8.05 Review Notes

Information on the formula sheet is not usually reproduced here...

The First Bits of the Course...

• For a free particle

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(x) = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

- General features of wavefunctions
 - The ground state must be even.
 - The number of nodes indicates how "high" the state is.
- To incorporate the fact a particle decays as $\exp(-t/\tau)$, add $-i\hbar/2\tau$ to the potential.
- The particle flux is given by $\overline{J(x,t) = \frac{\hbar}{m} \operatorname{Im}\left(\psi^* \frac{\partial \psi}{\partial x}\right)}$ with $\dot{\rho} + J' = 0$. To prove, write an expression for $\dot{\rho} = \frac{\mathrm{d}}{\mathrm{d}t}(\psi\psi^*)$ and simplify with a complexconjugated SE. Integrating the conservation law over all space, we end up with the fact total probability is conserved. For a fluid, $J = \rho v$ which gives us a nice definition of quantum velocity.

•
$$\left[\hat{x}, \hat{p}\right] = i\hbar$$

- General tips and tricks with Dirac Notation
 - o A crucial step in many derivations is that

 $\langle x$

$$|\hat{p}|p\rangle = p\langle x | p \rangle$$

$$= p \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

$$= -i\hbar \frac{d}{dx} \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

$$= -i\hbar \frac{d}{dx} \langle x | p \rangle$$

And similarly that

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$$\left\langle p \mid \hat{x} \mid x \right\rangle = x \left\langle p \mid x \right\rangle$$

$$= x \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar}$$

$$= i\hbar \frac{\mathrm{d}}{\mathrm{d}p} \left\langle x \mid p \right\rangle$$

- When working out expressions like $\langle x \mid \hat{p} \mid \psi \rangle$, write it as $\int \langle x \mid \hat{p} \mid p \rangle \langle p \mid \psi \rangle dp$.
- To find $\langle x \mid \hat{p} \mid y \rangle$, insert the identity into $\langle x \mid \hat{p} \mid \psi \rangle$ and compare.
- When showing that $e^{\hat{A}} | \alpha \rangle$ is an eigenstate (of *x*, say), easiest way to do it is

$$\hat{x}e^{\hat{A}}\left|\alpha\right\rangle = e^{\hat{A}}\left(e^{-\hat{A}}\hat{x}e^{\hat{A}}\right)\left|\alpha\right\rangle = e^{\hat{A}}\left(\hat{x} + \left[\hat{x},\hat{A}\right]\right)\left|\alpha\right\rangle$$

[This uses the fact that $e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A},\hat{B}]$, quoted on the formula sheet].

- To find the Fourier Transform of a function like xe^{ipx} , eliminate the x by expressing it as a derivative of the exponential.
- The function of the doubly differentiated delta function is to "pick out" the double derivative.
- To find the maximum and/or minimum value of an operator \hat{A} , consider a normalised eigenvector ψ and realise that $\langle \psi | \hat{A} | \psi \rangle = a \langle \psi | \psi \rangle$. Then, write \hat{A} in two ways that makes $\langle \psi | \hat{A} | \psi \rangle$ a norm, and realise it must therefore be greater than 0 (for example, $\langle \psi | \hat{a}^{\dagger} \hat{a} | \psi \rangle = \|\hat{a} \| \psi \| \ge 0$ and $\langle \psi | 1 \hat{a} \hat{a}^{\dagger} | \psi \rangle$).
- For a free particle, the wavelength is given by

$$\frac{\hbar^2 k^2}{2m} = E - V_{eff}$$

• Translation operators in QM

$$\begin{split} \hline \mathcal{U} &= e^{-ix_0\hat{p}/\hbar} & \left\langle x \left| \hat{\mathcal{U}} \right| \psi \right\rangle = \psi(x - x_0) & \hat{\mathcal{U}}^{\dagger} \hat{x} \hat{\mathcal{U}} = x + x_0 \\ \hline \mathcal{U} &= e^{i\phi\hat{J}_z} & \text{rotates the system by } \phi \text{ about the z-axis} \end{split}$$

- The postulates of QM:
 - At each instant, the state of a physical system is represented by a ket $|\psi\rangle$ in the space of states.

- Every observable attribute of a physical system is described by an Hermitian operator that acts on the kets that describe the system.
- The only possible result of the measurement of an observable A is one of the eigenvalues of the corresponding operator A.
- When a measurement of an observable A is made on a generic state $|\psi\rangle$, the probability of obtaining an eigenvalue a_n is given by the square of the inner product of $|\psi\rangle$ with the eigenstate $|a_n\rangle |\langle a_n |\psi\rangle|^2$.
- Immediately after the measurement of an observable A has yielded a value a_n , the state of the system is the normalised eigenstate $|a_n\rangle$.
- The time-evolution of a quantum system preserves the normalisation of the associated ket. The time evolution of the state of a quantum system is described by $|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle$ where U is unitary.

Uncertainty

- If $[\hat{A}, \hat{B}] = 0$, then A and B are compatible simultaneous eigenfunctions.
- The **complete set of commuting observables** is one in which each basis state is specified by a unique set of eigenvalues.
- For incompatible observables, the generalised uncertainty principle states that

$$\left(\Delta A\right)^{2} \left(\Delta B\right)^{2} \ge \left(\left\langle\psi \mid \frac{1}{2i}[\hat{A}, \hat{B}] \mid\psi\right\rangle\right)^{2}$$

We note that $\frac{1}{2i}[\hat{A},\hat{B}]$ is Hermitian and so has real expectation values. Thus, the RHS is always real and positive. Note that even if $[\hat{A},\hat{B}] \neq 0$, the expectation value of $i[\hat{A},\hat{B}]$ might still be 0.

• To prove the generalised uncertainty principle, consider

$$\left| f \right\rangle = \left(\hat{A} - \left\langle \hat{A} \right\rangle \right) \left| \psi \right\rangle$$
$$\left| g \right\rangle = \left(\hat{B} - \left\langle \hat{B} \right\rangle \right) \left| \psi \right\rangle$$

And

$$\begin{split} \left\langle f \mid f \right\rangle \left\langle g \mid g \right\rangle &\geq \left| \left\langle f \mid g \right\rangle \right|^2 \\ \left(\Delta A \right)^2 \left(\Delta B^2 \right) &\geq \underbrace{\left| \left\langle f \mid g \right\rangle + \left\langle g \mid f \right\rangle}{2} \right|^2 + \underbrace{\left| \left\langle f \mid g \right\rangle - \left\langle g \mid f \right\rangle}{2i} \right|^2 \\ \left(\Delta A \right)^2 \left(\Delta B^2 \right) &\geq \underbrace{\left| \left\langle \left[\hat{A}, \hat{B} \right] \\ 2i \right\rangle \right|^2} \end{split}$$

- For minimum uncertainty, we need
 - $\circ |g\rangle = \alpha |f\rangle$ (with complex α). This gives us equality in the Schwarz Inequality.

$$\circ \quad \left\langle f \mid g \right\rangle + \left\langle g \mid f \right\rangle = 0 \Rightarrow \alpha = i\lambda$$

And so $\left(\hat{B} - \left\langle \hat{B} \right\rangle \right) \left| \psi \right\rangle = i\lambda \left(\hat{A} - \left\langle \hat{A} \right\rangle \right) \left| \psi \right\rangle$

• For an eigenstate, the uncertainty of the operator is 0. To see why, consider $\langle \beta | \beta \rangle$ where $|\beta \rangle = (\hat{A} - a) |\alpha \rangle$. If $\langle \hat{A}^2 \rangle = \langle \hat{A} \rangle^2$.

Quantum Dynamics

0

- Time evolution operator defined such that $|\psi, t\rangle = \hat{U}(t, t_0) |\psi, t_0\rangle$
 - $\circ \quad \text{If } \hat{H} \text{ is independent of time}$

$$\hat{U}(t,t_0) = e^{-i(t-t_0)\hat{H}/\hbar}$$

If
$$\hat{H}$$
 dependent on time but $\left[\hat{H}(t), \hat{H}(t')\right] = 0$
$$\hat{U}(t, t_0) = e^{-\frac{i}{\hbar} \int_{t_0}^t \hat{H}(\tilde{t}) d\tilde{t}}$$

[Eg: field with constant position and varying direction].

- o If \hat{H} dependent of time and $\left[\hat{H}(t), \hat{H}(t')\right] \neq 0$, not 8.05
- For the first case above, insert the identity before and after \hat{U} to find that

$$\left|\psi,0\right\rangle = \sum_{n} C_{n}\left|n\right\rangle \Rightarrow \left|\psi,t\right\rangle = \sum_{n} C_{n} e^{-\frac{i}{\hbar}(t-t_{0})E_{n}}\left|n\right\rangle$$

• We can view expectation values in two different ways

$$\overbrace{\langle\psi,0|U^{\dagger}(t,0)}^{\text{Schrodinger}} \overbrace{\hat{A}}^{\hat{A}_{s}} \underbrace{|\psi,t\rangle_{s}}_{U(t,0)|\psi,0\rangle} = \underbrace{\langle\psi,0|}_{_{H}\langle\psi|} \underbrace{U^{\dagger}(t,0)\hat{A}U(t,0)}_{\stackrel{\tilde{A}_{H}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle_{H}}}{\overset{[\psi\rangle$$

In the Schrodinger Picture, the wavefunctions evolve with time and operators stay constant. In the Heisenberg picture, the opposite is true.

• Schrodinger and Heisenberg operators are related by the **Heisenberg** Equation of Motion

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \hat{A}_{\!_{H}}(t) = \left[\hat{A}_{\!_{H}}(t), \hat{H}_{\!_{H}}(t)\right] + i\hbar \underbrace{\dot{\hat{A}}_{\!_{H}}(t)}_{=\hat{\upsilon}^{\dagger}\dot{A}_{\!_{S}}\hat{\upsilon}}$$

This last term disappears if the Schrodinger operator does not vary with time, which is true most of the time. To solve this equation, find the **right-hand-side** and **integrate**. Taking **expectation values** of each side gives the **Ehrenfest Theorem**.

- A few notes
 - o Changing picture does not change the form of commutators

$$\begin{split} \left[\hat{A}_{\!_S}, \hat{B}_{\!_S} \right] &= \hat{C}_{\!_S} \Leftrightarrow \left[\hat{A}_{\!_H}, \hat{B}_{\!_H} \right] = \hat{C}_{\!_H} \\ \text{o} \quad \text{If } \left[\hat{H}(t), \hat{H}(t') \right] &= 0 \text{, then } \left[\hat{U}, \hat{H} \right] = 0 \text{ and } \hat{H}_{\!_H} = U^{\dagger} \hat{H}_{\!_S} \hat{U} = \hat{H}_{\!_S} \,. \end{split}$$

• If $\left[\hat{H}, \hat{A}\right] = 0$, then A is a conserved quantity.

Two-State Systems

- The matrix element $\langle 2|\hat{H}|1 \rangle$ is a measure of the tunnelling probability 1 $\rightarrow 2$.
- The **Hamiltonian** for a spin in a field B is

$$\hat{H} = -\gamma \boldsymbol{B} \cdot \hat{\boldsymbol{S}}$$

Where \boldsymbol{S} is a vector containing the spin operators as its components. By using the **Heisenberg Equation of Motion** for S_x , S_y and S_z and integrating, we can show that any spin **precesses** about \boldsymbol{B} with angular velocity $\omega = \gamma |\boldsymbol{B}|$.

- Any general two-state Hamiltonian can be written as a sum of the identity matrix and the Pauli matrices, and so can be thought of as a precessing spin.
- Now, consider instead a system with a **constant field** in the z-direction, and a rotating field in the x-y plane ($\omega_0 = \gamma B_0$ and $\omega_1 = \gamma B_1$)

$$\hat{H}(t) = -\frac{\hbar}{2}\omega_{_{0}}\hat{\sigma}_{_{3}} - \frac{\hbar}{2}\omega_{_{1}}\Big[\cos(\omega t)\hat{\sigma}_{_{1}} - \sin(\omega t)\hat{\sigma}_{_{2}}\Big]$$

Using the properties of the Pauli Matrices

$$\begin{split} \hat{H}(t) &= -\frac{\hbar}{2}\omega_0\hat{\sigma}_3 - \frac{\hbar}{2}\omega_1\exp\left(\frac{1}{2}i\omega t\sigma_3\right)\hat{\sigma}_1\exp\left(-\frac{1}{2}i\omega t\sigma_3\right) \\ &= -\exp\left(\frac{1}{2}i\omega t\sigma_3\right)\left[\frac{\hbar}{2}\omega_0\hat{\sigma}_3 + \frac{\hbar}{2}\omega_1\hat{\sigma}_1\right]\exp\left(-\frac{1}{2}i\omega t\sigma_3\right) \\ &= -\exp\left(\frac{1}{2}i\omega t\sigma_3\right)\left[\omega_0\hat{S}_z + \omega_1\hat{S}_x\right]\exp\left(-\frac{1}{2}i\omega t\sigma_3\right) \end{split}$$

So in other words, our Hamiltonian is **constant** in a **rotating frame**. So if the state is $|\psi_R(t)\rangle$ in the rotating frame, then in the lab frame, it is $|\psi(t)\rangle = \exp(\frac{1}{2}i\omega t\sigma_3)|\psi_R(t)\rangle$.

• Substitute $|\psi(t)\rangle = \exp\left(\frac{1}{2}i\omega t\sigma_3\right)|\psi_R(t)\rangle$ into the **LHS** of the SE to get

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \left| \psi_{\mathrm{R}}(t) \right\rangle = \left[(\omega - \omega_{0}) \hat{S}_{z} - \omega_{1} \hat{S}_{x} \right] \left| \psi_{\mathrm{R}}(t) \right\rangle$$

So in the rotating frame, there is **precession** about a **new field** B_{eff} . Since, typically, $\omega_1 \ll \omega_2$, the possible options are as follows

- ω very different from ω_0 the field basically precesses around the z axis (ie: nearly not at all for a spin up).
- $\omega \approx \omega_0$ the field precesses around the *x*-axis at a frequency ω_1 . Since our rotating frame is also moving around the *z*-axis, the spins spirals all the way down.
- **NMR** works as follows
 - We turn on a radio pulse with $\omega = \gamma_{\text{proton}} B_0$, for strength B_1 for a time $\Delta t = \pi / 2\gamma_{\text{proton}} B_1$. This brings the spin "down" and makes it maximally perpendicular to the z-axis.
 - We then switch the field off and look for radio emission of precessing spins at a frequency ω_0 resulting from such spins.

QM in Three-Dimensions

• Using all kinds of horribly complicated maths, we derive

$$oldsymbol{L}^2 + ig(oldsymbol{r}\cdotoldsymbol{p}ig)^2 = oldsymbol{r}^2 oldsymbol{p}^2 + i\hbaroldsymbol{r}\cdotoldsymbol{p} \Rightarrow oldsymbol{p}^2 = rac{(oldsymbol{r}\cdotoldsymbol{p})^2 - i\hbaroldsymbol{r}\cdotoldsymbol{p} + oldsymbol{L}^2}{oldsymbol{r}^2}$$

Using this relation and even more complicated maths, we get

$$\boldsymbol{H} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\boldsymbol{L}^2}{2mr^2} + V(r)$$

And finally, using a last dose of complicated maths, we find that a **maximal set of commuting operators** for this system is

$$\left\{H,\boldsymbol{L}^{\!2},L_{_{\!\boldsymbol{z}}}\right\}$$

• Start with eigenfunctions $|\ell, m\rangle$, and assume that

$$\begin{split} \boldsymbol{L}^{2}\left|\,\ell,m\right\rangle &= \hbar^{2}\ell(\ell+1) \left|\,\ell,m\right\rangle \\ & L_{z}\left|\,\ell,m\right\rangle &= \hbar m \left|\,\ell,m\right\rangle \end{split}$$

Use horrible maths once again to get

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

Then, derive facts about these as follows:

 $\circ \quad \text{Constraint on} \ \ell$

$$\begin{split} \left\langle \ell,m \mid \boldsymbol{L}^{\! 2} \mid \ell,m \right\rangle &= \left\| L_{\!_{i}} \left| \ell,m \right\rangle \right\| \geq 0 \\ \left\langle \ell,m \mid \boldsymbol{L}^{\! 2} \mid \ell,m \right\rangle &= \ell(\ell+1) \left\langle \ell,m \left| \ell,m \right\rangle \end{split}$$

And so

$$\ell(\ell+1) \ge 0 \Rightarrow \boxed{\ell \ge 0}$$

 \circ Constraint on m

$$\begin{split} \left\langle \ell, m \mid L_{-}L_{+} \mid \ell, m \right\rangle &= \left\| L_{+} \mid \ell, m \right\rangle \right\| \geq 0 \\ \left\langle \ell, m \mid L_{+}L_{-} \mid \ell, m \right\rangle &= \left\langle \ell, m \mid \boldsymbol{L}^{2} - L_{z}^{2} - \hbar L_{z} \mid \ell, m \right\rangle \end{split}$$

And so

$$\begin{split} \ell(\ell+1) &\geq m(m+1) \\ \text{When we have } \left| \ell, m_{\max} \right\rangle, \, \text{we have equality because } L_+ \left| \ell, m_{\max} \right\rangle = 0 \,, \\ \text{and so } m_{\max} &= \ell \,. \text{ Doing the same with } L_+ L_- \,, \, \text{we find} \\ \hline \left| -\ell \leq m \leq \ell \right| \end{split}$$

• Action of ladder operators – consider \hat{L}^2 and \hat{L}_z acting on $L_{\pm} | \ell, m \rangle$

to prove the lowering action. Write

$$\begin{split} L_{\pm} \left| \, \ell, m \right\rangle &= C_{\pm} \left| \, \ell, m \pm 1 \right\rangle \\ \left| C_{\pm}(\ell, m) \right|^2 &= \left\langle \ell, m \mid L_{\mp} L_{\pm} \mid \ell, m \right\rangle \end{split}$$

And then find ${\it C}_{\pm}$ by writing the product of ladder operators as above.

• To find
$$Y_{\ell m} = \left\langle \theta, \phi \, \Big| \, \ell, m \right\rangle$$

- Apply $\langle \theta, \phi |$ to the left of both sides of $L_{z} | \ell, m \rangle = \hbar m | \ell, m \rangle$
- o Separate variables, and get ϕ dependence directly.
- $\circ \quad \text{Apply } \left\langle \theta, \phi \right| \text{ to the left of both sides of } L_+ \left| \ell, \ell \right\rangle = 0 \text{ to find } Y_{\ell \ell}$
- Lower to find others.

Note that $Y_{1,0}$ is a dumbbell, but $Y_{1,\pm 1}$ are doughnuts.

- Half-integer ℓ is impossible for spatial wavefunctions, because they can otherwise be lowered forever.
- The parity operator Π is defined by $\Pi | \mathbf{r} \rangle = | -\mathbf{r} \rangle$, and it is hermitian and unitary. It can be shown that

$$\Pi \left| \ell, m \right\rangle = \left(-1 \right)^{\ell} \left| \ell, m \right\rangle$$

• Separating variables on the Schrodinger Equation gives

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2\ell(\ell+1)}{2mr^2} + V(r)\right)U(r) = EU(r)$$

Where

$$\psi(\boldsymbol{r}) = \frac{1}{r} U(r) Y_{\ell m}(\theta, \phi)$$

And normalisation implies that

$$\int_0^\infty \left| U(r) \right|^2 \mathrm{d}r = 1$$

- We can derive some asymptotic conditions on U:
 - If $U(r) \underset{r \to 0}{\rightarrow} r^{s}$, then $S = \ell + 1$, assuming that the potential is no more singular than 1/r. Can be shown by solving the above and normalising, or by requiring H to be Hermitian.

- Assuming that V vanishes at infinity, then $U(r) \sim e^{\pm r \sqrt{-2mE/\hbar^2}}$, and depending on whether E > 0 or E < 0, we get planes waves or decaying exponentials.
- When "sketching" states:
 - o The states starts off as $U(r) \sim r^{\ell+1}$
 - $\circ~{\rm At}~\infty$, we either have a sinusoidal function or a decaying exponential.
 - In between, we have oscillatory behaviour, where a higher potential (less energy) means a higher amplitude and a longer wavelength.

• The super symmetric method

- We define pairs of related Hamiltonians, $H^{(1)} = \mathcal{A}^{\dagger}\mathcal{A}$, $H^{(2)} = \mathcal{A}\mathcal{A}^{\dagger}$. [Note that in each of the Hamiltonians, only the sign of the \mathcal{W}' changes].
- o Important facts are that:
 - 1. $H^{(1)}$ and $H^{(2)}$ have the same energy spectrum, and if ϕ_n is an eigenstate of $H^{(1)}$, then $\mathcal{A}\phi_n$ is an eigenstate of $H^{(2)}$ with the same eigenvalue.
 - **2.** There is usually some sort of relationship between $H^{(1)}$ and $H^{(2)}$.
 - **3.** Only one of $H^{(1)}$ and $H^{(2)}$ can have a normalisable state with 0 energy.
- So the tactic for these problems is
 - Use **3** to get a state of $H^{(1)}$, say.
 - Use **2** to get the next level state, but for $H^{(2)}$.
 - Use 1 to make that into a state of $H^{(1)}$
 - Rinse, lather, repeat...

Spin

- Eigenvalues of the Pauli matrices are
 - $\begin{array}{lll} \circ & \frac{\sqrt{2}}{2}(1,-1) \ \text{and} \ \frac{\sqrt{2}}{2}(1,1) \ \text{for} \ \sigma_x. \\ \circ & \frac{\sqrt{2}}{2}(-i,1) \ \text{and} \ \frac{\sqrt{2}}{2}(1,-i) \ \text{for} \ \sigma_y. \end{array}$

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• We can decompose any 2 by 2 matrix into

$$\begin{bmatrix} \boldsymbol{M} = a_0 \boldsymbol{I} + \boldsymbol{a} \cdot \boldsymbol{\sigma} \\ a_0 = \frac{1}{2} \operatorname{tr} \left(\boldsymbol{M} \right) & \boldsymbol{a} = \frac{1}{2} \operatorname{tr} \left(\boldsymbol{M} \boldsymbol{\sigma} \right) \end{bmatrix}$$

Addition of Angular Momenta

- Two angular momenta L and L', with J = L + L' can be described in two difference bases
 - $\begin{array}{l} \circ \quad \hat{\boldsymbol{L}}^{2}, \hat{\boldsymbol{L}}'^{2}, \hat{\boldsymbol{L}}_{z}, \hat{\boldsymbol{L}}'_{z}, \text{ and states are } \left| \ell, \ell', m_{\ell}, m_{\ell}' \right\rangle \\ \circ \quad \hat{\boldsymbol{L}}^{2}, \hat{\boldsymbol{L}}'^{2}, \hat{\boldsymbol{J}}^{2}, \hat{\boldsymbol{J}}_{z}, \text{ and states are } \left| \ell, \ell', J, M_{j} \right\rangle \end{array}$
- It is useful to have the $L \cdot L'$ operator in the two bases

$$\hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{L}}' = \frac{1}{2} \Big(\hat{\boldsymbol{J}}^2 - \hat{\boldsymbol{L}}^2 - \hat{\boldsymbol{L}}'^2 \Big) \\ \hat{\boldsymbol{L}} \cdot \hat{\boldsymbol{L}}' = \hat{L}_z \hat{L}_z' + \hat{L}_x \hat{L}_x' + \hat{L}_y \hat{L}_y' = \hat{L}_z \hat{L}_z' + \frac{1}{2} \Big(\hat{L}_+ \hat{L}_-' + \hat{L}_- \hat{L}_+' \Big)$$

In systems in which both bases are referred to in the Hamiltonian, it pays to stay in the \hat{L}^2 , \hat{L}'^2 , \hat{L}'_z , \hat{L}'_z basis and diagonalise the Hamiltonian.

- The transformations between the two bases are listed in tables, and are obtained roughly as follows:
 - Start from the maximum J and M_j value (trivially obtained by adding all the maximum states). Lower using the ladder operators.
 - Find the state with J 1 and $M_j = J 1$ by using the fact it will be orthogonal to the $J, M_j = J - 1$ state. Lower.
 - o Rinse, lather, repeat...

Identical Particles

\$\heta_{ij}\$ is the exchange operator - it exchanges all the labels i and j in a state. It is Hermitian and unitary, and can have eigenvalues + 1 (bosons with integer spin) or -1 (fermions with half-integer spin).

- Constructing symmetric and antisymmetric wavefunctions
 - Consider **N** Fermions (1, 2, ..., N) which could be in any state $\alpha, \beta, ..., \nu$. The most general antisymmetric linear combination of these states is given by the Slater Determinant

$$\Psi(1,2,\cdots,N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} u_{\alpha}(1) & u_{\alpha}(2) & \cdots & u_{\alpha}(N) \\ u_{\beta}(1) & u_{\beta}(2) & \cdots & u_{\beta}(N) \\ \vdots & \vdots & & \vdots \\ u_{\nu}(1) & u_{\nu}(2) & \cdots & u_{\nu}(N) \end{vmatrix}$$

Thus, if we're looking for a state in which we know one particle is in α , one in β and one in γ , we simply calculate the above. Notes:

- Swapping one particle does exactly what is expected.
- If *any* states are identical, the determinant goes to 0 and the wavefunction **cannot** be anti-symmetrised.
- For *N* bosons, similar considerations apply, but with all the alternating signs in the Slater determinant changed to "positives".
- <u>General results</u> if we have N particles and j possible states, then the number of different three particle states possible is
 - o j^N if the particles are **distinguishable**.
 - o ${}^{N+j-1}C_{j-1}$ if the particles are **indistinguishable bosons**. [Placing j-1 barriers between N + j 1 states].
 - \circ ${}^{j}C_{N}$ if the particles are indistinguishable fermions.
- <u>Spatial and spin parts</u>
 - It is also possible to factor a wavefunction into **spin** and **spatial** wavefunctions. It is the **product of both** that has to satisfy appropriate symmetry.
 - We can **individually symmetrise/antisymmetrise** each part using the tactics above.
 - In general, for the $\ell \otimes \ell'$ spin case, states with resulting **even** J will be even, and states with resulting **odd** J will be odd.
- <u>Correlation and exchange forces</u>

- **Symmetric** wavefunctions result in particles appearing to "attract" each other, and vice-versa.
- Thus, energy levels in the Helium molecule are *lower* when spins are *aligned* (symmetric) because the spatial part then has to be *antisymmetric*, which results in less repulsion.
- Similarly, bonds are caused by *antisymmetric* spins, which then cause the electrons to attract.