FY2045 Quantum Mechanics I

Fall 2023

Henning Goa Hugdal

Week 9

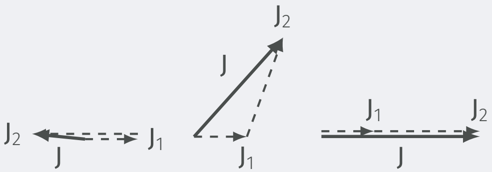
Addition of angular momenta

Addition of two angular momenta

How do we treat addition of angular momenta, $\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2$?

Classical case

$|\mathbf{J}|$ can vary continuously between $||\mathbf{J}_1| - |\mathbf{J}_2||$ and $|\mathbf{J}_1| + |\mathbf{J}_2|$



Quantum mechanical case

More complicated! Two questions arise:

i) What quantum numbers j can we have for $\mathbf{J}$, when $\mathbf{J}_1$ and $\mathbf{J}_2$ have quantum numbers j_1 and j_2.

ii) How do we express the eigenstates of $\mathbf{J}$ in terms of eigenstates of $\mathbf{J}_1$ and $\mathbf{J}_2$?

Two particles with spin ½

Two particles with quantum numbers $s_1 = s_2 = \frac{1}{2}$, and m_1, m_2. Four possible states:

$$\begin{aligned} &|\uparrow\uparrow\rangle\,,\ m = 1, \\ &|\uparrow\downarrow\rangle\,,\ m = 0, \\ &|\downarrow\uparrow\rangle\,,\ m = 0, \\ &|\downarrow\downarrow\rangle\,,\ m = -1, \end{aligned}$$

where $m = m_1 + m_2$. Since $m = 0, \pm 1$, we would expect $s = 1$, but we have one state too many!

Solution: Two different combinations for the total spin states $|sm\rangle$:

$$\left.\begin{aligned} |11\rangle &= |\uparrow\uparrow\rangle \\ |10\rangle &= \tfrac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle] \\ |1\text{-}1\rangle &= |\downarrow\downarrow\rangle \end{aligned}\right\} s = 1 \text{ (triplet)}$$

$$\left.|00\rangle = \tfrac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]\ \right\} s = 0 \text{ (singlet)}$$

The combination of two particles with spin ½ can carry total spin of **1 or 0**.

General addition of angular momenta

Adding two angular momenta described by

$$|j_1\, m_1\rangle\,, \quad m_1 = -j_1, -j_1+1, \ldots, j_1,$$
$$|j_2\, m_2\rangle\,, \quad m_2 = -j_2, -j_2+1, \ldots, j_2,$$

the total quantum number j can take the values

$$j = j_1 + j_2,\, j_1 + j_2 - 1,\, \ldots,\, |j_1 - j_2|.$$

The “new” or total spin states are

$$|j\, m\rangle = \sum_{m_1+m_2=m} C^{j_1 j_2 j}_{m_1 m_2 m}\, |j_1\, j_2\, m_1\, m_2\rangle\,,$$

where $C^{j_1 j_2 j}_{m_1 m_2 m}$ are **Clebsch-Gordan coefficients**.

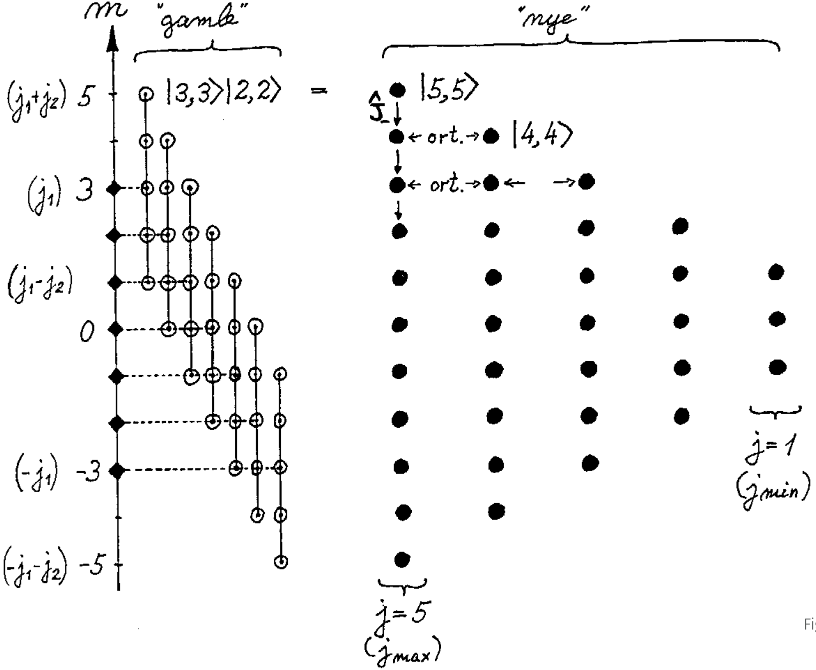


Figure by I. Øverbø.

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where $C^{j_1 j_2 j}_{m_1 m_2 m}$ are **Clebsch-Gordan coefficients**.

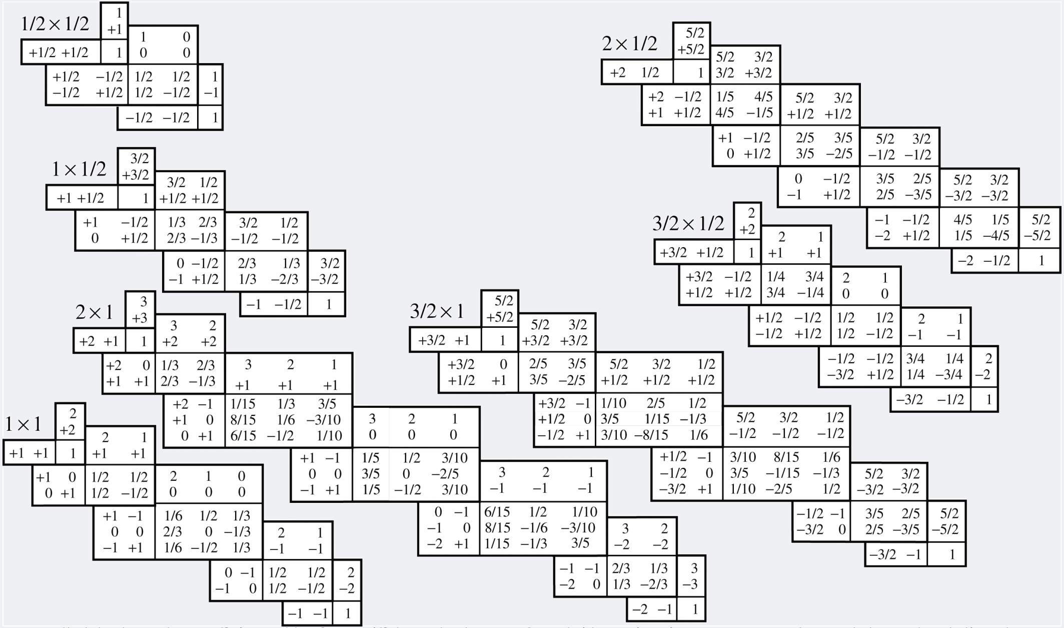
Two spin ½

$C^{j_1 j_2 j}_{m_1 m_2 m}$ given in table

1/2 × 1/2		1 +1	1 0	0 0	1 −1
+1/2	+1/2	$\boxed{1}$			
+1/2	−1/2		1/2	$\boxed{1/2}$	
−1/2	+1/2		1/2	$\boxed{-1/2}$	
−1/2	−1/2				1

Examples:

$$|11\rangle = C^{\frac{1}{2}\frac{1}{2}1}_{\frac{1}{2}\frac{1}{2}1}\, |\uparrow\uparrow\rangle = |\uparrow\uparrow\rangle$$
$$|00\rangle = C^{\frac{1}{2}\frac{1}{2}0}_{\frac{1}{2}-\frac{1}{2}0}\, |\uparrow\downarrow\rangle + C^{\frac{1}{2}\frac{1}{2}0}_{-\frac{1}{2}\frac{1}{2}0}\, |\downarrow\uparrow\rangle$$
$$= \frac{1}{\sqrt{2}}[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle].$$



All Clebsch-Gordan coefficient tables from Griffiths and Schroeter, ©Cambridge University Press 2018. Background changed and clipped.

Example — Electron with orbital angular momentum and spin

The electron in a hydrogen atom can have both orbital and spin angular momentum, $\mathbf{J} = \mathbf{L} + \mathbf{S}$;

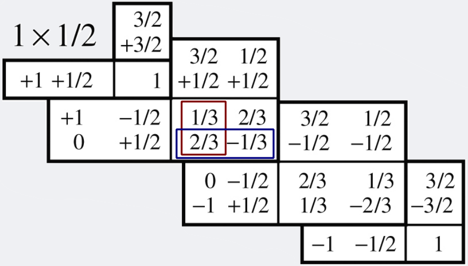
$$j = l - \frac{1}{2}, \text{ or } j = l + \frac{1}{2}, \text{ (assuming } l > 0\text{)}.$$

For $l = 1$, we can construct e.g. the "new" state

$$\left|\frac{3}{2}\,\frac{1}{2}\right\rangle = \frac{1}{\sqrt{3}}\left|1\,\frac{1}{2}\,1 - \frac{1}{2}\right\rangle + \sqrt{\frac{2}{3}}\left|1\,\frac{1}{2}\,0\,\frac{1}{2}\right\rangle,$$

or the "old" state

$$\left|1\,\frac{1}{2}\,0\,\frac{1}{2}\right\rangle = \sqrt{\frac{2}{3}}\left|\frac{3}{2}\,\frac{1}{2}\right\rangle - \frac{1}{\sqrt{3}}\left|\frac{1}{2}\,\frac{1}{2}\right\rangle.$$



Addition of several angular momenta

When adding several angular momenta

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3 + \ldots,$$

we do the additions in a step-wise fashion:

1) The combination $\mathbf{J}_{12} = \mathbf{J}_1 + \mathbf{J}_2$ has possible quantum numbers $|j_1 - j_2| \leq j_{12} \leq j_1 + j_2$,
2) The combination $\mathbf{J}_{13} = \mathbf{J}_{12} + \mathbf{J}_3$ has possible quantum numbers $|j_{12} - j_3| \leq j_{12} \leq j_{12} + j_3$,
3) ...

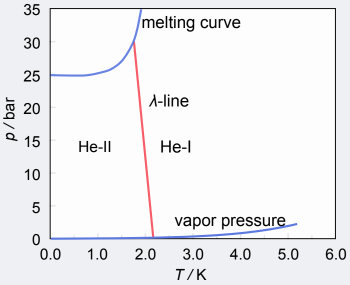
Example — Helium-4 vs. Helium-3

Helium-4

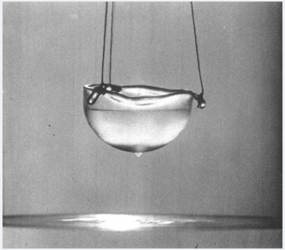
${}^4_2$He has two protons, **two** neutrons and two electrons.

Total spin $S = 0$ — this is a **boson**!

Can form Bose-Einstein condensate, becomes a superfluid below ~ 2 K.



Wikipedia, CC BY-SA 3.0. Background added.



By Alfred Leitner - Own work, Public Domain.

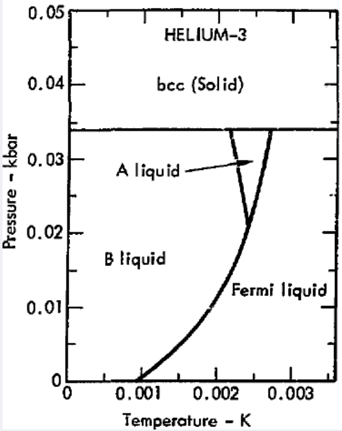
Example — Helium-4 vs. Helium-3

Helium-3

${}^{3}_{2}$He has two protons, **one** neutron and two electrons.

Total spin $S = \frac{1}{2}$ — this is a **fermion**!

A superfluid below $\sim 1\,\text{mK}$ — how?



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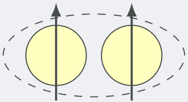
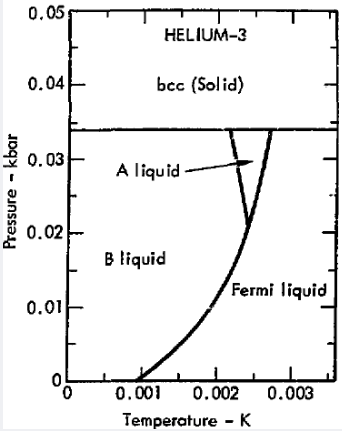
Helium-3 atoms can form pairs — with integer spin!



Helium-3 pair



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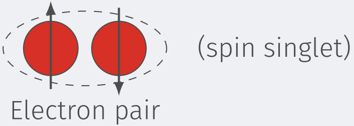
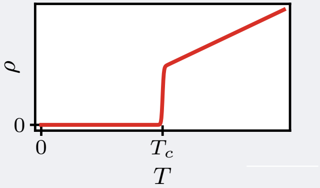
For more information see e.g. Nobel Focus: Helium Impersonates a Superconductor.

Tangent #1 — Superconductivity

Electrons can also form pairs!

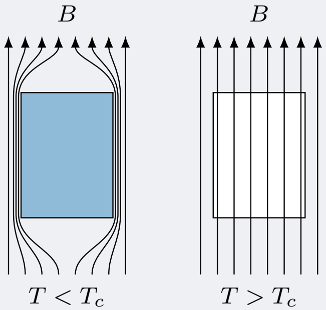




If they condense we get a charged superfluid — a **superconductor**.

Below a certain temperature T_c

- currents flow without resistance ($\rho = 0$),
- magnetic fields are expelled.

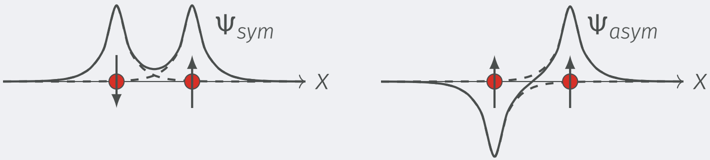


Tangent #2 — Ferromagnetism

Since electrons have magnetic moments due to spin, they behave like tiny magnets.

If many spins align spontaneously in the same direction we have a **ferromagnet**!

Why do they sometimes align in this way? Due to **exchange interactions**:



The antisymmetric configuration reduces the **electrostatic energy** of the electrons — hence parallel spins are favored.

Tangent #3 — Quantum information

In traditional computers the building blocks are **bits** that can be either 1 or 0.

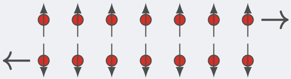
In quantum computers one wants to use quantum bits (**qubits**) that can be in states $|1\rangle$ or $|0\rangle$ — or a **superposition** of them.

Spin qubit

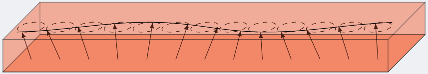
Use spins as bits?

$$|\uparrow\rangle = |1\rangle\,,$$
$$|\downarrow\rangle = |0\rangle\,.$$

Spin currents

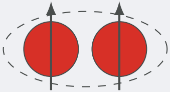


or



Spin supercurrents

Generate triplet electron pairs using e.g. magnets



Electron pair

Atoms and the periodic table

For a neutral atom of atomic number Z, with a nucleus with charge Ze and Z electrons with mass m_e and charge $-e$, we have the Hamiltonian

$$H = \sum_{j=1}^{Z} \Bigg\{ -\frac{\hbar^2}{2m_e}\nabla_j^2 - \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r_j} \qquad \text{(kinetic + el-nucl interaction)}$$

$$+ \frac{1}{2}\frac{1}{4\pi\epsilon_0}\sum_{k\neq j}\frac{e^2}{|\mathbf{r}_j - \mathbf{r}_k|}\Bigg\} \qquad \text{(el-el interaction).}$$

We need to solve $H\psi = E\psi$ for wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_Z)$, but can **only be solved exactly for hydrogen,** $Z = 1$. In practice one must use approximation methods.

We will sketch some **qualitative** features.

Helium — $Z = 2$

For $Z = 2$, we get

$$H = \left\{-\frac{\hbar^2}{2m_e}\nabla_1^2 - \frac{1}{4\pi\epsilon_0}\frac{2e^2}{r_1}\right\} + \left\{-\frac{\hbar^2}{2m_e}\nabla_2^2 - \frac{1}{4\pi\epsilon_0}\frac{2e^2}{r_2}\right\} + \frac{1}{4\pi\epsilon_0}\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$
$$\equiv H_1 + H_2 + H_{\mathrm{el-el}},$$

with hydrogenic Hamiltonians H_i, $i = 1, 2$ with nuclear charge $2e$, and electron-electron repulsion term $H_{\mathrm{el-el}}$.

If we ignore $H_{\mathrm{el-el}}$:

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi_{nlm}(\mathbf{r}_1)\psi_{n'l'm'}(\mathbf{r}_2),$$
$$E = 4(E_n + E_{n'}),$$

with hydrogen wavefunctions ψ_{nlm} with half the Bohr radius, and $E_n = -13.6/n^2$ eV.

Helium — Ground state

Using this approximation, we get

$$E_0 = \; -109\,\text{eV}$$

and

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2) = \psi_{100}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2),$$

with electrons in the singlet state.

This is lower than the experimental value

$$E_0^{\mathrm{exp}} = -78.975\,\text{eV},$$

since we neglected the **positive** $H_{\mathrm{el-el}}$,

$$H_{\mathrm{el-el}} = \frac{1}{4\pi\epsilon_0}\frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}.$$

Helium — Excited states

For excited states, one electron is in $n = 1$, one is in $n > 1$,

$$\psi_{nlm}\psi_{100}.$$

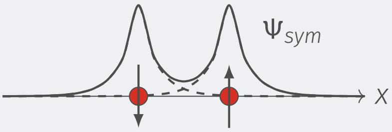
Total state must be antisymmetric:

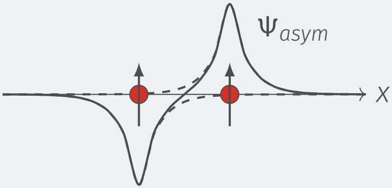
Parahelium

$$\underbrace{[\psi_{nlm}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2) + \psi_{nlm}(\mathbf{r}_2)\psi_{100}(\mathbf{r}_1)]}_{\text{symmetric}}\underbrace{[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]}_{\text{singlet}}$$

Orthohelium

$$\underbrace{[\psi_{nlm}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2) - \psi_{nlm}(\mathbf{r}_2)\psi_{100}(\mathbf{r}_1)]}_{\text{antisymmetric}}\underbrace{\begin{cases} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \\ |\downarrow\downarrow\rangle \end{cases}}_{\text{triplet}}$$





The expectation value for the separation is smaller for the symmetric wavefunction.

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$$\psi_{nlm}\psi_{100}.$$

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Orthohelium

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Interaction energy due to $H_{\mathrm{el-el}}$ higher for parahelium, giving parahelium states slightly higher energies than orthohelium states with the same (nlm).