2}, \frac{1}{2}\rangle_2 + |\frac{1}{2}, \frac{1}{2}\rangle_1|\frac{1}{2}, -\frac{1}{2}\rangle_2\right) \tag{365}$$

A state orthogonal to this has to satisfy
$$c_1 + c_2 = 0 \tag{366}$$

If we normalize the state we get
$$|l_T, m_T\rangle = |0, 0\rangle = \frac{1}{\sqrt{2}}\left(|\frac{1}{2}, -\frac{1}{2}\rangle_1|\frac{1}{2}, \frac{1}{2}\rangle_2 - |\frac{1}{2}, \frac{1}{2}\rangle_1|\frac{1}{2}, -\frac{1}{2}\rangle_2\right) \tag{367}$$

21   Computing $(\hat{L}^{(T)})^2$

Let us now compute
$$
\begin{aligned}
(\hat{L}^{(T)})^2 &= (\hat{L}_x^{(T)})^2 + (\hat{L}_y^{(T)})^2 + (\hat{L}_z^{(T)})^2 \\
&= (\hat{L}_x^{(1)} \otimes 1 + 1 \otimes \hat{L}_x^{(2)})^2 + (\hat{L}_y^{(1)} \otimes 1 + 1 \otimes \hat{L}_y^{(2)})^2 + (\hat{L}_z^{(1)} \otimes 1 + 1 \otimes \hat{L}_z^{(2)})^2 \\
&= \left((\hat{L}_x^{(1)})^2 \otimes 1 + 1 \otimes (\hat{L}_x^{(2)})^2 + 2\hat{L}_x^{(1)} \otimes \hat{L}_x^{(2)}\right) \\
&\quad + \left((\hat{L}_y^{(1)})^2 \otimes 1 + 1 \otimes (\hat{L}_y^{(2)})^2 + 2\hat{L}_y^{(1)} \otimes \hat{L}_y^{(2)}\right) \\
&\quad + \left((\hat{L}_z^{(1)})^2 \otimes 1 + 1 \otimes (\hat{L}_z^{(2)})^2 + 2\hat{L}_z^{(1)} \otimes \hat{L}_z^{(2)}\right) \\
&= (\hat{L}^{(1)})^2 \otimes 1 + 1 \otimes (\hat{L}^{(2)})^2 + 2\left(L_x^{(1)} \otimes L_x^{(2)} + L_y^{(1)} \otimes L_y^{(2)} + L_z^{(1)} \otimes L_z^{(2)}\right) \\
&= (\hat{L}^{(1)})^2 + (\hat{L}^{(2)})^2 + 2\vec{L}^{(1)} \cdot \vec{L}^{(2)} \tag{368}
\end{aligned}
$$

where in the last line we have not used the $\otimes$ symbol for simplicity. Thus we have
$$(\hat{L}^{(T)})^2 = (\hat{L}^{(1)})^2 + (\hat{L}^{(2)})^2 + 2\vec{L}^{(1)} \cdot \vec{L}^{(2)} \tag{369}$$

22 Measurement

We have written states as kets $|\psi\rangle$. The conjugate states are written as bras $\langle\chi|$. The dot product between these is written as $\langle\chi|\psi\rangle$.

Consider a Hermitian operator $\hat{O}$; all observables, in particular, are Hermitian operators. Let the eigenstates of $\hat{O}$ be called $|n\rangle$, corresponding the the eigenvalue λ_n.

The eigenstates $|n\rangle$ form a complete orthogonal set; we can normalize them so that we get

$$\langle n_i|n_j\rangle = \delta_{ij} \tag{370}$$

22.1 The identity operator

We can write the identity operator as follows

$$I = \sum_i |n_i\rangle\langle n_i| \tag{371}$$

To check this, suppose a general state $|\psi\rangle$ is expanded as

$$|\psi\rangle = \sum_k c_k |n_k\rangle \tag{372}$$

Then we have

$$\left(\sum_i |n\rangle\langle n_i|\right)|\psi\rangle = \left(\sum_i |n_i\rangle\langle n_i|\right)\sum_k c_k|n_k\rangle = \sum_i\sum_k c_k\delta_{ik}|n_i\rangle = \sum_i c_i|n_i\rangle = |\psi\rangle \tag{373}$$

which shows that $\sum_i |n_i\rangle\langle n_i|$ acts like the identity operator on every state.

22.2 Expressing n arbitrary operator

Now we argue that the operator $\hat{O}$ can be written in terms of its eigenvalues λ_i and the eigenstates $|n_i\rangle$. We will argue that

$$\hat{O} = \sum_i \lambda_i|n_i\rangle\langle n_i| \tag{374}$$

To check this, let us compute the action of the above expression on one of the eigenstates $|n_k\rangle$. We get

$$\left(\sum_i \lambda_i|n_i\rangle\langle n_i|\right)|n_k\rangle = \sum_i \lambda_i\delta_{ik}|n_i\rangle = \lambda_k|n_k\rangle \tag{375}$$

which agrees with the expectation $\hat{O}|n_k\rangle = \lambda_k|n_k\rangle$. Since our expression agrees with the action of $\hat{O}$ on all eigenstates $|n_k\rangle$, this agreement will automatically extend to all linear combinations of the $|n_k\rangle$, which means the agreement extends to all states $|\psi\rangle$.

22.3 Measurement

Suppose we start with a state $|\psi\rangle$ and make a measurement of an observable $\hat{O}$. The following are the rules of measurement:

(i) The measurement will have to yield one of the eigenvalues of $\hat{O}$; let this eigenvalue be λ_k, corresponding the the eigenstate $|n_k\rangle$.

(ii) After the measurement, the state of the system will be this eigenstate $|n_k\rangle$.

(iii) The probability of getting this outcome λ_k is given by

$$p_k = |\langle n_k|\psi\rangle|^2 \tag{376}$$

This expression can be understood by writing

$$|\psi\rangle = \sum_i c_i |n_i\rangle \tag{377}$$

The probability is then

$$p_k = |c_k|^2 = |\langle n_k|\psi\rangle|^2 \tag{378}$$

22.4 Two systems

Suppose we have two systems, called 1 and 2. First we look at the structure of states and dot products.

A product state of the full system can be written as

$$|\Psi\rangle = |\psi\rangle_1 |\chi\rangle_2 \tag{379}$$

Let another such state be

$$|\Psi'\rangle = |\psi'\rangle_1 |\chi'\rangle_2 \tag{380}$$

Then the dot product is

$$\langle \Psi'|\Psi\rangle = \langle \psi'|\psi\rangle \langle \chi'|\chi\rangle \tag{381}$$

A general state that can be written as

$$|\Psi\rangle = \sum_a \sum_b C_{ab} |\psi_a\rangle |\chi_b\rangle \tag{382}$$

where $|\psi_a\rangle_1$ is an orthonormal basis for system 1 and $|\chi_b\rangle_2$ is an orthonormal basis for system 2. We have the following kinds of questions that can be asked:

(i) What is the probability that we get a state

$$|\Psi'\rangle = \sum_c \sum_d D_{cd} |\psi_a\rangle |\chi_b\rangle \tag{383}$$

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Since we have a complete states of a complete system (formed by systems 1 and 2), we just have

$$P = |\langle \Psi' | \Psi \rangle|^2 \tag{384}$$

(ii) What is the probability to find a state

$$|\psi'\rangle_1 = \sum_c D_c |\psi_c\rangle_1 \tag{385}$$

Now we compute

$$|\chi'\rangle_2 = {}_1\langle \psi' | \Psi \rangle \tag{386}$$

to get a state is system 2. Then we have

$$P = ||\chi'\rangle_2|^2 = {}_2\langle \chi' | \chi' \rangle_2 \tag{387}$$

(iii) Suppose we measure system 1 and find the eigenvalue λ_k corresponding to the eigenstate $|n_k\rangle$ for an operator $\hat{O}$ acting on system 1. What is the probability of finding a state $|\chi'\rangle_2$ for system 2 after this first measurement?

Note that $\hat{O}$ is an observable on system 1, and does not affect system 2. Suppose the measurement of system 1 gives the eigenstate $|n_k\rangle$. Then the full state after measurement will have the form

$$|\Psi'\rangle = D(|n_k\rangle\langle n_k| \otimes I)|\Psi\rangle \tag{388}$$

where D is a constant that we will have to find to normalize $|\Psi'\rangle$. We can then proceed as in (i) above.

22.5 Applying this to problem 10.13

(i) We can write the singlet state as

$$|\Psi\rangle_0 = \frac{1}{\sqrt{2}} \left(|\chi_+\rangle_1 |\chi_-\rangle_2 - |\chi_-\rangle_1 |\chi_+\rangle_2 \right) \tag{389}$$

By inspection, we can see that if the spin of system 1 is $|\chi_+\rangle_1$, then there is no amplitude for the spin of the second system to also be up; i..e, $|\chi_+\rangle_2$. Thus the probability is zero.

Formally, we can proceed as follows. After the spin of the first system is measured an found to be $|\chi_+\rangle_1$, the state of the system is

$$
\begin{aligned}
|\Psi'\rangle_0 &= D\left((|n_k\rangle\langle n_k| \otimes I)\right) \frac{1}{\sqrt{2}} \left(|\chi_+\rangle_1 |\chi_-\rangle_2 - |\chi_-\rangle_1 |\chi_+\rangle_2 \right) \\
&= D\left((|\chi_+\rangle_{11}\langle\chi_+| \otimes \sum_l |n_l\rangle_{22}\langle n_l|) \right) \frac{1}{\sqrt{2}} \left(|\chi_+\rangle_1 |\chi_-\rangle_2 - |\chi_-\rangle_1 |\chi_+\rangle_2 \right) \\
&= D\left((|\chi_+\rangle_{11}\langle\chi_+| \otimes (|\chi_+\rangle_{22}\langle\chi_+| + |\chi_-\rangle_{22}\langle\chi_-|) \right) \frac{1}{\sqrt{2}} \left(|\chi_+\rangle_1 |\chi_-\rangle_2 - |\chi_-\rangle_1 |\chi_+\rangle_2 \right) \\
&= 0
\end{aligned} \tag{390}
$$

(ii) We can write the spins in the y basis. Then the singlet is

$$|\Psi\rangle_0 = \frac{1}{\sqrt{2}} \left(|\chi_+^y\rangle_1 |\chi_-^y\rangle_2 - |\chi_-^y\rangle_1 |\chi_+^y\rangle_2 \right) \tag{391}$$

where we noted with a superscript that these are y direction spins. The measurement of the first spin giving the result $|\chi_+^y\rangle_1$ will give the final state as

$$|\chi_+^y\rangle_1 |\chi_-^y\rangle_2 \tag{392}$$

The probability that the second system is in spin state $|\chi_+^x\rangle_2$ is

$$P = |\langle \chi_+^x | \chi_-^y \rangle|^2 = \frac{1}{2} \tag{393}$$

where we used the explicit form of these eigenstates in the z basis

$$|\chi_+^x\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\chi_-^y\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \tag{394}$$

To do this formally, we can proceed as follows. After the spin of the first system is measured an found to be $|\chi_+^y\rangle_1$, the state of the system is

$$
\begin{aligned}
|\Psi'\rangle_0 &= D\left((|n_k\rangle\langle n_k| \otimes I) \right) \frac{1}{\sqrt{2}} \left(|\chi_+\rangle_1 |\chi_-\rangle_2 - |\chi_-\rangle_1 |\chi_+\rangle_2 \right) \\
&= D\left((|\chi_+^y\rangle_{11}\langle \chi_+^y| \otimes \sum_l |n_l\rangle_{22}\langle n_l|) \right) \frac{1}{\sqrt{2}} \left(|\chi_+\rangle_1 |\chi_-\rangle_2 - |\chi_-\rangle_1 |\chi_+\rangle_2 \right) \\
&= D\left((|\chi_+^y\rangle_{11}\langle \chi_+^y| \otimes (|\chi_+\rangle_{22}\langle \chi_+| + |\chi_-\rangle_{22}\langle \chi_-|)) \frac{1}{\sqrt{2}} \left(|\chi_+\rangle_1 |\chi_-\rangle_2 - |\chi_-\rangle_1 |\chi_+\rangle_2 \right) \right) \\
&= D\left(-\frac{1}{\sqrt{2}} {}_1\langle \chi_+^y | \chi_-\rangle_1 |\chi_+^y\rangle_1 |\chi_+\rangle_2 + \frac{1}{\sqrt{2}} {}_1\langle \chi_+^y | \chi_+\rangle_1 |\chi_+^y\rangle_1 |\chi_-\rangle_2 \right) \\
&= D\left(-\frac{1}{\sqrt{2}} (-\frac{i}{\sqrt{2}}) |\chi_+^y\rangle_1 |\chi_+\rangle_2 + \frac{1}{\sqrt{2}} (\frac{1}{\sqrt{2}}) |\chi_+^y\rangle_1 |\chi_-\rangle_2 \right) \\
&= D |\chi_+^y\rangle_1 \left(\frac{i}{2} |\chi_+\rangle_2 + \frac{1}{2} |\chi_-\rangle_2 \right)
\end{aligned}
\tag{395}
$$

The normalized state is

$$|\Psi'\rangle_0 = |\chi_+^y\rangle_1 \left(\frac{1}{\sqrt{2}} (i|\chi_+\rangle_2 + |\chi_-\rangle_2) \right) \tag{396}$$

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To find the probability that the second system is in the $|\sigma_+^x\rangle_2$ state, we compute

$$
\begin{aligned}
A &= {}_2\langle\chi_+^x|\left(\frac{1}{\sqrt{2}}\left(i|\chi_+\rangle_2 + |\chi_-\rangle_2\right)\right) \\
&= \left(\frac{1}{\sqrt{2}}{}_2\langle\chi_+| + \frac{1}{\sqrt{2}}{}_2\langle\chi_-|\right)\left(\frac{1}{\sqrt{2}}\left(i|\chi_+\rangle_2 + |\chi_-\rangle_2\right)\right) \\
&= \frac{1}{2}(i+1)
\end{aligned}
\tag{397}
$$

Then the probability is

$$
P = |A|^2 = \frac{1}{2}
\tag{398}
$$

(iii) Suppose the first spin has the form

$$
|\psi\rangle_1 = \cos\alpha_1|\chi_+\rangle + \sin\alpha_1 e^{i\beta_1}|\chi_-\rangle
\tag{399}
$$

and the second spin has the form

$$
|\chi\rangle_2 = \cos\alpha_2|\chi_+\rangle + \sin\alpha_2 e^{i\beta_2}|\chi_-\rangle
\tag{400}
$$

Thus the overall state is

$$
|\Psi\rangle = \left(\cos\alpha_1|\chi_+\rangle_1 + \sin\alpha_1 e^{i\beta_1}|\chi_-\rangle_1\right)\left(\cos\alpha_2|\chi_+\rangle_2 + \sin\alpha_2 e^{i\beta_2}|\chi_-\rangle_2\right)
\tag{401}
$$

Let us ask for the probability for this to be in the singlet state

$$
|\Psi\rangle_0 = \frac{1}{\sqrt{2}}\left(|\chi_+\rangle_1|\chi_-\rangle_2 - |\chi_-\rangle_1|\chi_+\rangle_2\right)
\tag{402}
$$

The amplitude for a singlet is

$$
\begin{aligned}
A_0 &= \langle\Psi_0|\Psi\rangle \\
&= \frac{1}{\sqrt{2}}\left({}_1\langle\chi_+|{}_2\langle\chi_-| - {}_1\langle|\chi_-|{}_2\langle\chi_+|\right)\left(\cos\alpha_1|\chi_+\rangle_1 + \sin\alpha_1 e^{i\beta_1}|\chi_-\rangle_1\right)\left(\cos\alpha_2|\chi_+\rangle_2 + \sin\alpha_2 e^{i\beta_2}|\chi_-\rangle_2\right) \\
&= \frac{1}{\sqrt{2}}\cos\alpha_1\sin\alpha_2 e^{i\beta_2} - \frac{1}{\sqrt{2}}\sin\alpha_1 e^{i\beta_1}\cos\alpha_2
\end{aligned}
\tag{403}
$$

The probability for a singlet is

$$
P_0 = |A_0|^2 = \frac{1}{2}|\cos\alpha_1\sin\alpha_2 e^{i\beta_2} - \sin\alpha_1 e^{i\beta_1}\cos\alpha_2|^2
\tag{404}
$$

The probability of a triplet is then

$$
P_1 = 1 - P_0 = 1 - \frac{1}{2}|\cos\alpha_1\sin\alpha_2 e^{i\beta_2} - \sin\alpha_1 e^{i\beta_1}\cos\alpha_2|^2
\tag{405}
$$

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23 Particle in a magnetic field

23.1 The classical Hamiltonian

We have

$$H = \frac{1}{2m}(\vec{p} - q\vec{A})^2 \tag{406}$$

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{1}{2m}(p_x - qA_x) \tag{407}$$

Thus

$$p_x = m\dot{x} + qA_x \tag{408}$$

We have

$$\dot{p}_x = -\frac{\partial H}{\partial x} = -\frac{1}{m}(p_x - qA_x)(-q)A_{x,x} - \frac{1}{m}(p_y - qA_y)(-q)A_{y,x} - \frac{1}{m}(p_z - qA_z)(-q)A_{z,x} \tag{409}$$

This is

$$m\ddot{x} + q(A_{x,x}\dot{x} + A_{x,y}\dot{y} + A_{x,z}\dot{z}) = q(\dot{x}A_{x,x} + \dot{y}A_{y,x} + \dot{z}A_{z,x}) \tag{410}$$

$$m\ddot{x} = q(\dot{y}(A_{y,x} - A_{x,y}) - \dot{z}(A_{x,z} - A_{z,x})) \tag{411}$$

$$m\ddot{x} = q(\dot{y}B_z - \dot{z}B_y) \tag{412}$$

$$m\ddot{x} = q(\vec{v} \times \vec{B})_x \tag{413}$$

23.2 General notations

Minimal coupling is

$$\vec{p} \rightarrow \vec{p} - q\vec{A} \tag{414}$$

Thus for the electron we have

$$\vec{p} \rightarrow \vec{p} + e\vec{A} \tag{415}$$

The Hamiltonian is

$$H = \frac{1}{2m}(\vec{p} + e\vec{A})^2 - e\Phi \tag{416}$$

The schrodinger equation is

$$i\hbar\partial_t\psi = \frac{1}{2m}(-i\hbar\vec{\nabla} + e\vec{A})^2\psi - e\Phi\psi \tag{417}$$

This is

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\triangle\psi - \frac{ie\hbar}{m}\vec{A}\cdot\vec{\nabla}\psi - \frac{ie\hbar}{2m}(\vec{\nabla}\cdot\vec{A})\psi + \frac{e^2}{2m}A^2\psi - e\Phi\psi \tag{418}$$

(Here there may be a factor of 2 error in the third term on the RHS.)

For a coulomb potential

$$\Phi = \frac{1}{4\pi\epsilon_0}\frac{Ze}{r} \tag{419}$$

(Here there may be a sign error in the text.)

23.3 The gauge potential

Suppose we have a constant magnetic field $\hat{B}$. Then we get this from

$$\vec{A} = -\frac{1}{2}\vec{r} \times \vec{B} \tag{420}$$

As an example, let

$$\vec{B} = B_z \hat{z} \tag{421}$$

Then we have

$$\vec{r} \times \vec{B} = B_z(y\hat{x} - x\hat{y}) \tag{422}$$

and

$$\vec{A} = -\frac{1}{2}B_z(y\hat{x} - x\hat{y}) \tag{423}$$

We check that

$$\vec{\nabla} \cdot \vec{A} = 0 \tag{424}$$

23.4 Weak constant magnetic field

We have

$$
\begin{aligned}
(-\frac{ie\hbar}{m})\vec{A} \cdot \vec{\nabla}\psi &= (-\frac{ie\hbar}{m})(-\frac{1}{2})(\vec{r} \times \vec{B}) \cdot \vec{\nabla}\psi \\
&= (-\frac{ie\hbar}{m})(-\frac{1}{2})\vec{\nabla}\psi \cdot (\vec{r} \times \vec{B}) \\
&= (-\frac{ie\hbar}{m})(-\frac{1}{2})\vec{B} \cdot (\vec{\nabla}\psi \times \vec{r}) \\
&= -(-\frac{ie\hbar}{m})(-\frac{1}{2})\vec{B} \cdot (\vec{r} \times \vec{\nabla}\psi) \\
&= -(-\frac{ie\hbar}{m})(-\frac{1}{2})\frac{1}{(-i\hbar)}\vec{B} \cdot (\vec{r} \times (-i\hbar\vec{\nabla})\psi) \\
&= (\frac{e}{2m})\vec{B} \cdot (\vec{r} \times \vec{p}\psi) \\
&= (\frac{e}{2m})\vec{B} \cdot (\vec{r} \times \vec{p})\psi \\
&= (\frac{e}{2m})\vec{B} \cdot \vec{L}\psi
\end{aligned}
\tag{425}
$$

23.5 Problem 16-1

We have the for the 3-d oscillator

$$H = -\frac{\hbar^2}{2m}\triangle + \frac{1}{2}m\omega^2 r^2 \tag{426}$$

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This is spherically symmetric, and we can write its solutions as

$$\psi = R_{n_r,l}(r)Y_{lm}(\theta, \phi), \quad n = 0, 1, 2, \ldots \tag{427}$$

The energy levels are

$$E = \hbar\omega(2n_r + l + \frac{3}{2}) \tag{428}$$

where n, l are independent integers.

Now the Hamiltonian is

$$H' = H - \frac{q}{2m}B_z L_z \tag{429}$$

Thus the energy levels are

$$E = \hbar\omega(2n + l + \frac{3}{2}) - \frac{q\hbar}{2m}B_z m_z \tag{430}$$

23.6   Radial equation for 3-d Harmonic oscillator

The equation is

$$\frac{d^2 H(y)}{dy^2} + (\frac{l + \frac{3}{2}}{y} - 1)\frac{dH(y)}{dy} + \frac{\lambda - 2l - 3}{4y}H(y) = 0 \tag{431}$$

We let

$$H = \sum_{n \geq 0} a_n y^n \tag{432}$$

This gives

$$n(n-1)a_n y^{n-2} + (\frac{l + \frac{3}{2}}{y} - 1)na_n y^{n-1} + (\frac{\lambda - 2l - 3}{4})a_n y^{n-1} = 0 \tag{433}$$

The coefficient of y^{n-1} is

$$(n+1)na_{n+1} + (l + \frac{3}{2})(n+1)a_{n+1} - na_n + \frac{lambda - 2l - 3}{4}a_n = 0 \tag{434}$$

This gives

$$\frac{a_{n+1}}{a_n} = \frac{n - \frac{\lambda - 2l - 3}{4}}{l + \frac{3}{2} + n} \tag{435}$$

Thus we need

$$n_r - \frac{\lambda - 2l - 3}{4} = 0 \tag{436}$$

for some $n_r = 0, 1, 2, \ldots$. This gives

$$\lambda = 4n_4 + 2l + 3 \tag{437}$$

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24 Landau levels

24.1 Classical particle in a constant magnetic field

We had

$$H = \frac{(\vec{p} + e\vec{A})^2}{2m} \tag{438}$$

Thus

$$\dot{x} = \frac{\partial H}{\partial p_x} = p_x + eA_x \tag{439}$$

etc. Thus

$$\vec{v} = \frac{1}{m}(\vec{p} + e\vec{A}) \tag{440}$$

Thus the mechanical angular momentum is

$$m\vec{r} \times \vec{v} = \vec{r} \times \vec{p} + e\vec{r} \times \vec{A} \tag{441}$$

In the gauge

$$\vec{A} = -\frac{1}{2}\vec{r} \times \vec{B} \tag{442}$$

we have

$$m\vec{r} \times \vec{v} = \vec{r} \times \vec{p} - \frac{1}{2}e\vec{r} \times (\vec{r} \times \vec{B}) = \vec{L} - \frac{1}{2}e\left((\vec{r} \cdot \vec{B})\vec{r} - r^2\vec{B}\right) \tag{443}$$

We take the z component and assume that we are in the $z = 0$ plane. Then we get

$$mrv = L_z + \frac{eB}{2}r^2 \tag{444}$$

From the rotation equation, we have

$$m\frac{v^2}{r} = evB, \quad v = \frac{erB}{m}, \quad mvr = eBr^2 \tag{445}$$

Thus we have

$$eBr^2 = L_z + \frac{1}{2}eBr^2, \quad L_z = \frac{1}{2}eBr^2 \tag{446}$$

We now set

$$L_z = n\hbar \tag{447}$$

Thuis gives

$$\frac{1}{2}eBr^2 = n\hbar, \quad r^2 = \frac{2n\hbar}{eB} \tag{448}$$

The energy is

$$E = \frac{1}{2}mv^2 = \frac{1}{2}m\frac{e^2r^2B^2}{m^2} = \frac{1}{2}\frac{eB2n\hbar}{m} = \frac{eM}{m}n\hbar \tag{449}$$

Writing

$$\frac{eB}{m} = \omega \tag{450}$$

we have

$$E = n\hbar\omega \tag{451}$$

so the level spacing is $\hbar\omega$ though the levels are highly degenerate because of the arbitrary choice of position.

If we do all this in the gauge

$$\vec{A} = Bx\hat{y} \tag{452}$$

then instead of

$$mrv = L_z + \frac{eB}{2}r^2 \tag{453}$$

we get

$$mrv = L_z + eBx^2 \tag{454}$$

If we average over a circular orbit, we see that we get the same numbers.

24.2   The constant magnetic field in different gauges

We have taken

$$\vec{A} = -\frac{1}{2}\vec{r} \times \vec{B} \tag{455}$$

This gave

$$\vec{A} = -\frac{1}{2}B(y\hat{x} - x\hat{y}) \tag{456}$$

When we take the curl of this we get

$$(\vec{\nabla} \times \vec{A})_z = \partial_x A_y - \partial_y A_x = \frac{1}{2}B + \frac{1}{2}B = B \tag{457}$$

We could also take

$$\vec{A} = -By\hat{x} \tag{458}$$

or

$$\vec{A} = Bx\hat{y} \tag{459}$$

We will take the latter.

24.3   The Hamiltonian

In the gauge

$$\vec{A} = Bx\hat{y} \tag{460}$$

we have

$$A_x = 0, \quad A_y = Bx, \quad A_z = 0 \tag{461}$$

Thus we have

$$H = \frac{1}{2m}(\vec{p} + e\vec{A})^2 = \frac{1}{2m}(p_x^2 + (p_y + eBx)^2 + p_z^2) = \frac{1}{2m}(p_x^2 + 2eBp_yx + e^2B^2x^2 + p_z^2) \tag{462}$$

Here the order of p_y, x did not matter since they commute. We see that

$$[H, p_y] = 0, \quad [H, p_z] = 0 \tag{463}$$

Thus we can choose simultaneous eigenfunctions of H, p_y, p_z. This can be seen more directly from the equation, where we can take

$$\psi = e^{ik_yy}e^{ik_zz} \tag{464}$$

We will set

$$k_y \equiv k, \quad k_z = 0 \tag{465}$$

Then

$$p_y = -i\hbar\partial_y \to -i\hbar(ik) \to \hbar k \tag{466}$$

Then we get

$$H\psi = \frac{1}{2m}(p_x^2 + \hbar^2k^2 + 2eBx\hbar k + e^2B^2x^2) = \frac{1}{2m}(p_x^2 + e^2B^2(x + \frac{\hbar k}{eB})^2) \tag{467}$$

This is a harmonic oscillator, with

$$\frac{1}{2}m\omega^2 = \frac{1}{2m}e^2B^2, \quad \omega = \frac{eB}{m} \tag{468}$$

Thus the energy levels are

$$(n + \frac{1}{2})\hbar\omega \tag{469}$$

But note that k is arbitrary, so the levels are highly degenerate.

24.4 Relation to classical frequencies

In the classical theory, we have the force

$$\vec{F} = -e\vec{v} \times B \tag{470}$$

This gives rise to circular motion with

$$\frac{mv^2}{r} = F = evB, \quad v = \frac{erB}{m} \tag{471}$$

This gives a time period

$$T = \frac{2\pi r}{v} = \frac{2\pi r m}{erB} = \frac{2\pi m}{eB} \tag{472}$$

The frequency and angular frequency are then

$$\nu = \frac{1}{T} = \frac{eB}{2\pi m}, \quad \omega = 2\pi\nu = \frac{eB}{m} \tag{473}$$

24.5 Boundary conditions

We have a strip of length L_2 in the y direction. It is better to use a periodic box. Then

$$k = \frac{2\pi n}{L_2} \tag{474}$$

Thus the x locations, for a given value of the excitation of the harmonic oscillator, are

$$x_n = -\frac{\hbar k}{eB} = -\frac{2\pi\hbar n^*}{L_2 eB} \tag{475}$$

This has the range $0 \leq x \leq L_1$. Thus

$$\frac{2\pi\hbar|n^*_{max}|}{L_2 eB} = L_1 \tag{476}$$

which gives

$$|n^*_{max}| = \frac{eBL_1 L_2}{2\pi\hbar} = \frac{eBL_1 L_2}{h} \tag{477}$$

We see that $\frac{\hbar}{eB}$ has the dimensions of an area, so we define a magnetic length

$$l_B = \sqrt{\frac{\hbar}{eB}} \tag{478}$$

Thus the number of states in the sample per unit area for each Landau level are

$$n_B = \frac{1}{2\pi l_B^2} \tag{479}$$

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24.6 Problem 16-2

We have

$$H = \frac{1}{2I}(\vec{L})^2 = \frac{1}{2I}(\vec{r} \times \vec{p})^2 \tag{480}$$

In a magnetic field $\vec{p}$ changes to

$$\vec{p} \to \vec{p} - q\vec{A} \tag{481}$$

In a constant magnetic field this is, using $\vec{A} = -\frac{1}{2}\vec{r} \times \vec{B}$,

$$\vec{p} \to \vec{p} + \frac{1}{2}q\vec{r} \times \vec{B} \tag{482}$$

Thus

$$\vec{r} \times \vec{p} \to \vec{r} \times (\vec{p} + \frac{1}{2}q\vec{r} \times \vec{B}) = \vec{L} + \frac{1}{2}q\left(\vec{r} \cdot \vec{B})\vec{r} - r^2\vec{B}\right) \tag{483}$$

The full Hamiltonian is given by

$$H = \frac{1}{2I}\left(\vec{L} + \frac{1}{2}q\left(\vec{r} \cdot \vec{B})\vec{r} - r^2\vec{B}\right)\right)^2 \tag{484}$$

In the limit of small B, we have

$$(\vec{L} + \frac{1}{2}q\left(\vec{r} \cdot \vec{B})\vec{r} - r^2\vec{B}\right))^2 \approx \vec{L}^2 - qr^2\vec{B} \cdot \vec{L} \tag{485}$$

where we have noted that in computing

$$\vec{L} \cdot \vec{r} \to (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)\hat{x} + \ldots \tag{486}$$

we never get any terms that do not commute, and so $\vec{L} \cdot \vec{r} = 0$. The same is true for $\vec{r} \cdot \vec{L}$. Thus we set

$$\vec{L} \cdot \vec{r} = 0, \quad \vec{r} \cdot \vec{L} = 0 \tag{487}$$

and also note that we can write our terms so that the term $(\vec{r} \cdot B)$ is to the left or right of the above terms.

Thus we get

$$H \approx \frac{1}{2I}\vec{L}^2 - \frac{q}{2M}\vec{B} \cdot \vec{L} \tag{488}$$

where we have used that

$$I = Mr^2 \tag{489}$$

The spectrum is

$$\frac{\hbar^2}{2I}l(l+1) - \frac{qB\hbar m_z}{2M} \tag{490}$$

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25   The Hall effect

25.1   Conductivity

Ohm's law says

$$V = IR \tag{491}$$

Let the resistor have cross sectional area A ad length L. Then we have

$$R \propto \frac{1}{A}, \quad R \propto L \tag{492}$$

so we can write

$$R = \rho \frac{L}{A} \tag{493}$$

where ρ is called the resistivity. We can write for the potential drop across the resistor

$$V = \mathcal{E}L \tag{494}$$

where $\mathcal{E}$ is the electric field. The current can be written in terms of the current density j which gives the current per unit area

$$I = Aj \tag{495}$$

Thus we have

$$\mathcal{E}L = (Aj)(\rho \frac{L}{A}) \tag{496}$$

which is

$$j = \frac{1}{\rho} \mathcal{E} \tag{497}$$

We define the conductivity σ as

$$\sigma = \frac{1}{\rho} \tag{498}$$

which gives

$$j = \sigma \mathcal{E} \tag{499}$$

For simple cases, j will have the same direction as $\mathcal{E}$. Thus we can write

$$\vec{j} = \sigma \vec{\mathcal{E}} \tag{500}$$

But more generally, the two vectors will be proportional, but not necessarily in the same direction. This can happen if there is a magnetic field, since the magnetic field will try to drive the electrons sideways as they move forward along the direction of $\mathcal{E}$. Thus we write

$$j_i = \sum_j \sigma_{ij} \mathcal{E}_j \tag{501}$$

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Thinking of σ_{ij} as a matrix $\hat{\sigma}$, we can write this as

$$\vec{j} = \hat{\sigma}\vec{\mathcal{E}} \tag{502}$$

The resistivity is defined as

$$\hat{\rho} = \hat{\sigma}^{-1} \tag{503}$$

so we have

$$\vec{\mathcal{E}} = \hat{\rho}\vec{j} \tag{504}$$

25.2   The physics of conductivity

The force on a charge q is

$$\vec{F} = q\vec{\mathcal{E}} + q\vec{v} \times \vec{B} \tag{505}$$

Suppose first that we have $B = 0$. In a constant electric field, it would seem that electrons will continue to speed up with time. But these electrons collide with the ions in the material, and after every collision we can assume that their velocity gets set back to zero. Between collisions, we have

$$m\frac{dv}{dt} = q\mathcal{E}, \quad v = \frac{q\mathcal{E}t}{m} \tag{506}$$

Let the time between collisions be τ. The maximum velocity will be

$$v_{max} = \frac{q\mathcal{E}\tau}{m} \tag{507}$$

and the average velocity will be

$$v_{av} = \frac{q\mathcal{E}\tau}{2m} \tag{508}$$

The current density is then

$$j = qnv_{av} = \frac{q^2 n\mathcal{E}\tau}{2m} \tag{509}$$

where n is the number density of charges. We thus get

$$\sigma = \frac{q^2 n\tau}{2m} \tag{510}$$

We can write the effect of the collisions as an effective force F_{eff}. This force applies a momentum change

$$\Delta p = -mv_{max} = -m\frac{q\mathcal{E}\tau}{m} = -q\mathcal{E}\tau \tag{511}$$

after every interval τ. Thus the average force is

$$F_{av} = \frac{\Delta p}{\tau} = -q\mathcal{E} \tag{512}$$

This is as expected; the average frictional force from collisions has to cancel the force from the electric field.

Now let us do this more abstractly, so that we can use this when a magnetic field is also present. The frictional force changes the velocity from v_{max} to zero after every time interval τ. Thus

$$|f| \propto \frac{mv_{max}}{\tau} \tag{513}$$

Since $v_{max} \propto v_{av}$, we can write

$$\vec{f} = -\frac{cm\vec{v}_{av}}{\tau} \tag{514}$$

where c is a constant of order unity. If the collisions happen very frequently (i.e., τ is small) then we can write $v_{av} = v$ where v is the velocity of the particle. Then we have

$$\vec{f} = -\frac{cm\vec{v}}{\tau} \tag{515}$$

Since τ is not a very precisely defined quantity, we can redefine $\frac{c}{\tau} \to \tau$, which gives $c = 1$ and

$$\vec{f} = -\frac{m\vec{v}}{\tau} \tag{516}$$

Now consider the charge in a region with both electric and magnetic fields. We have

$$m\frac{d\vec{v}}{dt} = q\vec{\mathcal{E}} + q\vec{v} \times \vec{B} - \frac{m}{\tau}\vec{v} \tag{517}$$

In steady state, we will have

$$\frac{d\vec{v}}{dt} = 0 \tag{518}$$

Then we get

$$q\vec{\mathcal{E}} + q\vec{v} \times \vec{B} - \frac{m}{\tau}\vec{v} = 0 \tag{519}$$

Let us assume that we are in a 2-d plane $x - y$ and

$$\vec{\mathcal{E}} = \mathcal{E}\hat{x}, \vec{B} = B\hat{z} \tag{520}$$

Then

$$q\mathcal{E}_x + qv_yB - \frac{m}{\tau}v_x = 0 \tag{521}$$

$$q\mathcal{E}_y - qv_xB - \frac{m}{\tau}v_y = 0 \tag{522}$$

Thus

$$\begin{pmatrix} -\frac{m}{\tau} & qB \\ -qB & -\frac{m}{\tau} \end{pmatrix} \begin{pmatrix} v_x \\ v_y \end{pmatrix} = \begin{pmatrix} -q\mathcal{E}_x \\ -q\mathcal{E}_y \end{pmatrix} \tag{523}$$

The current density is

$$\vec{j} = qn\vec{v} \tag{524}$$

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Thus

$$\begin{pmatrix} \frac{m}{\tau} & -qB \\ qB & \frac{m}{\tau} \end{pmatrix} \begin{pmatrix} j_x \\ j_y \end{pmatrix} = \begin{pmatrix} q^2 n \mathcal{E}_x \\ q^2 n \mathcal{E}_y \end{pmatrix} \tag{525}$$

which is

$$\frac{1}{q^2 n} \begin{pmatrix} \frac{m}{\tau} & -qB \\ qB & \frac{m}{\tau} \end{pmatrix} \begin{pmatrix} j_x \\ j_y \end{pmatrix} = \begin{pmatrix} \mathcal{E}_x \\ \mathcal{E}_y \end{pmatrix} \tag{526}$$

Thus

$$\hat{\rho} = \frac{1}{q^2 n} \begin{pmatrix} \frac{m}{\tau} & -qB \\ qB & \frac{m}{\tau} \end{pmatrix} \tag{527}$$

$$\hat{\sigma} = \frac{q^2 n}{(\frac{m}{\tau})^2 + q^2 B^2} \begin{pmatrix} \frac{m}{\tau} & qB \\ -qB & \frac{m}{\tau} \end{pmatrix} \tag{528}$$

We note that

$$\rho_{xy} = -\frac{B}{qn} = \frac{B}{en} \tag{529}$$

is independent of τ. (In the second step we have replaced $q = -e$.)

With quantum effects, we had seen that if we fill the lowest Landau level

$$n = \frac{eB}{h} \tag{530}$$

Thus

$$\rho_{xy} = \frac{h}{e^2} \tag{531}$$

If we fill ν Landau levels, then

$$n = \frac{eB}{h} \nu \tag{532}$$

and

$$\rho_{xy} = \frac{h}{e^2} \frac{1}{\nu} \tag{533}$$

We have

$$B = \frac{n}{\nu} \frac{h}{e} \tag{534}$$

Here n is the number density, so it has units of $(Area)^{-1}$. Thus $\frac{h}{e}$ has units of $B \times Area$, which are the units of flux. We define the basic flux quantum as

$$\Phi_0 = \frac{h}{e} \tag{535}$$

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26 Time dependent perturbation theory

Let the Hamiltonian be

$$\hat{H} = \hat{H}_0 + \lambda V(t) \tag{536}$$

We define

$$\hat{H}_0|\phi_k\rangle = E_k|\phi_k\rangle \tag{537}$$

The Schrodinger equation is

$$i\hbar\partial_t|\psi(t)\rangle = (\hat{H}_0 + \lambda V(t))|\psi(t)\rangle \tag{538}$$

We expand

$$|\psi(t)\rangle = \sum_k c_k(t)e^{-i\frac{E_k}{\hbar}t}|\phi_k\rangle \tag{539}$$

Then

$$i\hbar\sum_k \dot{c}_k(t)e^{-i\frac{E_k}{\hbar}t}|\phi_k\rangle + \sum_k c_k(t)E_k e^{-i\frac{E_k}{\hbar}t}|\phi_k\rangle = \sum_k c_k(t)E_k e^{-i\frac{E_k}{\hbar}t}|\phi_k\rangle + \lambda\sum_k c_k(t)V(t)e^{-i\frac{E_k}{\hbar}t}|\phi_k\rangle \tag{540}$$

$$i\hbar\sum_k \dot{c}_k(t)e^{-i\frac{E_k}{\hbar}t}|\phi_k\rangle = \lambda\sum_k c_k(t)V(t)e^{-i\frac{E_k}{\hbar}t}|\phi_k\rangle \tag{541}$$

We take the inner product with $\langle\phi_l|$ on each side. This gives

$$i\hbar\dot{c}_l(t)e^{-i\frac{E_l}{\hbar}t} = \lambda\sum_k c_k(t)e^{-i\frac{E_k}{\hbar}t}\langle\phi_l|V(t)|\phi_k\rangle \tag{542}$$

$$\dot{c}_l(t) = -\frac{i}{\hbar}\lambda\sum_k c_k(t)e^{-i\frac{(E_k-E_l)}{\hbar}t}\langle\phi_l|V(t)|\phi_k\rangle \tag{543}$$

Thus

$$c_l(t) = c_l(0) - \frac{i}{\hbar}\lambda\sum_k \int_{t'=0}^{t} dt' c_k(t')e^{-i\frac{(E_k-E_l)}{\hbar}t'}\langle\phi_l|V(t')|\phi_k\rangle \tag{544}$$

This is all exact, but since we have $c_n(t)$ on both sides we cannot solve this equation. Thus we insert

$$c_k(t) \rightarrow c_k(0) \tag{545}$$

on the RHS, Then we get

$$c_l(t) = c_l(0) - \frac{i}{\hbar}\lambda\sum_k \int_{t'=0}^{t} dt' c_k(0)e^{-i\frac{(E_k-E_l)}{\hbar}t'}\langle\phi_l|V(t')|\phi_k\rangle \tag{546}$$

$$c_l(t) = c_l(0) - \frac{i}{\hbar}\lambda\sum_k c_k(0)\int_{t'=0}^{t} dt' e^{-i\frac{(E_k-E_l)}{\hbar}t'}\langle\phi_l|V(t')|\phi_k\rangle \tag{547}$$

26.1 Harmonic oscillator with a time-dependent frequency

We write
$$\omega^2(t) = \omega_0^2 + \lambda q(t) \tag{548}$$

We have
$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2(t)\hat{x}^2 = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2 + \frac{1}{2}m\lambda q(t)\hat{x}^2 \tag{549}$$

Thus
$$V(t) = \frac{1}{2}mq(t)\hat{x}^2 \tag{550}$$

We have
$$|\phi_k\rangle = \frac{1}{\sqrt{k!}}(\hat{A}^\dagger)^k|0\rangle \tag{551}$$

We also have
$$A = \sqrt{\frac{m\omega}{2\hbar}}x + i\frac{1}{\sqrt{2m\omega\hbar}}p \tag{552}$$

$$A^\dagger = \sqrt{\frac{m\omega}{2\hbar}}x - i\frac{1}{\sqrt{2m\omega\hbar}}p \tag{553}$$

Thus
$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{A} + \hat{A}^\dagger) \tag{554}$$

$$\hat{x}^2 = \frac{\hbar}{2m\omega}(\hat{A} + \hat{A}^\dagger)^2 \tag{555}$$

Thus
$$V(t) = \frac{1}{2}mq(t)\frac{\hbar}{2m\omega}(\hat{A} + \hat{A}^\dagger)^2 = q(t)\frac{\hbar}{4\omega}(\hat{A} + \hat{A}^\dagger)^2 \tag{556}$$

Thus we get
$$\langle\phi_l|V(t)|\phi_k\rangle = q(t)\frac{\hbar}{4\omega}\frac{1}{\sqrt{l!}}\frac{1}{\sqrt{k!}}\langle 0|\hat{A}^l(\hat{A} + \hat{A}^\dagger)^2(\hat{A}^\dagger)^k|0\rangle \tag{557}$$

For a given l, we have three possibilities:

(i) $k = l + 2$. Then we have
$$\langle 0|\hat{A}^l(\hat{A} + \hat{A}^\dagger)^2(\hat{A}^\dagger)^k|0\rangle = \langle 0|\hat{A}^l(\hat{A})^2(\hat{A}^\dagger)^{l+2}|0\rangle \tag{558}$$

$$= \langle 0|\hat{A}^{l+2}(\hat{A}^\dagger)^{l+2}|0\rangle = (l+2)! \tag{559}$$

(ii) $k = l$. Then we have
$$\langle 0|\hat{A}^l(\hat{A} + \hat{A}^\dagger)^2(\hat{A}^\dagger)^k|0\rangle = \langle 0|\hat{A}^l(\hat{A}\hat{A}^\dagger + \hat{A}^\dagger\hat{A})^2(\hat{A}^\dagger)^l|0\rangle = \langle 0|\hat{A}^l(2\hat{A}\hat{A}^\dagger - 1)^2(\hat{A}^\dagger)^l|0\rangle \tag{560}$$

$$= 2\langle 0|\hat{A}^{l+1}(\hat{A}^\dagger)^{l+1}|0\rangle - \langle 0|\hat{A}^l(\hat{A}^\dagger)^l|0\rangle = 2(l+1)! - l! = [2(l+1)-1]l! = (2l+1)l! \quad (561)$$

(iii) $k = l - 2$. This needs $l \geq 2$. Then we have

$$\langle 0|\hat{A}^l(\hat{A} + \hat{A}^\dagger)^2(\hat{A}^\dagger)^k|0\rangle = \langle 0|\hat{A}^l(\hat{A}^\dagger)^2(\hat{A}^\dagger)^{l-2}|0\rangle \quad (562)$$

$$= \langle 0|\hat{A}^l(\hat{A}^\dagger)^l|0\rangle = l! \quad (563)$$

We have

$$E_k = (k + \frac{1}{2})\hbar\omega \quad (564)$$

(i) $k = l + 2$:

$$\int_{t'=0}^t dt' e^{-i\frac{(E_k - E_l)}{\hbar}t'}\langle\phi_l|V(t')|\phi_k\rangle = \int_{t'=0}^t dt' e^{-2i\omega t'}q(t')\frac{\hbar}{4\omega}\frac{1}{\sqrt{l!}}\frac{1}{\sqrt{(l+2)!}}(l+2)! \quad (565)$$

$$= \frac{\hbar}{4\omega}\sqrt{(l+2)(l+1)}\int_{t'=0}^t dt' e^{-2i\omega t'}q(t') \quad (566)$$

(ii) $k = l$:

$$\int_{t'=0}^t dt' e^{-i\frac{(E_k - E_l)}{\hbar}t'}\langle\phi_l|V(t')|\phi_k\rangle = \int_{t'=0}^t dt' q(t')\frac{\hbar}{4\omega}\frac{1}{\sqrt{l!}}\frac{1}{\sqrt{l!}}(2l+1)l! \quad (567)$$

$$= \frac{\hbar}{4\omega}(2l+1)\int_{t'=0}^t dt' q(t') \quad (568)$$

(i) $k = l - 2$:

$$\int_{t'=0}^t dt' e^{-i\frac{(E_k - E_l)}{\hbar}t'}\langle\phi_l|V(t')|\phi_k\rangle = \int_{t'=0}^t dt' e^{2i\omega t'}q(t')\frac{\hbar}{4\omega}\frac{1}{\sqrt{l!}}\frac{1}{\sqrt{(l-2)!}}l! \quad (569)$$

$$= \frac{\hbar}{4\omega}\sqrt{l(l-1)}\int_{t'=0}^t dt' e^{2i\omega t'}q(t') \quad (570)$$

27 The Fermi Golden Rule

27.1 The 2-level system

Consider a 2-level system

$$i\hbar\partial_t\psi = \alpha\sigma_1\psi \tag{571}$$

Suppose we start with the state $|\psi_+\rangle = (1,0)$. Then we see that

$$\partial_t\psi = -\frac{i}{\hbar}\sigma_1|\psi_+\rangle = -\frac{i}{\hbar}|\psi_-\rangle \tag{572}$$

But since the Hamiltonian is Hermitian, we will oscillate between these two states. To see this, we look at the eigenstates

$$|\psi_+\rangle = \frac{1}{\sqrt{2}}(1,1), \quad |\psi_-\rangle = \frac{1}{\sqrt{2}}(1,-1), \quad |\psi_i\rangle = (1,0) = \frac{1}{\sqrt{2}}\left(|\psi_+\rangle + |\psi_-\rangle\right) \tag{573}$$

The eigenvalues of the Hamiltonian are

$$E_+ = \alpha, \quad E_- = -\alpha \tag{574}$$

Thus the state at any later time is

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}}\left(e^{-\frac{i}{\hbar}\alpha t}|\psi_+\rangle + e^{\frac{i}{\hbar}\alpha t}|\psi_-\rangle\right) \tag{575}$$

In particular, at

$$\frac{\alpha}{\hbar}t = 2n\pi \tag{576}$$

the state returns to its initial form $|\psi_+\rangle$.

27.2 The exponential

We have

$$i\hbar\partial_t\Psi = H\Psi \tag{577}$$

Thus

$$\partial_t\Psi = -\frac{i}{\hbar}H\Psi \tag{578}$$

If H is time independent, we get

$$\Psi(t) = e^{-\frac{i}{\hbar}Ht}\Psi(0) \tag{579}$$

We can break this into steps

$$e^{-\frac{i}{\hbar}Ht} = e^{-\frac{i}{\hbar}H\Delta t}e^{-\frac{i}{\hbar}H\Delta t}\ldots e^{-\frac{i}{\hbar}H\Delta t} \tag{580}$$

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Suppose we have

$$H = H_0 + H_1 \tag{581}$$

with H_1 small. Then we have at first order

$$e^{-\frac{i}{\hbar}Ht} = e^{-\frac{i}{\hbar}H_0\Delta t}(1 - \frac{i}{\hbar}H_1\Delta t)e^{-\frac{i}{\hbar}H_0\Delta t}\ldots e^{-\frac{i}{\hbar}H_0\Delta t} \tag{582}$$

The first order term is

$$e^{-\frac{i}{\hbar}H_0(t-t')}(-\frac{i}{\hbar}H_1\Delta t)e^{-\frac{i}{\hbar}H_0t'} = e^{-\frac{i}{\hbar}H_0(t-t')}(-\frac{i}{\hbar}H_1dt')e^{-\frac{i}{\hbar}H_0t'} \tag{583}$$

Suppose this acts on a state with energy E_1 and transitions it to a state with energy E_2. Then we have

$$e^{-\frac{i}{\hbar}E_2(t-t')}(-\frac{i}{\hbar}H_1\Delta t)e^{-\frac{i}{\hbar}H_0t'} = e^{-\frac{i}{\hbar}H_0(t-t')}(-\frac{i}{\hbar}\langle\psi_2|H_1\psi_1\rangle dt')e^{-\frac{i}{\hbar}E_1t'} \tag{584}$$

The amplitude in state $|\psi_2\rangle$ at time t is

$$\tilde{c}(t) = \int_{t'=0}^{t} e^{-\frac{i}{\hbar}H_0(t-t')}(-\frac{i}{\hbar}\langle\psi_2|H_1|\psi_1\rangle dt')e^{-\frac{i}{\hbar}E_1t'} \tag{585}$$

27.3   Transition to a band

But in a special case we can have a behavior where the amplitude in an initial state leaves and does not come back, at least for very large times. Suppose e start in a state with energy E_0. Consider a band of states $|\psi_n\rangle$ with energies E_n. Let the amplitude to transition, per unit time, into the state $|\psi_n\rangle$ be $-\frac{i}{\hbar}R_n$; thus the amplitude to transition back per unit time will be $-\frac{i}{\hbar}R_n^*$. Then the amplitude in state $|\psi_n\rangle$ at time t is

$$\tilde{c}_n(t) = \int_{t'=0}^{t} e^{-i\frac{E_0}{\hbar}t'}(-\frac{i}{\hbar}R_n dt')e^{-i\frac{E_n}{\hbar}(t-t')} = -\frac{i}{\hbar}R_n e^{-i\frac{E_n}{\hbar}t}\int_{t'=0}^{t} dt' e^{\frac{i(E_n-E_0)}{\hbar}t'} \tag{586}$$

This gives

$$\begin{aligned}
\tilde{c}_n(t) &= -\frac{i}{\hbar}R_n e^{-i\frac{E_n}{\hbar}t}\frac{\hbar}{i(E_n-E_0)}(e^{\frac{i(E_n-E_0)}{\hbar}t} - 1) \\
&= -\frac{i}{\hbar}R_n e^{-\frac{1}{2}i\frac{(E_n+E_0)}{\hbar}t}\frac{\hbar}{i(E_n-E_0)}2i\sin\frac{(E_n-E_0)t}{2\hbar} \\
&= -R_n e^{-\frac{1}{2}i\frac{(E_n+E_0)}{\hbar}t}\left(\frac{\sin\frac{(E_n-E_0)t}{2\hbar}}{\frac{(E_n-E_0)}{2\hbar}}\right) \tag{587}
\end{aligned}$$

The probability at time t is

$$P_n(t) = |R_n|^2\left(\frac{\sin\frac{(E_n-E_0)t}{2\hbar}}{\frac{(E_n-E_0)}{2\hbar}}\right)^2 \tag{588}$$

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Let the level spacing be Δ. Then we have

$$\sum_n \rightarrow \frac{1}{\Delta} \int dE \tag{589}$$

Let us also assume that $R_n \approx R$ in the range of interest. Then we get

$$
\begin{aligned}
P(t) = \sum_n P_n(t) \;\; &\rightarrow \;\; \frac{|R|^2}{\Delta} \int dE \left(\frac{\sin \frac{(E-E_0)t}{2\hbar}}{\frac{(E-E_0)}{2\hbar}} \right)^2 \\
&= \;\; \frac{2\hbar |R|^2 t}{\Delta} \int d\left(\frac{(E-E_0)t}{2\hbar} \right) \left(\frac{\sin \frac{(E-E_0)t}{2\hbar}}{\frac{(E-E_0)t}{2\hbar}} \right)^2
\end{aligned}
\tag{590}
$$

We have

$$\int dx \frac{\sin^2 x}{x^2} = \pi \tag{591}$$

Thus

$$\frac{P(t)}{t} = \frac{2\pi\hbar |R|^2}{\Delta} = 2\pi\hbar |R|^2 \rho \tag{592}$$

where

$$\rho = \frac{1}{\Delta} \tag{593}$$

is the number of energy levels per unit interval in energy; i.e., the level density.

27.4 Delta functions

We have

$$\int dx \frac{\sin^2 x}{x^2} = \pi \tag{594}$$

Thus we can say that

$$\frac{1}{\pi} \frac{\sin^2 x}{x^2} \tag{595}$$

acts like a bump-function with integral unity, and width $\Delta x \sim 1$. We then have

$$\frac{1}{\pi} \frac{\sin^2(xt)}{(xt)^2} \sim \delta(xt) \sim \frac{1}{t} \delta(x) \tag{596}$$

Thus

$$\frac{1}{\pi} \frac{\sin^2(xt)}{(x)^2} = \frac{1}{\pi} t^2 \frac{\sin^2(xt)}{(xt)^2} = t\delta(x) \tag{597}$$

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and

$$\frac{\sin^2(xt)}{(x)^2} = \pi t \delta(x) \tag{598}$$

Thus we can write

$$P(t) = \sum_{states} |R_n|^2 \left(\frac{\sin \frac{(E-E_0)t}{2\hbar}}{\frac{(E-E_0)}{2\hbar}} \right)^2 = \sum_{states} |R_n|^2 \pi t \delta(\frac{(E-E_0)}{2\hbar}) = \sum_{states} |R_n|^2 2\pi\hbar t \delta(E-E_0) \tag{599}$$

With

$$\sum_{states} = \rho \int dE \tag{600}$$

and

$$R_n \to R \tag{601}$$

we get

$$P(t) = \int dE \rho |R|^2 2\pi\hbar t \delta(E-E_0) \tag{602}$$

$$\frac{P(t)}{t} = 2\pi\hbar |R|^2 \rho \int dE \delta(E-E_0) = 2\pi\hbar |R|^2 \rho \tag{603}$$

More generally, we have

$$\sum_{states} = \sum_{\vec{k}} = \frac{V}{(2\pi)^2} \int d^3k = \frac{V}{(2\pi\hbar)^3} \int d^3p \tag{604}$$

28   Summary of perturbation methods

28.1   Time independent perturbation theory, eigenvalue method

In the time independent case we had (nondegenerate case)

$$H = H^{(0)} + \lambda H^{(1)} \tag{605}$$

We find

$$E^{(1)} = \langle \psi_{k_0}^{(0)} | H^{(1)} | \psi_{k_0}^{(0)} \rangle \tag{606}$$

$$C_k = \frac{\langle \psi_k^{(0)} | H^{(1)} | \psi_{k_0}^{(0)} \rangle}{(E_{k_0}^{(0)} - E_k^{(0)})}, \qquad k \neq k_0 \tag{607}$$

We had to be careful to diagonalize $\hat{H}^{(1)}$ in the degenerate case.

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28.2 Time dependent perturbation theory, evolution computation

We take

$$\hat{H} = \hat{H}_0 + \lambda V(t) \tag{608}$$

$$|\psi(t)\rangle = \sum_k \tilde{c}_k(t)|\phi_k\rangle = \sum_k c_k(t) e^{-i\frac{E_k}{\hbar}t}|\phi_k\rangle \tag{609}$$

$$c_l(t) = c_l(0) - \frac{i}{\hbar}\lambda \sum_k c_k(0) \int_{t'=0}^{t} dt' e^{-i\frac{(E_k - E_l)}{\hbar}t'} \langle\phi_l|V(t')|\phi_k\rangle \tag{610}$$

As a special case, we can take a slow evolution from the time independent problem $\hat{H} = \hat{H}^{(0)}$ to the new time independent case $\hat{H} = \hat{H}^{(0)} + \lambda V$. Then we get the adiabatic theorem, that the energy eigenstate $|\psi_k\rangle_0$ of the initial Hamiltonian changes to the corresponding eigenstate $|\psi_k\rangle_\lambda$ of the final Hamiltonian.

28.3 Both time-independent and time-dependent cases, expanding exponential

We have

$$e^{-\frac{i}{\hbar}Ht} = e^{-\frac{i}{\hbar}H\Delta t}e^{-\frac{i}{\hbar}H\Delta t}\ldots e^{-\frac{i}{\hbar}H\Delta t} \tag{611}$$

The first order term from an interval Δt is

$$e^{-\frac{i}{\hbar}H_0(t-t')}(-\frac{i}{\hbar}\lambda H_1\Delta t)e^{-\frac{i}{\hbar}H_0 t'} = e^{-\frac{i}{\hbar}H_0(t-t')}(-\frac{i}{\hbar}\lambda H_1 dt')e^{-\frac{i}{\hbar}H_0 t'} \tag{612}$$

Suppose we start with energy E_1 and take the inner product with a state with energy E_2. Then we get that the amplitude in state $|\psi_2\rangle$ at time t is

$$\tilde{c}(t) = \int_{t'=0}^{t} e^{-\frac{i}{\hbar}E_2(t-t')}(-\frac{i}{\hbar}\langle\psi_2|H_1|\psi_1\rangle dt')e^{-\frac{i}{\hbar}E_1 t'} = -\frac{i}{\hbar}e^{-\frac{i}{\hbar}E_2 t}\int_{t'=0}^{t} dt' \langle\psi_2|H_1|\psi_1\rangle e^{\frac{i}{\hbar}(E_2 - E_1)t'} \tag{613}$$

If $H^{(1)} = V$ is time-independent, then we get

$$\tilde{c}(t) = -\frac{i}{\hbar}\langle\psi_2|H_1|\psi_1\rangle e^{-\frac{i}{\hbar}E_2 t}\int_{t'=0}^{t} dt' e^{\frac{i}{\hbar}(E_2 - E_1)t'} \tag{614}$$

28.4 Summary of the Ferni-Golden rule analysis

(i) First we assume that there is evolution under H_0 from $t = 0$ to $t = t'$. Then in a time interval dt' we have the action of H_1. Then from $t' + dt'$ to t, we have evolution under H_0 again.

(ii) We assume that

$$\langle\psi_k|H_1|\psi_0\rangle = R_k \tag{615}$$

$$\langle \psi_0 | H_1 | \psi_0 \rangle = 0 \tag{616}$$

so the Hamiltonian makes transitions from $|\psi_0\rangle$ to the band $|\psi_k\rangle$.

(iii) This gives for the first order term

$$|\psi(t)\rangle = \int_{t'=0}^{t} e^{-\frac{i}{\hbar}H_0(t-t')}(-\frac{i}{\hbar}dt' H_1)e^{-\frac{i}{\hbar}H_0 t'}|\psi_0\rangle \tag{617}$$

(iv) We write

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}E_0 t}|\psi_0\rangle + \sum_k \tilde{c}_k(t)|\psi_k\rangle \tag{618}$$

We take the inner product with $\langle \psi_k |$. This gives

$$\tilde{c}_k(t) = \langle \psi_k | \int_{t'=0}^{t} e^{-\frac{i}{\hbar}H_0(t-t')}(-\frac{i}{\hbar}dt' H_1)e^{-\frac{i}{\hbar}H_0 t'}|\psi_0\rangle \tag{619}$$

$$\tilde{c}_k(t) = \langle \psi_k | \int_{t'=0}^{t} e^{-\frac{i}{\hbar}E_k(t-t')}(-\frac{i}{\hbar}dt' H_1)e^{-\frac{i}{\hbar}E_0 t'}|\psi_0\rangle \tag{620}$$

$$\tilde{c}_k(t) = -\frac{i}{\hbar} \int_{t'=0}^{t} dt' e^{-\frac{i}{\hbar}E_k(t-t')} \langle \psi_k | H_1(t')|\psi_0\rangle e^{-\frac{i}{\hbar}E_0 t'} \tag{621}$$

(v) In the time independent case we write

$$\langle \psi_k | H_1 | \psi_0 \rangle \equiv R_k \tag{622}$$

$$\tilde{c}_k(t) = -\frac{i}{\hbar} R_k \int_{t'=0}^{t} dt' e^{-\frac{i}{\hbar}E_k(t-t')} e^{-\frac{i}{\hbar}E_0 t'} \tag{623}$$

$$\tilde{c}_k(t) = -\frac{i}{\hbar} R_k e^{-\frac{i}{\hbar}E_k t} \int_{t'=0}^{t} dt' e^{\frac{i}{\hbar}(E_k - E_0)t'} \tag{624}$$

$$\tilde{c}_k(t) = -\frac{i}{\hbar} R_k e^{-\frac{1}{2}i\frac{(E_k + E_0)}{\hbar}t} \left(\frac{\sin \frac{(E_k - E_0)t}{2\hbar}}{\frac{(E_k - E_0)}{2\hbar}} \right) \tag{625}$$

(vi) The probability at time t is

$$P_k(t) = \frac{1}{\hbar^2}|R_k|^2 \left(\frac{\sin \frac{(E_k - E_0)t}{2\hbar}}{\frac{(E_k - E_0)}{2\hbar}} \right)^2 \tag{626}$$

This oscillates with time.

(vii) Let the level spacing be Δ. Then we have

$$\sum_k \rightarrow \frac{1}{\Delta} \int dE \tag{627}$$

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Let us also assume that $R_k \approx R$ in the range of interest. Then we get

$$P(t) = \sum_k P_k(t) \quad \rightarrow \quad \frac{|R|^2}{\hbar^2 \Delta} \int dE \left(\frac{\sin \frac{(E-E_0)t}{2\hbar}}{\frac{(E-E_0)}{2\hbar}} \right)^2$$

$$= \frac{2|R|^2 t}{\hbar \Delta} \int d\left(\frac{(E-E_0)t}{2\hbar} \right) \left(\frac{\sin \frac{(E-E_0)t}{2\hbar}}{\frac{(E-E_0)t}{2\hbar}} \right)^2 \tag{628}$$

We have

$$\int dx \frac{\sin^2 x}{x^2} = \pi \tag{629}$$

Thus

$$\frac{P(t)}{t} = \frac{2\pi}{\hbar} \frac{|R|^2}{\Delta} = \frac{2\pi}{\hbar} |R|^2 \rho \tag{630}$$

where

$$\rho = \frac{1}{\Delta} \tag{631}$$

is the number of energy levels per unit interval in energy; i.e., the level density.

(viii) We find

$$\frac{\sin^2(xt)}{(x)^2} = \pi t \delta(x) \tag{632}$$

(ix) Thus we can write

$$P(t) = \sum_{states} \frac{1}{\hbar^2} |R_k|^2 \left(\frac{\sin \frac{(E-E_0)t}{2\hbar}}{\frac{(E-E_0)}{2\hbar}} \right)^2 = \sum_{states} \frac{1}{\hbar^2} |R_k|^2 \pi t \delta(\frac{(E-E_0)}{2\hbar}) = \sum_{states} |R_k|^2 \frac{2\pi}{\hbar} t \delta(E-E_0) \tag{633}$$

With

$$\sum_{states} = \rho \int dE \tag{634}$$

and

$$R_k \rightarrow R \tag{635}$$

we get

$$P(t) = \int dE \rho |R|^2 \frac{2\pi}{\hbar} t \delta(E-E_0) \tag{636}$$

$$\frac{P(t)}{t} = \frac{2\pi |R|^2 \rho}{\hbar} \int dE \delta(E-E_0) = \frac{2\pi}{\hbar} |R|^2 \rho \tag{637}$$

(x) More generally, we have

$$\sum_{states} = \sum_{\vec{k}} = \frac{V}{(2\pi)^2} \int d^3k = \frac{V}{(2\pi\hbar)^3} \int d^3p \tag{638}$$

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29 Scattering

29.1 The classical problem

We have a scatterer, and a beam of particles incident on it. The beam is described by a flux F. We have

$$F = nv \tag{639}$$

where n is the number density of particles in the beam, and v is their velocity. The flux F gives the number of particles crossing a unit transverse area per unit time.

We define the cross section σ as the area which is cut out from this beam and scattered in different directions. We cannot usually directly look at the scatter itself, as it is small. Thus to find σ we will look at the particles that are scattered. Imagine a large sphere of radius R. The particles will be leaving normal to the surface of this sphere. Suppose that N particles are crossing this sphere per unit time. Then N particles must have been cut out from the beam per unit time. We have

$$N = F\sigma \tag{640}$$

Thus we get

$$\sigma = \frac{N}{F} \tag{641}$$

where N is the number of particles scattered per unit time and F is the flux.

We can also compute the cross section for scattering into some given solid angle. For a circle on a 2-d plane, we define the angle in radians as

$$\theta = \frac{s}{R} \tag{642}$$

where s is the arc length and R is the radius. Similarly, in 3-d we define the solid angle in steradians as

$$\Omega = \frac{A}{R^2} \tag{643}$$

where A is the area on the surface of the sphere and R is the radius. Infinitesimal solid angles will be denoted $d\Omega$. If dN are the particles scattered in an infinitesimal solid angle $d\Omega$ per unit time, then we define

$$d\sigma = \frac{dN}{F} \tag{644}$$

and we write

$$\frac{d\sigma}{d\Omega} = \frac{1}{F}\frac{dN}{d\Omega} \tag{645}$$

where $\frac{dN}{d\Omega}$ is the number of particle scattered per unit solid angle in the given direction.

29.2 The set-up

We take a cubical box of size L on each axis. Thus the total volume is

$$V = L^3 \tag{646}$$

We assume periodic boundary conditions on the box. The leading order Hamiltonian is that of a particle of mass m.

$$H_0 = \frac{\vec{\hat{p}}^2}{2m} \tag{647}$$

We have a potential $\lambda V(\vec{r})$ localized somewhere in this box, where λ is small. We start with a wavefunction

$$|\psi_i\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \tag{648}$$

We take a final wavefunction of the form

$$|\psi_f\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}'\cdot\vec{r}} \tag{649}$$

The energies under H_0 of the initial wavefunction is

$$E_0 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \tag{650}$$

29.3 Flux

We have

$$\vec{F} = \frac{\hbar}{2im}\left(\psi^*(x)\vec{\nabla}\psi(x) - (\vec{\nabla}\psi^*(x))\psi(x)\right) = \frac{\hbar}{2im}(\frac{1}{V}2i\vec{k}) = \frac{\hbar\vec{k}}{Vm} \tag{651}$$

This agrees with the classical intuition

$$F = nv = \frac{1}{V}\frac{p}{m} = \frac{\hbar k}{Vm} \tag{652}$$

29.4 Fermi-Golden rule

Now we have to find the analogue of N, the number of particles scattered per unit time. The probability $P(t)$ tells us how many particle shave entered one of the scattered states after time t. So the number of particles scattering per unit time is

$$N = \frac{P(t)}{t} \tag{653}$$

The fermi golden rule says that

$$P(t) = \sum_{states} |\tilde{c}_{\vec{k}'}(t)|^2 \rightarrow \int dE \frac{2\pi}{\hbar}\rho\delta(E - E_0)|R|^2 t \tag{654}$$

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Here we could sum over all states $\vec{k}'$, or restrict to those in a certain angular range $d\Omega$:

$$P_{d\Omega}(t) = \sum_{states,d\Omega} |\tilde{c}_{\vec{k}'}(t)|^2 \to \int dE \frac{2\pi}{\hbar} \rho_{d\Omega} \delta(E - E_0)|R|^2 t \tag{655}$$

29.5   Density of states

The density of states is given by the condition

$$k_x = \frac{2\pi n_x}{L}, \quad k_y = \frac{2\pi n_y}{L}, \quad k_z = \frac{2\pi n_z}{L} \tag{656}$$

$$\sum_{states} = \sum_{\vec{n}} \to \int d^3 n = \frac{L^3}{(2\pi)^3} \int d^3 k = \frac{V d^3 k}{(2\pi)^3} \tag{657}$$

In terms of energy,

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \tag{658}$$

$$dE = \frac{\hbar^2 k}{m} dk, \quad \frac{dE}{dk} = \frac{\hbar^2 k}{m} \tag{659}$$

$$d^3 k = k^2 dk d\Omega = k^2 \frac{dk}{dE} dE d\Omega = k^2 \frac{m}{\hbar^2 k} dE d\Omega = \frac{km}{\hbar^2} dE d\Omega \tag{660}$$

Thus

$$\sum_{states} \to \frac{V d^3 k}{(2\pi)^3} = \frac{V}{(2\pi)^3} \frac{km}{\hbar^2} dE d\Omega \tag{661}$$

We write

$$\sum_{states} = \rho dE \tag{662}$$

and for a given angular range

$$\sum_{states,d\Omega} = \int \rho_{d\Omega} dE \tag{663}$$

We then find

$$\rho_{d\Omega} = \frac{V}{(2\pi)^3} \frac{km}{\hbar^2} d\Omega \tag{664}$$

29.6   The cross section

The cross section is defined by the number of particles that scatter per unit time. Thus this is

$$\sigma = \frac{1}{F}\frac{1}{t} P(t) = \frac{1}{F}\frac{1}{t} \sum_{states} |\tilde{c}_{\vec{k}'}(t)|^2 \tag{665}$$

The Fermi-Golden rule says that

$$\sum_{states} |\tilde{c}_{\vec{k}'}(t)|^2 \rightarrow \frac{2\pi}{\hbar} \int dE \rho \delta(E - E_0)|R|^2 \, t \tag{666}$$

Here we note that in our case R can depend on the angle of scattering θ_s. in our case it does not as the density of states in the box is isotropic. Thus we write

$$\sum_{states} |\tilde{c}_{\vec{k}'}(t)|^2 \rightarrow \frac{2\pi}{\hbar} \int_{E,\theta_s} dE \rho(\theta_s)\delta(E - E_0)|R(\theta_s)|^2 \, t \tag{667}$$

Thus we get

$$\sigma = \frac{1}{F}\frac{1}{t}\sum_{states} |\tilde{c}_{\vec{k}'}(t)|^2 \rightarrow \frac{1}{F}\frac{2\pi}{\hbar} \int_{E,\theta_s} dE \rho(\theta_s)\delta(E - E_0)|R(\theta_s)|^2 \tag{668}$$

If we limit both sides to a small angular direction $d\Omega$, then we write

$$
\begin{aligned}
d\sigma &= \frac{1}{F}\frac{1}{t}P_{d\Omega}(t) = \frac{1}{F}\frac{1}{t}\sum_{states,d\Omega} |\tilde{c}_{\vec{k}'}(t)|^2 \\
&\rightarrow \frac{1}{F}\frac{2\pi}{\hbar} \int_E dE \rho_{d\Omega}(\theta_s)\delta(E - E_0)|R(\theta_s)|^2 \\
&= \frac{1}{F}\frac{2\pi}{\hbar} \rho_{d\Omega}(\theta_s)|R(\theta_s)|^2
\end{aligned}
\tag{669}
$$

Thus we write

$$\frac{d\sigma}{d\Omega} = \frac{1}{F}\frac{2\pi}{\hbar}\frac{d\rho}{d\Omega}(\theta_s)|R(\theta_s)|^2 \tag{670}$$

29.7   Putting it together

We have

$$d\sigma = \frac{1}{F}\frac{1}{t}P_{d\Omega}(t) = \frac{1}{F}\frac{1}{t}\sum_{states,d\Omega} |\tilde{c}_{\vec{k}'}(t)|^2 \tag{671}$$

Using the Fermi Golden rule we get

$$d\sigma \rightarrow \frac{1}{F}\frac{2\pi}{\hbar} \int dE \delta(E - E_0)\rho_{d\Omega}|R|^2 = \frac{1}{F}\frac{2\pi}{\hbar}\rho_{d\Omega}|R|^2 \tag{672}$$

We can use

$$\rho_{d\Omega} = \frac{V}{(2\pi)^3}\frac{km}{\hbar^2}d\Omega \tag{673}$$

This gives

$$d\sigma = \frac{1}{F}\frac{2\pi}{\hbar}\frac{V}{(2\pi)^3}\frac{km}{\hbar^2}d\Omega|R|^2 \qquad (674)$$

This can be written as

$$\frac{d\sigma}{d\Omega} = \frac{1}{F}\frac{2\pi}{\hbar}\frac{V}{(2\pi)^3}\frac{km}{\hbar^2}|R|^2 \qquad (675)$$

We had

$$F = \frac{\hbar k}{Vm} \qquad (676)$$

This gives

$$\frac{d\sigma}{d\Omega} = \frac{Vm}{\hbar k}\frac{2\pi}{\hbar}\frac{V}{(2\pi)^3}\frac{km}{\hbar^2}|R|^2 \qquad (677)$$

29.8   Computing R

We have

$$R = \lambda\langle\psi_{\vec{k}'}|V|\psi_{\vec{k}}\rangle \qquad (678)$$

This gives

$$R = \lambda\int d^3\vec{r}\frac{1}{V}e^{-i\vec{k}'\cdot\vec{r}}V(\vec{r})e^{i\vec{k}\cdot\vec{r}} = \lambda\frac{1}{V}\int d^3\vec{r}e^{i\Delta\vec{k}\cdot\vec{r}}V(\vec{r}) \qquad (679)$$

where

$$\Delta\vec{k} = \vec{k}' - \vec{k} \qquad (680)$$

Thus we see that R has the form

$$R = \frac{\lambda A}{V} \qquad (681)$$

where

$$A = \int d^3\vec{r}e^{-i\Delta\vec{k}\cdot\vec{r}}V(\vec{r}) \qquad (682)$$

We then find that

$$\frac{d\sigma}{d\Omega} = \frac{Vm}{\hbar k}\frac{2\pi}{\hbar}\frac{V}{(2\pi)^3}\frac{km}{\hbar^2}\frac{\lambda^2|A|^2}{V^2} = \frac{\lambda^2 m^2}{(2\pi)^2\hbar^4}|A|^2 \qquad (683)$$

29.9   An example

As an example, we take the Yukawa potential

$$V = \frac{1}{r}e^{-\mu r} \qquad (684)$$

Then we have to compute

$$A = \int d^3\vec{r}e^{-i\Delta\vec{k}\cdot\vec{r}}V(\vec{r}) \qquad (685)$$

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We have, writing the angle through which we scatter as θ_s

$$|\Delta \vec{k}|^2 = |\vec{k}' - \vec{k}|^2 = k'^2 + k^2 - 2k'k\cos\theta_s = 2k^2 - 2k^2\cos\theta_s = 2k^2(1 - \cos\theta_s) = 4k^2\sin^2\frac{\theta_s}{2} \tag{686}$$

Thus

$$|\Delta\vec{k}| = 2k\sin\frac{\theta_s}{2} \tag{687}$$

We have

$$A = \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta \int_0^\infty r^2 dr \frac{1}{r} e^{-\mu r} e^{-i|\Delta\vec{k}|r\cos\theta} \tag{688}$$

This is

$$A = \int_0^{2\pi} d\phi \int_0^1 d(\cos\theta) \int_0^\infty r^2 dr \frac{1}{r} e^{-\mu r} e^{-i|\Delta\vec{k}|r\cos\theta} \tag{689}$$

$$A = 2\pi \int_0^\infty r^2 dr \frac{1}{r} e^{-\mu r} \frac{(e^{-i|\Delta\vec{k}|r} - e^{i|\Delta\vec{k}|r})}{(-i|\Delta\vec{k}|r)} \tag{690}$$

This is

$$A = 2\pi \int_0^\infty r^2 dr \frac{1}{r} e^{-\mu r} \frac{(-2i)\sin|\Delta\vec{k}|r}{(-i|\Delta\vec{k}|r)} = 4\pi \int_0^\infty r^2 dr \frac{1}{r} e^{-\mu r} \frac{\sin|\Delta\vec{k}|r}{(|\Delta\vec{k}|r)} \tag{691}$$

This gives

$$A = \frac{4\pi}{|\Delta\vec{k}|} \int_0^\infty dr e^{-\mu r} \sin|\Delta\vec{k}|r = \frac{4\pi}{|\Delta\vec{k}|} \left(\frac{|\Delta\vec{k}|}{|\Delta\vec{k}|^2 + \mu^2} \right) = \frac{4\pi}{|\Delta\vec{k}|^2 + \mu^2} \tag{692}$$

We had

$$\frac{d\sigma}{d\Omega} = \frac{\lambda^2 m^2}{(2\pi)^2 \hbar^4} |A|^2 \tag{693}$$

This gives

$$\frac{d\sigma}{d\Omega} = \frac{\lambda^2 m^2}{(2\pi)^2 \hbar^4} \frac{(4\pi)^2}{(|\Delta\vec{k}|^2 + \mu^2)^2} = \frac{4\lambda^2 m^2}{\hbar^4} \frac{1}{(|\Delta\vec{k}|^2 + \mu^2)^2} \tag{694}$$

We had

$$|\Delta\vec{k}| = 2k\sin\frac{\theta_s}{2} \tag{695}$$

Using this gives

$$\frac{d\sigma}{d\Omega} = \frac{4\lambda^2 m^2}{\hbar^4} \frac{1}{(4k^2\sin^2\frac{\theta_s}{2} + \mu^2)^2} = 4\lambda^2 m^2 \frac{1}{(4\hbar^2 k^2\sin^2\frac{\theta_s}{2} + \hbar^2\mu^2)^2} \tag{696}$$

We had

$$E_0 = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} \tag{697}$$

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Thus

$$\hbar^2 k^2 = 2mE_0 \tag{698}$$

$$\frac{d\sigma}{d\Omega} = \frac{4\lambda^2 m^2}{(8mE_0 \sin^2 \frac{\theta_s}{2} + \hbar^2 \mu^2)^2} = \frac{\lambda^2}{(4E_0 \sin^2 \frac{\theta_s}{2} + \frac{\hbar^2 \mu^2}{2m})^2} \tag{699}$$

Integrating gives

$$\sigma = \frac{4\pi\lambda^2}{\frac{\hbar^2 \mu^2}{2m}(4E + \frac{\hbar^2 \mu^2}{2m})} \tag{700}$$

30 The photoelectric effect

We have a photon with energy

$$E = h\nu \tag{701}$$

incident on an atom. The atom has an electron in the wavefunction

$$|\psi_i\rangle \rightarrow \psi(r, \theta, \phi) \tag{702}$$

with energy $E_{e,i}$. The photon gets absorbed, and its energy gets transferred to the electron which is ejected. Let the final wavefunction of the electron be

$$|\psi_f\rangle \rightarrow \frac{1}{\sqrt{V}} e^{i\vec{k}_f \cdot \vec{r}} \tag{703}$$

30.1 The photon wavefunction

The photon is a transverse wave, with a polarization given by a unit vector $\vec{\epsilon}$. The transverse nature is given through

$$\vec{\epsilon} \cdot \vec{k}_\gamma = 0 \tag{704}$$

The main thing we need to know is the strength of the $\vec{A}$ field for a single photon. This is given by computing the energy density of the $\vec{E}, \vec{B}$ fields found from $\vec{A}$, multiplying by the volume V, and setting this equal to $\hbar\omega$. We will derive this in the subsection below, but for now we note the result:

$$|\psi_\gamma\rangle \rightarrow \vec{\epsilon} \frac{1}{\sqrt{V}} \sqrt{\frac{\hbar}{2\omega\epsilon_0}} e^{i\vec{k}_\gamma \cdot \vec{r}} \tag{705}$$

The flux is given by noting that we have one particle in volume V, so $\rho = \frac{1}{V}$ and the speed is $v = c$.

$$F = \rho v = \frac{1}{V} c \tag{706}$$

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30.2 Deriving the amplitude of the photon field

For a nonrelativistic particle we had taken a wavefunction of the form

$$|\psi\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{r}} \tag{707}$$

But the photon is a relativistic particle: it moves ta the speed of light. We can still expand it as a plane wave

$$\vec{A} = \sum_{\vec{k}} \left(\vec{A}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} \right) \tag{708}$$

But we have to do more work to see exactly what the coefficient $A_{\vec{k}}$ is. To do this we will use the fact that the energy of the photon should be

$$E_\gamma = h\nu = \hbar\omega \tag{709}$$

To get this energy we will use the fact that for a classical electromagnetic field, the energy density is

$$U = \frac{\epsilon_0}{2} |\vec{E}|^2 + \frac{1}{2\mu_0} |\vec{B}|^2 \tag{710}$$

The fields themselves are given in terms of the vector potential $\vec{A}$ as

$$\vec{B} = \vec{\nabla} \times \vec{A} \tag{711}$$

$$\vec{E} = -\dot{\vec{A}} - \vec{\nabla}\Phi \rightarrow -\dot{\vec{A}} \tag{712}$$

where we have noted that in our situation we have no scalar potential; thus $\Phi = 0$.

First we note that the energy is $E = \hbar\omega$, so the time dependence of the wavefunction must be

$$\vec{A} = \sum_{\vec{k}} \left(\vec{A}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} e^{-i\frac{E}{\hbar}t} \right) = \sum_{\vec{k}} \left(\vec{A}_{\vec{k}}^* e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t} \right) \tag{713}$$

To use the above classical relations, we note that the classical vector potential $\vec{A}$ is real, so we must add in the complex conjugate of the form we had taken above

$$\vec{A} = \sum_{\vec{k}} \left(\vec{A}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} e^{-i\omega t} + \vec{A}_{\vec{k}}^* e^{i\vec{k}\cdot\vec{r}} e^{i\omega t} \right) \tag{714}$$

We consider a given Fourier mode $\vec{k}$ and consider it at time $t = 0$

$$\vec{B} = \vec{\nabla} \times \vec{A} = i\vec{k} \times \vec{A}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} - i\vec{k} \times \vec{A}_{\vec{k}}^* e^{-i\vec{k}\cdot\vec{r}} \tag{715}$$

$$\vec{E} = -\dot{\vec{A}} = i\omega \vec{A}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}} - i\omega \vec{A}_{\vec{k}}^* e^{-i\vec{k}\cdot\vec{r}} \tag{716}$$

We have to compute $|\vec{E}|^2, |\vec{B}|^2$ and integrate over all space, The integration kills all terms that are oscillating as $e^{i\vec{K}\cdot\vec{r}}$ for any $\vec{K}$. This leaves only the terms that come from one factor having $\vec{A}_{\vec{k}}$ and one factor $\vec{A}^*_{\vec{k}}$. We get

$$|\vec{B}|^2 = 2(\vec{k} \times \vec{A}_{\vec{k}}) \cdot (\vec{k} \cdot \vec{A}^*_{\vec{k}} = 2k^2|\vec{A}_{\vec{k}}|^2 \tag{717}$$

where we have used that

$$(\vec{A} \times \vec{B}) \cdot (\vec{C} \times \vec{D}) = (\vec{A} \cdot \vec{C})(\vec{B} \cdot \vec{D}) - (\vec{A} \cdot \vec{D})(\vec{B} \cdot \vec{C}) \tag{718}$$

and the fact that $\vec{A}$ os transverse

$$\vec{k} \cdot \vec{A}_{\vec{k}} = 0 \tag{719}$$

Similarly, we find

$$|\vec{E}|^2 = 2\omega^2|\vec{A}_{\vec{k}}|^2 \tag{720}$$

the energy density is then

$$U = \frac{\epsilon_0}{2}|\vec{E}|^2 + \frac{1}{2\mu_0}|\vec{B}|^2 = \epsilon_0\omega^2|\vec{A}_{\vec{k}}|^2 + \frac{1}{\mu_0}k^2|\vec{A}_{\vec{k}}|^2 \tag{721}$$

We use that

$$\epsilon_0\mu_0 = \frac{1}{c^2}, \quad \omega = ck \tag{722}$$

Then we get

$$U = 2\epsilon_0\omega^2|\vec{A}_{\vec{k}}|^2 \tag{723}$$

We set the total energy to $E = \hbar\omega$

$$E = UV = 2\epsilon_0\omega^2|\vec{A}_{\vec{k}}|^2 V = \hbar\omega \tag{724}$$

which gives

$$|\vec{A}_{\vec{k}}| = \sqrt{\frac{\hbar}{2\epsilon_0\omega V}} \tag{725}$$

30.3 The interaction

The interaction between the electron and a gauge field is given by

$$H = \frac{1}{2m}(\vec{p} + e\vec{A}) \cdot (\vec{p} \cdot \vec{A}) = \frac{1}{2m}\left(p^2 + e\vec{p} \cdot \vec{A} + e\vec{A} \cdot \vec{p} + e^2 A^2\right) \tag{726}$$

We have

$$\vec{p} \cdot \vec{A} = -i\hbar\vec{\nabla} \cdot \vec{A} = -i\hbar(\vec{\nabla} \cdot \vec{A}) + \vec{A} \cdot \vec{p} \tag{727}$$

We have

$$\vec{\nabla} \cdot \vec{A} = \vec{\nabla} \cdot \frac{1}{\sqrt{V}}\vec{\epsilon} \cdot (i\vec{k}_\gamma)e^{i\vec{k}_\gamma \cdot \vec{r}} = 0 \tag{728}$$

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This gives

$$H = \frac{1}{2m}\left(p^2 + e^2 A^2 + 2e\vec{A}\cdot\vec{p}\right) \tag{729}$$

Thus

$$H = H^{(0)} + \lambda H^{(0)} \tag{730}$$

with

$$\lambda = \frac{e}{m}, \quad H^{(1)} = \vec{A}\cdot\vec{p} \tag{731}$$

30.4 The matrix element

We are going from an initial state containing one photon and one electron in a given wavefunction, to a band of states which has one electron in some momentum state. The cross section is then given by the fermi golden rule, for which we need the amplitude

$$R = \lambda\langle\psi_f|\hat{H}^{(1)}|\psi_i\rangle \tag{732}$$

We have

$$R = \lambda\int d^3\vec{r}\left(\frac{1}{\sqrt{V}}e^{-i\vec{k}_f\cdot\vec{r}}\right)\left(\vec{\epsilon}\frac{1}{\sqrt{V}}\sqrt{\frac{\hbar}{2\omega\epsilon_0}}e^{i\vec{k}_\gamma\cdot\vec{r}}\cdot(-i\hbar\vec{\nabla})\right)(\psi_i(\vec{r})) \tag{733}$$

We can integrate by parts. Note that $\vec{\epsilon}\cdot\vec{k}_\gamma = 0$, so we just get the derivative acting on the first term. This gives

$$R = i\hbar\lambda\sqrt{\frac{\hbar}{2\omega\epsilon_0}}\vec{\epsilon}\cdot(i\vec{k}_f)\frac{1}{V}\int d^3\vec{r}e^{-i\vec{\Delta}k\cdot\vec{r}}\psi_i(\vec{r}) = -\hbar\lambda\frac{1}{V}\sqrt{\frac{\hbar}{2\omega\epsilon_0}}(\vec{\epsilon}\cdot\vec{k}_f)\int d^3\vec{r}e^{-i\vec{\Delta}k\cdot\vec{r}}\psi_i(\vec{r}) \tag{734}$$

where we have defined

$$\vec{\Delta}k = \vec{k}_f - \vec{k}_\gamma \tag{735}$$

As an example, let us take the wavefunction ψ_{100}

$$\psi_{100} = 2(\frac{Z}{a_0})^{\frac{3}{2}}e^{-\frac{Zr}{a_0}} \tag{736}$$

The spherical harmonic is

$$Y_{00} = \frac{1}{\sqrt{4\pi}} \tag{737}$$

Thus we have

$$\psi_i(\vec{r}) = 2(\frac{Z}{a_0})^{\frac{3}{2}}e^{-\frac{Zr}{a_0}}\frac{1}{\sqrt{4\pi}} = \frac{1}{\sqrt{\pi}}(\frac{Z}{a_0})^{\frac{3}{2}}e^{-\frac{Zr}{a_0}} \tag{738}$$

Thus we need to compute

$$I = \int d^3\vec{r}e^{-i\vec{\Delta}k\cdot\vec{r}}e^{-\frac{Zr}{a_0}} = 2\pi\int_{-1}^{1}d(\cos\theta)\int drr^2 e^{-\mu r}e^{-i\Delta kr\cos\theta} \tag{739}$$

We write

$$\mu = \frac{Z}{a_0} \tag{740}$$

Doing the θ integral gives

$$I = 2\pi \frac{1}{-i\Delta k} \int drr e^{-\mu r} (-2i \sin \Delta k r) = 4\pi \frac{1}{\Delta k} \int_0^\infty drr e^{-\mu r} \sin(\Delta k r) \tag{741}$$

$$I = 4\pi \frac{1}{\Delta k} \frac{2\Delta k \mu}{((\Delta k)^2 + \mu^2)^2} = 8\pi \mu \frac{1}{((\Delta k)^2 + \mu^2)^2} \tag{742}$$

$$R = -\hbar \lambda \frac{1}{V} \sqrt{\frac{\hbar}{2\omega \epsilon_0}} (\vec{\epsilon} \cdot \vec{k}_f) 8\pi \mu \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} \frac{1}{((\Delta k)^2 + \mu^2)^2} \tag{743}$$

30.5   The cross section

We have

$$d\sigma = \frac{1}{F} \frac{1}{t} P_{d\Omega}(t) = \frac{1}{F} \frac{1}{t} \sum_{states, d\Omega} |\tilde{c}_{\vec{k}'}(t)|^2 \tag{744}$$

Using the Fermi Golden rule we get

$$d\sigma \to \frac{1}{F} \frac{2\pi}{\hbar} \int dE \delta(E - E_0) \rho_{d\Omega} |R|^2 = \frac{1}{F} \frac{2\pi}{\hbar} \rho_{d\Omega} |R|^2 \tag{745}$$

We can use

$$\rho_{d\Omega} = \frac{V}{(2\pi)^3} \frac{k_f m}{\hbar^2} d\Omega \tag{746}$$

This gives

$$d\sigma = \frac{1}{F} \frac{2\pi}{\hbar} \frac{V}{(2\pi)^3} \frac{k_f m}{\hbar^2} d\Omega |R|^2 \tag{747}$$

This can be written as

$$\frac{d\sigma}{d\Omega} = \frac{1}{F} \frac{2\pi}{\hbar} \frac{V}{(2\pi)^3} \frac{k_f m}{\hbar^2} |R|^2 \tag{748}$$

We had

$$F = \frac{c}{V} \tag{749}$$

This gives

$$\frac{d\sigma}{d\Omega} = \frac{V}{c} \frac{2\pi}{\hbar} \frac{V}{(2\pi)^3} \frac{k_f m}{\hbar^2} |R|^2 \tag{750}$$

30.6 Putting it together

We get

$$\frac{d\sigma}{d\Omega} = \frac{V}{c}\frac{2\pi}{\hbar}\frac{V}{(2\pi)^3}\frac{k_f m}{\hbar^2}\left(\hbar^2\lambda^2\frac{1}{V^2}\frac{\hbar}{2\omega\epsilon_0}(\vec{\epsilon}\cdot\vec{k}_f)^2(8\pi)^2\mu^2\frac{1}{\pi}(\frac{Z}{a_0})^3\frac{1}{((\Delta k)^2+\mu^2)^4}\right) \tag{751}$$

$$\frac{d\sigma}{d\Omega} = \frac{1}{c}\frac{2\pi}{\hbar}\frac{1}{(2\pi)^3}\frac{k_f m}{\hbar^2}\left(\hbar^2\frac{e^2}{m^2}\frac{\hbar}{2\omega\epsilon_0}(\vec{\epsilon}\cdot\vec{k}_f)^2(8\pi)^2(\frac{Z}{a_0})^2\frac{1}{\pi}(\frac{Z}{a_0})^3\frac{1}{((\Delta k)^2+\frac{Z^2}{a_0^2})^4}\right) \tag{752}$$

$$\frac{d\sigma}{d\Omega} = Z^5 a_0^3\frac{1}{c}\frac{1}{\hbar}\frac{k_f m}{\hbar^2}\left(\hbar^2\frac{e^2}{m^2}\frac{\hbar}{\omega\epsilon_0}(\vec{\epsilon}\cdot\vec{k}_f)^2 8\frac{1}{\pi}\frac{1}{((\Delta k)^2 a_0^2+Z^2)^4}\right) \tag{753}$$

We have

$$a_0 = \frac{\hbar^2(4\pi\epsilon_0)}{me^2} \tag{754}$$

$$\frac{d\sigma}{d\Omega} = Z^5 a_0^2\frac{\hbar^2(4\pi\epsilon_0)}{me^2}\frac{1}{c}\frac{1}{\hbar}\frac{k_f m}{\hbar^2}\left(\hbar^2\frac{e^2}{m^2}\frac{\hbar}{\omega\epsilon_0}(\vec{\epsilon}\cdot\vec{k}_f)^2 8\frac{1}{\pi}\frac{1}{((\Delta k)^2 a_0^2+Z^2)^4}\right) \tag{755}$$

$$\frac{d\sigma}{d\Omega} = 32 Z^5 a_0^2\left(\frac{p_f c}{\hbar\omega}\right)\left(\frac{\vec{\epsilon}\cdot\vec{p}_f}{mc}\right)^2\frac{1}{((\Delta k)^2 a_0^2+Z^2)^4} \tag{756}$$

31 Identical particles

Suppose we have two bosons which are identical, scattering in the center of mass frame. The initial state then has the form

$$|\psi_i\rangle = \frac{1}{\sqrt{2}}\left(|\psi(p_{1i})\rangle_1|\psi(p_{2i})\rangle_2 + |\psi(p_{2i})\rangle_1|\psi(p_{1i})\rangle_2\right) \tag{757}$$

The Hamiltonian is symmetric, and thus a symmetric wavefunction evolves to a symmetric one. The final wavefunction thus has the form

$$|\psi_f\rangle = \frac{1}{\sqrt{2}}\left(|\psi(p_{1f})\rangle_1|\psi(p_{2f})\rangle_2 + |\psi(p_{2f})\rangle_1|\psi(p_{1f})\rangle_2\right) \tag{758}$$

Let

$$R_1 = {}_1\langle\psi(p_{1f})|{}_2\langle\psi(p_{2f})|\lambda H^{(1)}|\psi(p_{1f})\rangle_1|\psi(p_{2f})\rangle_2 \tag{759}$$

and

$$R_2 = {}_1\langle\psi(p_{2f})|{}_2\langle\psi(p_{1f})|\lambda H^{(1)}|\psi(p_{1f})\rangle_1|\psi(p_{2f})\rangle_2 \tag{760}$$

We note that since the particles are identical, we also have

$$R_1 = {}_1\langle\psi(p_{2f})|{}_2\langle\psi(p_{1f})|\lambda H^{(1)}|\psi(p_{2f})\rangle_1|\psi(p_{1f})\rangle_2 \tag{761}$$

and

$$R_2 = {}_1\langle\psi(p_{1f})|{}_2\langle\psi(p_{2f})|\lambda H^{(1)}|\psi(p_{2f})\rangle_1|\psi(p_{1f})\rangle_2 \tag{762}$$

Consider angle $0 < \theta_s < \frac{\pi}{2}$. We assume that one f the particles scatters in this angle; the other will then scatter with $\frac{\pi}{2} < \theta_s < \pi$. Then we find that

$$|R|^2 \to = |\frac{1}{2}(2R_1 + 2R_2)|^2 = |R_1 + R_2|^2 \tag{763}$$

Similarly, for fermions we find

$$|R|^2 \to = |\frac{1}{2}(2R_1 - 2R_2)|^2 = |R_1 - R_2|^2 \tag{764}$$

In particular, for fermions we see that scattering at $\theta_s = \frac{\pi}{2}$ will vanish.

32   Quantum information

In classical theory, we can have a bit of information which can take two states $0, 1$. Thus information can be coded in a string

$$S = 10001011001... \tag{765}$$

In quantum theory the analogue is a 2-state system, which has states of the form

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{766}$$

Normalization tells us that

$$|\alpha|^2 + |\beta|^2 = 1 \tag{767}$$

32.1   Gates

In classical theory we have operations called gates, which can change the state of bits. For example, if we have one bit, the operation can flip the bit

$$0 \to 1, \quad 1 \to 0 \tag{768}$$

This is called the NOT gate, since it converts the bit to the state that it is 'not'.

We can also map both states to the same state

$$0 \to 0, \quad 1 \to 0 \tag{769}$$

In quantum theory, we can manipulate the bit by acting with operators. Thus we can apply

$$|\psi\rangle \to \sigma^x|\psi\rangle \tag{770}$$

Thus will implement the flip

$$\sigma_x \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \sigma_x \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{771}$$

Thus σ^x gives the NOT gate. But we cannot map both states to the same state, as this would not be a unitary operation. The general unitary map is of the form

$$U = e^{iH} = e^{i\phi} e^{i\alpha \hat{n} \cdot \vec{\sigma}} \tag{772}$$

where $\hat{n}$ is a unit vector and ϕ, α are real numbers. A gate of particular importance is the Hadamard gate

$$H = \frac{1}{\sqrt{2}} (\sigma^x + \sigma^z) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{773}$$

If we have two bits, then we can do a joint operation on the two bits. In classical theory, we have the Controlled Not (CNOT) gate, where if the first bit is 0 then the second bit is left unchanged, while if the first bit is 1, then the second bit is flipped. The first bit is left unchanged in either case. Thus we have

$$00 \to 00, \quad 01 \to 01, \quad 10 \to 11, \quad 11 \to 10 \tag{774}$$

This is a unitary map, and we can implement CNOT in the quantum theory as well.

32.2 Quantum teleportation

We start with Alice and Bob having na entangled pair

$$\frac{1}{\sqrt{2}} (0_A 0_B + 1_A 1_B) \tag{775}$$

Now Alice is given a state

$$\psi = \alpha 0 + \beta 1 \tag{776}$$

Thus the overall state is

$$\Psi = \frac{1}{\sqrt{2}} (\alpha 0 + \beta 1)(0_A 0_B + 1_A 1_B) \tag{777}$$

We first do a CNOT on Alice's bits. This gives

$$\Psi_1 = \frac{1}{\sqrt{2}} \alpha 0 (0_A 0_B + 1_A 1_B) + \frac{1}{\sqrt{2}} \beta 1 (1_A 0_B + 0_A 1_B) \tag{778}$$

We then do a Hadamard on Alice's first bit. This gives

$$\Psi_2 = \frac{1}{2} \alpha (0 + 1)(0_A 0_B + 1_A 1_B) + \frac{1}{2} \beta (0 - 1)(1_A 0_B + 0_A 1_B) \tag{779}$$

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Expanding gives

$$
\begin{aligned}
\Psi_2 \;=\; & \frac{1}{2}00_A(\alpha 0_B + \beta 1_B) \\
+\; & \frac{1}{2}01_A(\alpha 1_B + \beta 0_B) \\
+\; & \frac{1}{2}10_A(\alpha 0_B - \beta 1_B) \\
+\; & \frac{1}{2}11_A(\alpha 1_B - \beta 0_B)
\end{aligned}
\tag{780}
$$

Now Alice measures her bits:

(i) If she finds 00_A, she conveys this information to Bob, and Bob knows that he already has the state ψ.

(ii) If she finds 01_A, Bob has the state $\alpha 1_B + \beta 0_B$. She tells Bob that she has 01_A, and Bob applies the NOT σ^x to get ψ.

(iii) If she finds 10_A, Bob has the state $\alpha 0_B - \beta 1_B$. She tells Bob that she has 10_A, and Bob applies the Z gate σ^z to get ψ.

(iv) If she finds 11_A, Bob has the state $\alpha 1_B - \beta 0_B$. She tells Bob that she has 11_A, and Bob applies $\sigma^z \sigma^x$ to get ψ.

The above operations can be summarized by saying that if Alice's bits are $M_1 M_2$, then the operation needed is

$$
(\sigma^z)^{M_1}(\sigma^x)^{M_2}
\tag{781}
$$

32.3   The Deutch algorithm

(1) We start with two bits. We put the first in the state 0 and the second in the state 1. Thus we have

$$
\psi_0 = 01
\tag{782}
$$

(2) We apply a Hadamard to each bit. This gives

$$
\psi_1 = \frac{1}{2}(0+1)(0-1)
\tag{783}
$$

(3) We apply the map f which does

$$
xy \to x(y + f(x))
\tag{784}
$$

Thus
$$x0 \rightarrow x(0 + f(x)) = xf(x) \tag{785}$$
$$x1 \rightarrow x(1 + f(x)) \tag{786}$$

Thus
$$x(0 - 1) \rightarrow x\left(f(x) + (1 + f(x))\right) \tag{787}$$

We note that this is
$$\begin{aligned}
f(x) = 0 &\quad \rightarrow \quad x(0 - 1) \\
f(x) = 1 &\quad \rightarrow \quad x(1 - 0)
\end{aligned}$$
$$\tag{788}$$

Thus we have
$$x(0 - 1) \rightarrow (-1)^{f(x)} x(0 - 1) \tag{789}$$

(4) Thus applied to ψ_2 we get

$$\psi_3 = \frac{1}{2}(-1)^{f(0)}0(0 - 1) + \frac{1}{2}(-1)^{f(1)}1(0 - 1) \tag{790}$$

Now there are two possibilities:

$$\begin{aligned}
f(0) = f(1) &\rightarrow f(0) + f(1) = 0 : \quad \rightarrow \quad \psi_3 = \frac{1}{2}(-1)^{f(0)}(0 + 1)(0 - 1) \\
f(0) \neq f(1) &\rightarrow f(0) + f(1) = 1 : \quad \rightarrow \quad \psi_3 = \frac{1}{2}(-1)^{f(0)}(0 - 1)(0 - 1)
\end{aligned}$$
$$\tag{791}$$

(5) We do a Hadamard on the first bit, getting

$$\begin{aligned}
f(0) + f(1) = 0 : &\quad \rightarrow \quad \psi_4 = \frac{1}{\sqrt{2}}(-1)^{f(0)}0(0 - 1) \\
f(0) + f(1) = 1 : &\quad \rightarrow \quad \psi_4 = \frac{1}{\sqrt{2}}(-1)^{f(0)}1(0 - 1)
\end{aligned}$$
$$\tag{792}$$

We can write this as
$$\psi_4 = \frac{1}{\sqrt{2}}(-1)^{f(0)}\left(f(0) + f(1)\right)(0 - 1) \tag{793}$$

Thus if we measure the first bit, then we can find the value of

$$f(0) + f(1) \tag{794}$$

33 The Aharonov-Bohm effect

The goal of this effect is to see if the vector potential $\vec{A}$ can have physical effects even if $\vec{\nabla} \times \vec{A} = \vec{B} = 0$.

33.1 Solving for the wavefunction

Consider a particle of mass m with Hamiltonian

$$H_0 = \frac{p^2}{2m} \tag{795}$$

Now consider this particle in a vector potential $\vec{A}(\vec{r})$. The Hamiltonian is

$$H_A = \frac{(\vec{p} - q\vec{A})^2}{2m} \tag{796}$$

Suppose we have a wavefunction at some time $t = t_0$ given by $\psi_0(\vec{r})$. Consider another wavefunction

$$\psi_A(\vec{r}) = e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \vec{\psi_0}(\vec{r}) \tag{797}$$

Now we see that

$$
\begin{aligned}
(\vec{p} - q\vec{A})\psi_A(\vec{r}) &= (-i\hbar\vec{\nabla} - q\vec{A})e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \vec{\psi_0}(\vec{r}) \\
&= e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \left((-i\hbar\vec{\nabla})\psi_0(\vec{r}) + q\vec{A}(\vec{r})\psi_0(\vec{r}) - q\vec{A}(\vec{r})\psi_0(\vec{r}) \right) \\
&= e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} (-i\hbar\vec{\nabla})\psi_0(\vec{r}) \\
&= e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \vec{p}\psi_0(\vec{r})
\end{aligned}
\tag{798}
$$

Thus we see that for any function $\psi(\vec{r})$

$$(\vec{p} - q\vec{A})e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \psi(\vec{r}) = e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \vec{p}\psi(\vec{r}) \tag{799}$$

Thus

$$
\begin{aligned}
(\vec{p} - q\vec{A})^2 e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \psi(\vec{r}) &= (\vec{p} - q\vec{A})e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \vec{p}\psi(\vec{r}) \\
&= e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} (\vec{p})^2 \psi(\vec{r})
\end{aligned}
\tag{800}
$$

and

$$\frac{(\vec{p} - q\vec{A})^2}{2m} e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \psi(\vec{r}) = e^{i\frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}')\cdot d\vec{r}'} \frac{(\vec{p})^2}{2m} \psi(\vec{r}) \tag{801}$$

which is
$$H_A \psi_A = e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} H_0 \psi_0 \tag{802}$$

Suppose we have an eigenfunction
$$H_0 \psi_0 = E_0 \psi_0 \tag{803}$$

We wish to solve the eigenvalue problem
$$H_A \psi_A = E_A \psi_A \tag{804}$$

We write
$$\psi_A = e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_0 \tag{805}$$

Then
$$H_A \psi_A = e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} H_0 \psi_0 = e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} E_0 \psi_0 = E_0 \psi_A \tag{806}$$

Thus ψ_A is an eigenfunction of H_A with eigenvalue $E_A = E_0$.

Similarly, suppose we have solved an evolution problem
$$i\hbar \partial_t \psi_0(\vec{r}, t) = H_0 \psi_0(\vec{r}, t) \tag{807}$$

We wish to find a solution to
$$i\hbar \partial_t \psi_A(\vec{r}, t) = H_A \psi_A(\vec{r}, t) \tag{808}$$

We write
$$\psi_A = e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_0 \tag{809}$$

Then
$$
\begin{aligned}
i\hbar \partial_t \psi_A(\vec{r}, t) &= e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} (i\hbar \partial_t) \psi_0(\vec{r}, t) \\
&= e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} H_0 \psi_0(\vec{r}, t) \\
&= H_A e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_0(\vec{r}, t) \\
&= H_A \psi_A(\vec{r}, t)
\end{aligned} \tag{810}
$$

Thus the above constructed $\psi_A(\vec{r}, t)$ solves the evolution equation for H_A of $\psi_0(\vec{r}, t)$ solved the equation for H_0.

33.2 The effect of $\vec{B} \neq 0$

It may seem from this that it is always trivial to solve for H_A of we can solve for H_0. In 1-d this is true, but in higher dimensions, different paths in the exponent lead to different functions. Thus this solution makes sense only if all paths give the same result. But this means that

$$\int_C \vec{A} \cdot \vec{dr} = 0 \tag{811}$$

for all loops C. By the Stokes theorem, this means that

$$\int \int_S (\vec{\nabla} \times \vec{A}) \cdot \hat{n} dS = 0 \tag{812}$$

This gives

$$\vec{\nabla} \times \vec{A} = \vec{B} = 0 \tag{813}$$

everywhere.

Consider a tube with magnetic flux B, but no flux outside. Then for a loop around the tube

$$\int_C \vec{A} \cdot d\vec{r} = \int \int_S \vec{B} \cdot \hat{n} dS = F \tag{814}$$

where F is the total flux through the tube. Thus $\vec{A}$ is not zero outside the tube.

33.3 The Aharonov-Bohm effect

Consider a two slit experiment. We first consider the wave coming out of the slit 1 alone. We solve the waveequation first solving in the absence of any $\vec{B}$ to get a wavefunction ψ_1. Then in the presence of $\vec{A}$, we get the solution as

$$\psi_{1A} = e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_1 \tag{815}$$

Now consider the wave from slit 2. We solve the waveequation first solving in the absence of any $\vec{B}$ to get a wavefunction ψ_2. Then in the presence of $\vec{A}$, we get the solution as

$$\psi_{2A} = e^{i \frac{q}{\hbar} \int_0^x \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_2 \tag{816}$$

This time note that we have used the $\vec{A}$ which is correct for the other paths around the slit.

Consider the interference pattern at any point $\vec{r}$ on the screen. From slit 1, with $\vec{B} = 0$, we get an amplitude

$$\psi_1(\vec{r}, t) \tag{817}$$

With $\vec{B}$ turned on, we get the amplitude

$$\psi_{1A}(\vec{r}, t) = e^{i \frac{q}{\hbar} \int_0^{x,(1)} \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_1(\vec{r}, t) \tag{818}$$

From slit 2, with $\vec{B} = 0$, we get an amplitude

$$\psi_2(\vec{r}, t) \tag{819}$$

With $\vec{B}$ turned on, we get the amplitude

$$\psi_{2A}(\vec{r}, t) = e^{i\frac{q}{\hbar} \int_0^{x,(2)} \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_2(\vec{r}, t) \tag{820}$$

where the path in the second case goes below the flux tube.

In the absence of flux the net amplitude at $\vec{r}$ was

$$\psi_{T0} = \psi_1 + \psi_2 \tag{821}$$

With $\vec{B}$ turned on, the net amplitude is

$$\psi_{TA} = e^{i\frac{q}{\hbar} \int_0^{x,(1)} \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_1 + e^{i\frac{q}{\hbar} \int_0^{x,(2)} \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_2 \tag{822}$$

We can write this as

$$\psi_{TA} = \psi_1 + e^{i\frac{q}{\hbar} \int_0^{x,(C)} \vec{A}(\vec{r}') \cdot d\vec{r}'} \psi_2 \tag{823}$$

where

$$e^{i\frac{q}{\hbar} \int_0^{x,(C)} \vec{A}(\vec{r}') \cdot d\vec{r}'} = e^{i\frac{q}{\hbar} \int_0^{x,(2)} \vec{A}(\vec{r}') \cdot d\vec{r}'} e^{-i\frac{q}{\hbar} \int_0^{x,(1)} \vec{A}(\vec{r}') \cdot d\vec{r}'} \tag{824}$$

Thus we will see a shift in the interference pattern when we turn the $\vec{B}$ field on.