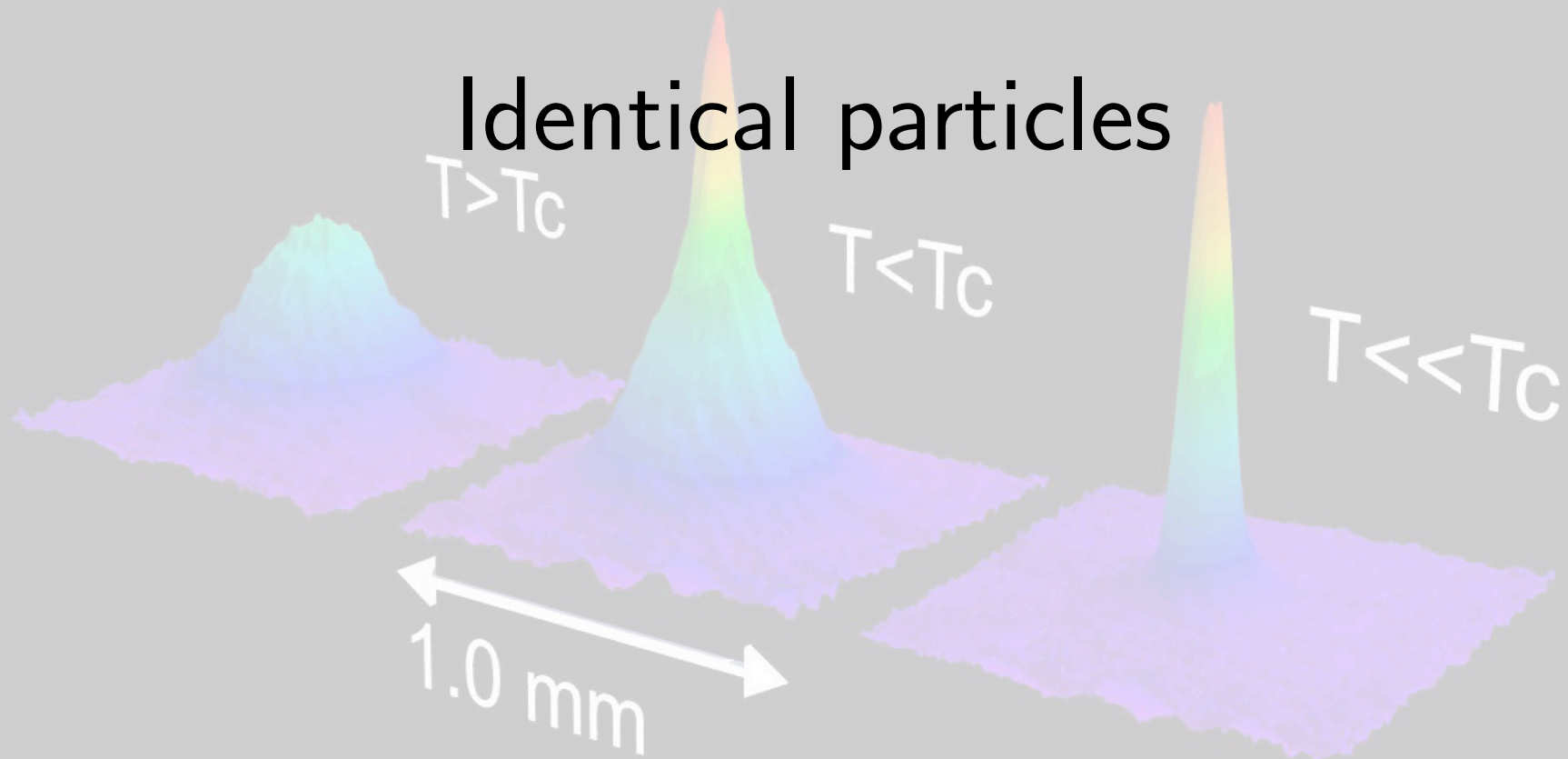


Lecture 11

Identical particles



Identical particles

- Until now, our focus has largely been on the study of quantum mechanics of *individual* particles.
- However, most physical systems involve interaction of many (ca. 10^{23} !) particles, e.g. electrons in a solid, atoms in a gas, etc.
- In classical mechanics, particles are always distinguishable – at least formally, “trajectories” through phase space can be traced.
- In quantum mechanics, particles can be **identical** and **indistinguishable**, e.g. electrons in an atom or a metal.
- The intrinsic uncertainty in position and momentum therefore demands separate consideration of distinguishable and indistinguishable quantum particles.
- Here we define the quantum mechanics of many-particle systems, and address (just) a few implications of particle indistinguishability.

Quantum statistics: preliminaries

- Consider two identical particles confined to one-dimensional box.
By “identical”, we mean particles that can not be discriminated by some internal quantum number, e.g. electrons of same spin.
- The two-particle wavefunction $\psi(x_1, x_2)$ only makes sense if

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2 \Rightarrow \psi(x_1, x_2) = e^{i\alpha} \psi(x_2, x_1)$$

- If we introduce **exchange operator** $\hat{P}_{\text{ex}} \psi(x_1, x_2) = \psi(x_2, x_1)$, since $\hat{P}_{\text{ex}}^2 = \mathbb{I}$, $e^{2i\alpha} = 1$ showing that $\alpha = 0$ or π , i.e.

$$\begin{aligned} \psi(x_1, x_2) &= \psi(x_2, x_1) && \text{bosons} \\ \psi(x_1, x_2) &= -\psi(x_2, x_1) && \text{fermions} \end{aligned}$$

[N.B. in two-dimensions (such as fractional quantum Hall fluid) “quasi-particles” can behave as though $\alpha \neq 0$ or π – **anyons!**]

Quantum statistics: preliminaries

- But which sign should we choose?

$\psi(x_1, x_2) = \psi(x_2, x_1)$	bosons
$\psi(x_1, x_2) = -\psi(x_2, x_1)$	fermions

- All elementary particles are classified as fermions or bosons:

Three Generations of Matter (Fermions)

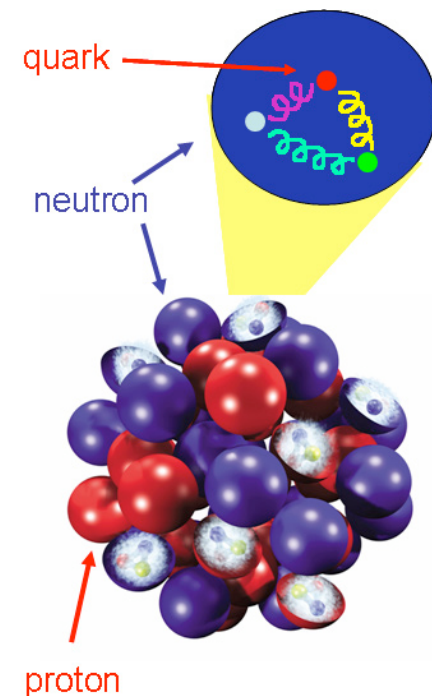
	I	II	III	
mass→	3 MeV	1.24 GeV	172.5 GeV	0
charge→	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0
spin→	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1 γ
name→	u up	c charm	t top	photon
	6 MeV	95 MeV	4.2 GeV	0
	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	0
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
Quarks	d down	s strange	b bottom	g gluon
	<2 eV	<0.19 MeV	<18.2 MeV	90.2 GeV
	0	0	0	0
	$\frac{1}{2}$ ν	$\frac{1}{2}$ ν	$\frac{1}{2}$ ν	1
	e electron neutrino	μ muon neutrino	τ tau neutrino	Z ⁰ weak force
	0.511 MeV	106 MeV	1.78 GeV	80.4 GeV
	-1	-1	-1	± 1
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
Leptons	e electron	μ muon	τ tau	W [±] weak force

Bosons (Forces)

- Particles with **half-integer spin are fermions** and their wavefunction must be antisymmetric under particle exchange.
e.g. electron, positron, neutron, proton, quarks, muons, etc.
- Particles with **integer spin (including zero) are bosons** and their wavefunction must be symmetric under particle exchange.
e.g. pion, kaon, photon, gluon, etc.

Quantum statistics: remarks

- Within non-relativistic quantum mechanics, correlation between spin and statistics can be seen as an empirical law.
- However, the **spin-statistics relation** emerges naturally from the unification of quantum mechanics and special relativity.
- The rule that fermions have half-integer spin and bosons have integer spin is internally consistent:
e.g. Two identical nuclei, composed of n nucleons (fermions), would have integer or half-integer spin and would transform as a “composite” fermion or boson according to whether n is even or odd.



Quantum statistics: fermions

- To construct wavefunctions for three or more fermions, let us suppose that they do not interact, and are confined by a spin-independent potential,

$$\hat{H} = \sum_i \hat{H}_s[\hat{\mathbf{p}}_i, \mathbf{r}_i], \quad \hat{H}_s[\hat{\mathbf{p}}, \mathbf{r}] = \frac{\hat{\mathbf{p}}^2}{2m} + V(\mathbf{r})$$

- Eigenfunctions of Schrödinger equation involve products of states of single-particle Hamiltonian, \hat{H}_s .
- However, simple products $\psi_a(1)\psi_b(2)\psi_c(3)\cdots$ do not have required antisymmetry under exchange of any two particles.
Here a, b, c, \dots label eigenstates of \hat{H}_s , and $1, 2, 3, \dots$ denote *both* space and spin coordinates, i.e. 1 stands for (\mathbf{r}_1, s_1) , etc.

Quantum statistics: fermions

- We could achieve antisymmetrization for particles 1 and 2 by subtracting the same product with 1 and 2 interchanged,

$$\psi_a(1)\psi_b(2)\psi_c(3) \mapsto [\psi_a(1)\psi_b(2) - \psi_a(2)\psi_b(1)]\psi_c(3)$$

- However, wavefunction must be antisymmetrized under *all* possible exchanges. So, for 3 particles, we must add together all 3! permutations of 1, 2, 3 in the state a, b, c with factor -1 for each particle exchange.
- Such a sum is known as a **Slater determinant**:

$$\psi_{abc}(1, 2, 3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \psi_a(1) & \psi_b(1) & \psi_c(1) \\ \psi_a(2) & \psi_b(2) & \psi_c(2) \\ \psi_a(3) & \psi_b(3) & \psi_c(3) \end{vmatrix}$$

and can be generalized to N , $\psi_{i_1, i_2, \dots, i_N}(1, 2, \dots, N) = \det(\psi_i(n))$

Quantum statistics: fermions

$$\psi_{abc}(1, 2, 3) = \frac{1}{\sqrt{3!}} \begin{vmatrix} \psi_a(1) & \psi_b(1) & \psi_c(1) \\ \psi_a(2) & \psi_b(2) & \psi_c(2) \\ \psi_a(3) & \psi_b(3) & \psi_c(3) \end{vmatrix}$$

- Antisymmetry of wavefunction under particle exchange follows from antisymmetry of Slater determinant, $\psi_{abc}(1, 2, 3) = -\psi_{abc}(1, 3, 2)$.
- Moreover, determinant is non-vanishing only if all three states a , b , c are different – manifestation of **Pauli's exclusion principle**: two identical fermions can not occupy the same state.
- Wavefunction is exact for non-interacting fermions, and provides a useful platform to study weakly interacting systems from a perturbative scheme.

Quantum statistics: bosons

- In bosonic systems, wavefunction must be symmetric under particle exchange.
- Such a wavefunction can be obtained by expanding all of terms contributing to Slater determinant and setting all signs positive.
i.e. bosonic wave function describes uniform (equal phase) superposition of all possible permutations of product states.

Space and spin wavefunctions

- When Hamiltonian is spin-independent, wavefunction can be factorized into spin and spatial components.
- For two electrons (fermions), there are four basis states in spin space: the (antisymmetric) spin $S = 0$ singlet state,

$$|\chi_S\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)$$

and the three (symmetric) spin $S = 1$ triplet states,

$$|\chi_T^1\rangle = |\uparrow_1\uparrow_2\rangle, \quad |\chi_T^0\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1\downarrow_2\rangle + |\downarrow_1\uparrow_2\rangle), \quad |\chi_T^{-1}\rangle = |\downarrow_1\downarrow_2\rangle$$

Space and spin wavefunctions

- For a general state, total wavefunction for two electrons:

$$\Psi(\mathbf{r}_1, s_1; \mathbf{r}_2, s_2) = \psi(\mathbf{r}_1, \mathbf{r}_2)\chi(s_1, s_2)$$

where $\chi(s_1, s_2) = \langle s_1, s_2 | \chi \rangle$.

- For two electrons, total wavefunction, Ψ , must be antisymmetric under exchange.
i.e. spin singlet state must have symmetric spatial wavefunction;
spin triplet states have antisymmetric spatial wavefunction.
- For three electron wavefunctions, situation becomes challenging... see notes.
- The conditions on wavefunction antisymmetry imply spin-dependent correlations even where the Hamiltonian is spin-independent, and leads to numerous physical manifestations...

Example I: Specific heat of hydrogen H₂ gas

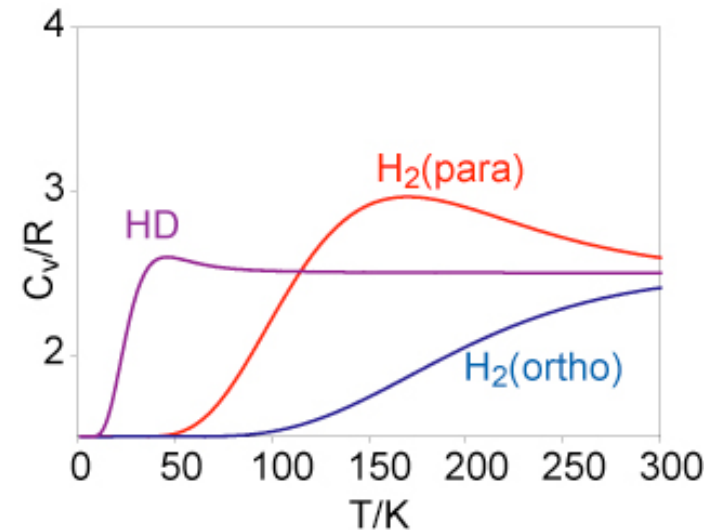
- With two spin 1/2 proton degrees of freedom, H₂ can adopt a spin singlet (parahydrogen) or spin triplet (ortho-hydrogen) wavefunction.
- Although interaction of proton spins is negligible, spin statistics constrain available states:

Since parity of state with rotational angular momentum ℓ is given by $(-1)^\ell$, parahydrogen having symmetric spatial wavefunction has ℓ even, while for ortho-hydrogen ℓ must be odd.

- Energy of rotational level with angular momentum ℓ is

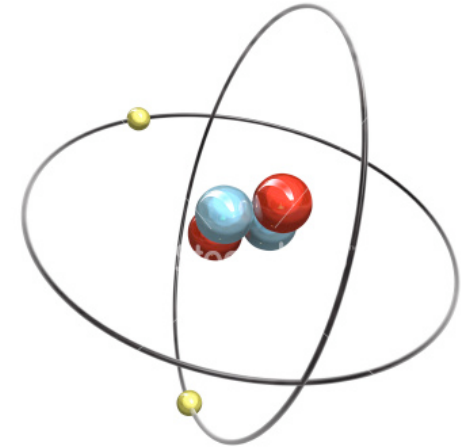
$$E_\ell^{\text{rot}} = \frac{1}{2I} \hbar^2 \ell(\ell + 1)$$

where I denotes moment of inertia \rightsquigarrow
very different specific heats (cf. IB).



Example II: Excited states spectrum of Helium

- Although, after hydrogen, helium is simplest atom with two protons ($Z = 2$), two neutrons, and two bound electrons, the Schrödinger equation is analytically intractable.



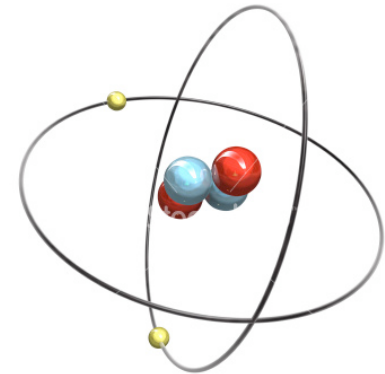
- In absence of electron-electron interaction, electron Hamiltonian

$$\hat{H}^{(0)} = \sum_{n=1}^2 \left[\frac{\hat{\mathbf{p}}_n^2}{2m} + V(r_n) \right], \quad V(r) = -\frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r}$$

is separable and states can be expressed through eigenstates, ψ_{nlm} , of hydrogen-like Hamiltonian.

Example II: Excited states spectrum of Helium

$$\hat{H}^{(0)} = \sum_{n=1}^2 \left[\frac{\hat{\mathbf{p}}_n^2}{2m} + V(r_n) \right]$$



- In this approximation, ground state wavefunction involves both electrons in 1s state \rightsquigarrow antisymmetric spin singlet wavefunction, $|\Psi_{\text{g.s.}}\rangle = (|100\rangle \oplus |100\rangle)|\chi_S\rangle$.
- Previously, we have used perturbative theory to determine how ground state energy is perturbed by electron-electron interaction,

$$\hat{H}^{(1)} = \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

- What are implications of particle statistics on spectrum of lowest excited states?

Example II: Excited states spectrum of Helium

- Ground state wavefunction belongs to class of states with symmetric spatial wavefunctions, and antisymmetric spin (singlet) wavefunctions – **parahelium**.
- In the absence of electron-electron interaction, $\hat{H}^{(1)}$, first excited states in the same class are degenerate:

$$|\psi_{\text{para}}\rangle = \frac{1}{\sqrt{2}} (|100\rangle \otimes |2\ell m\rangle + |2\ell m\rangle \otimes |100\rangle) |\chi_S\rangle$$

- Second class have antisymmetric spatial wavefunction, and symmetric (triplet) spin wavefunction – **orthohelium**. Excited states are also degenerate:

$$|\psi_{\text{ortho}}\rangle = \frac{1}{\sqrt{2}} (|100\rangle \otimes |2\ell m\rangle - |2\ell m\rangle \otimes |100\rangle) |\chi_T^{m_s}\rangle$$

Example II: Excited states spectrum of Helium

$$|\psi_{p,o}\rangle = \frac{1}{\sqrt{2}} (|100\rangle \otimes |2\ell m\rangle \pm |2\ell m\rangle \otimes |100\rangle) |\chi_{S,T}^{m_s}\rangle$$

- Despite degeneracy, since off-diagonal matrix elements between different m, ℓ values vanish, we can invoke first order perturbation theory to determine energy shift for ortho- and parahelium,

$$\begin{aligned} \Delta E_{n\ell}^{p,o} &= \langle \psi_{p,o} | \hat{H}^{(1)} | \psi_{p,o} \rangle \\ &= \frac{1}{2} \frac{e^2}{4\pi\epsilon_0} \int d^3r_1 d^3r_2 \frac{|\psi_{100}(\mathbf{r}_1)\psi_{n\ell 0}(\mathbf{r}_2) \pm \psi_{n\ell 0}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \end{aligned}$$

(+) parahelium and (-) orthohelium.

- N.B. since matrix element is independent of m , $m = 0$ value considered here applies to all values of m .

Example II: Excited states spectrum of Helium

$$\Delta E_{nl}^{\text{p,o}} = \frac{1}{2} \frac{e^2}{4\pi\epsilon_0} \int d^3 r_1 d^3 r_2 \frac{|\psi_{100}(\mathbf{r}_1)\psi_{nl0}(\mathbf{r}_2) \pm \psi_{nl0}(\mathbf{r}_1)\psi_{100}(\mathbf{r}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

- Rearranging this expression, we obtain

$$\Delta E_{nl}^{\text{p,o}} = J_{nl} \pm K_{nl}$$

where diagonal and cross-terms given by

$$J_{nl} = \frac{e^2}{4\pi\epsilon_0} \int d^3 r_1 d^3 r_2 \frac{|\psi_{100}(\mathbf{r}_1)|^2 |\psi_{nl0}(\mathbf{r}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

$$K_{nl} = \frac{e^2}{4\pi\epsilon_0} \int d^3 r_1 d^3 r_2 \frac{\psi_{100}^*(\mathbf{r}_1)\psi_{nl0}^*(\mathbf{r}_2)\psi_{100}(\mathbf{r}_2)\psi_{nl0}(\mathbf{r}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

Example II: Excited states spectrum of Helium

$$J_{nl} = \frac{e^2}{4\pi\epsilon_0} \int d^3r_1 d^3r_2 \frac{|\psi_{100}(\mathbf{r}_1)|^2 |\psi_{nl0}(\mathbf{r}_2)|^2}{|\mathbf{r}_1 - \mathbf{r}_2|} > 0$$

- Physically, J_{nl} represents electrostatic interaction energy associated with two charge distributions $|\psi_{100}(\mathbf{r}_1)|^2$ and $|\psi_{nl0}(\mathbf{r}_2)|^2$.

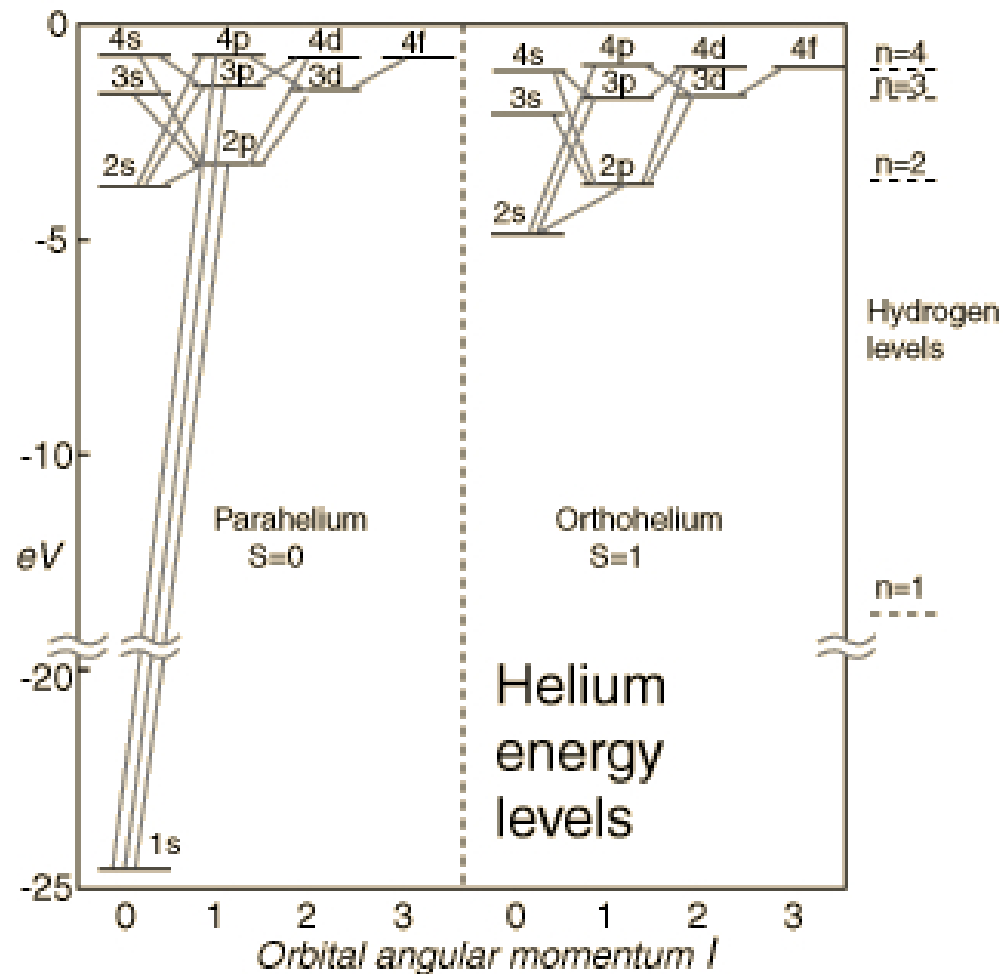
$$K_{nl} = \frac{e^2}{4\pi\epsilon_0} \int d^3r_1 d^3r_2 \frac{\psi_{100}^*(\mathbf{r}_1) \psi_{nl0}^*(\mathbf{r}_2) \psi_{100}(\mathbf{r}_2) \psi_{nl0}(\mathbf{r}_1)}{|\mathbf{r}_1 - \mathbf{r}_2|}$$

- K_{nl} represents **exchange term** reflecting antisymmetry of total wavefunction.
- Since $K_{nl} > 0$ and $\Delta E_{nl}^{\text{p,o}} = J_{nl} \pm K_{nl}$, there is a positive energy shift for parahelium and a negative for orthohelium.

Example II: Excited states spectrum of Helium

$$|\psi_{p,o}\rangle = \frac{1}{\sqrt{2}} (|100\rangle \otimes |nlm\rangle \pm |nlm\rangle \otimes |100\rangle) |\chi_{S,T}^{m_s}\rangle$$

$$\Delta E_{nl}^{p,o} = J_{nl} \pm K_{nl}$$



Example II: Excited states spectrum of Helium

- Finally, noting that, with $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$,

$$\begin{aligned}\frac{1}{\hbar^2} 2\mathbf{S}_1 \cdot \mathbf{S}_2 &= \frac{1}{\hbar^2} [(\mathbf{S}_1 + \mathbf{S}_2)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2] \\ &= S(S + 1) - 2 \times 1/2(1/2 + 1) = \begin{cases} 1/2 & \text{triplet} \\ -3/2 & \text{singlet} \end{cases}\end{aligned}$$

the energy shift can be written as

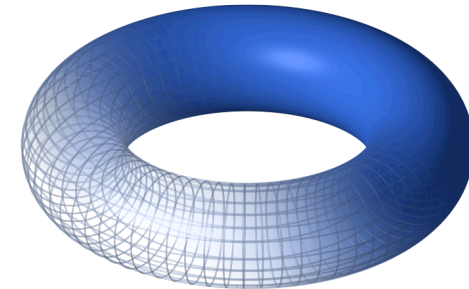
$$\Delta E_{nl}^{p,o} = J_{nl} - \frac{1}{2} \left(1 + \frac{4}{\hbar^2} \mathbf{S}_1 \cdot \mathbf{S}_2 \right) K_{nl}$$

- From this result, we can conclude that electron-electron interaction leads to effective **ferromagnetic** interaction between spins.
- Similar phenomenology finds manifestation in metallic systems as **Stoner ferromagnetism**.

Ideal quantum gases

- Consider free (i.e. non-interacting) non-relativistic quantum particles in a box of size L^d

$$\hat{H}_0 = \sum_{i=1}^N \frac{\hat{\mathbf{p}}_i^2}{2m}$$

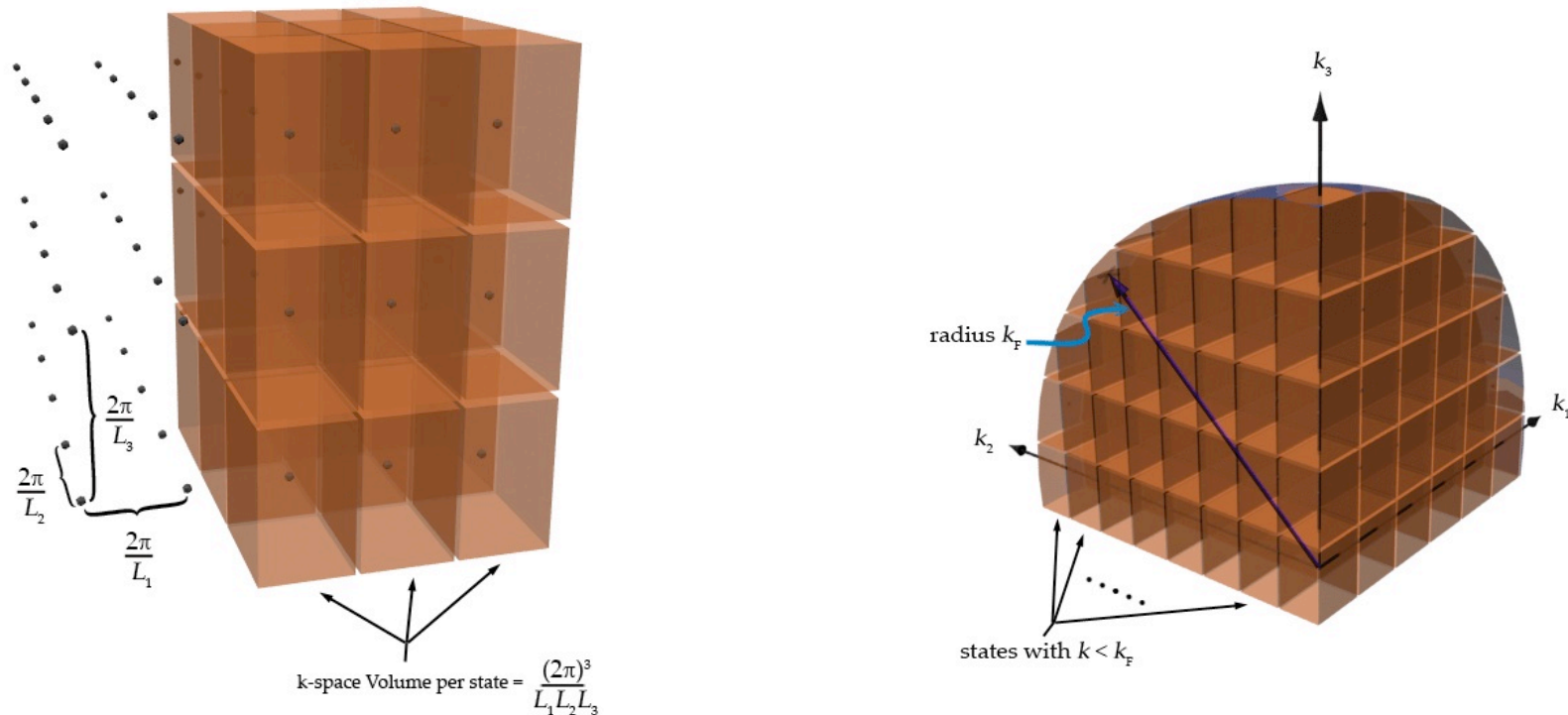


- For periodic boundary conditions, normalized eigenstates of Hamiltonian are plane waves, $\phi_{\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r} | \mathbf{k} \rangle = \frac{1}{L^{d/2}} e^{i\mathbf{k} \cdot \mathbf{r}}$, with

$$\mathbf{k} = \frac{2\pi}{L} (n_1, n_2, \dots, n_d), \quad n_i \text{ integer}$$

Ideal quantum gases: fermions

- In (spinless) fermionic system, Pauli exclusion prohibits multiple occupancy of single-particle states.



- Ground state obtained by filling up all states to **Fermi energy**, $E_F = \hbar^2 k_F^2 / 2m$ with k_F the **Fermi wavevector**.

Ideal quantum gases: fermions

- Since each state is associated with a k -space volume $(2\pi/L)^d$, in three-dimensional system, total number of occupied states is given by $N = \left(\frac{L}{2\pi}\right)^3 \frac{4}{3}\pi k_F^3$, i.e. the particle density $n = N/L^3 = k_F^3/6\pi^2$,

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m} (6\pi^2 n)^{2/3}, \quad n(E) = \frac{1}{6\pi^2} \left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

- This translates to **density of states per unit volume**:

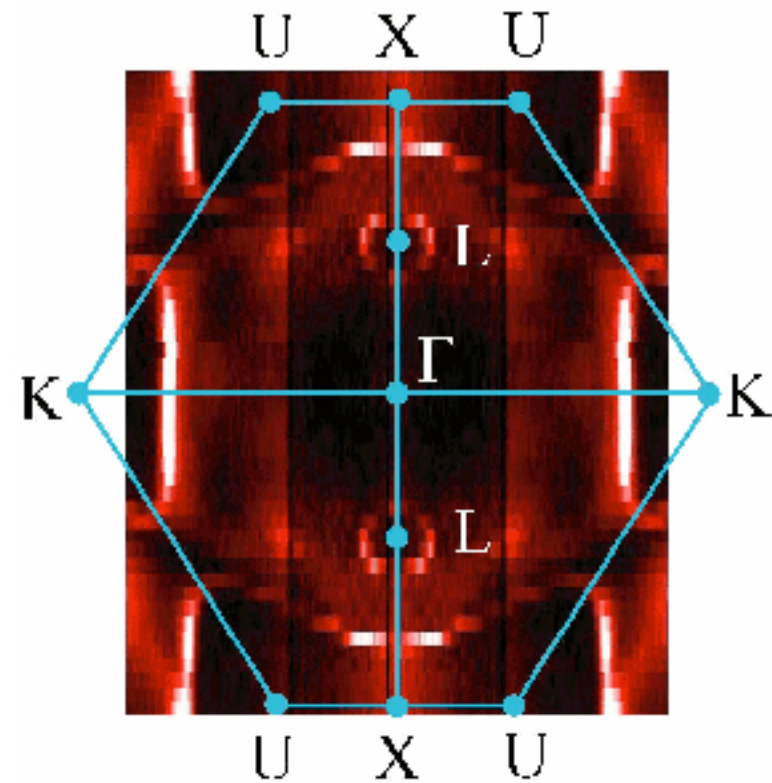
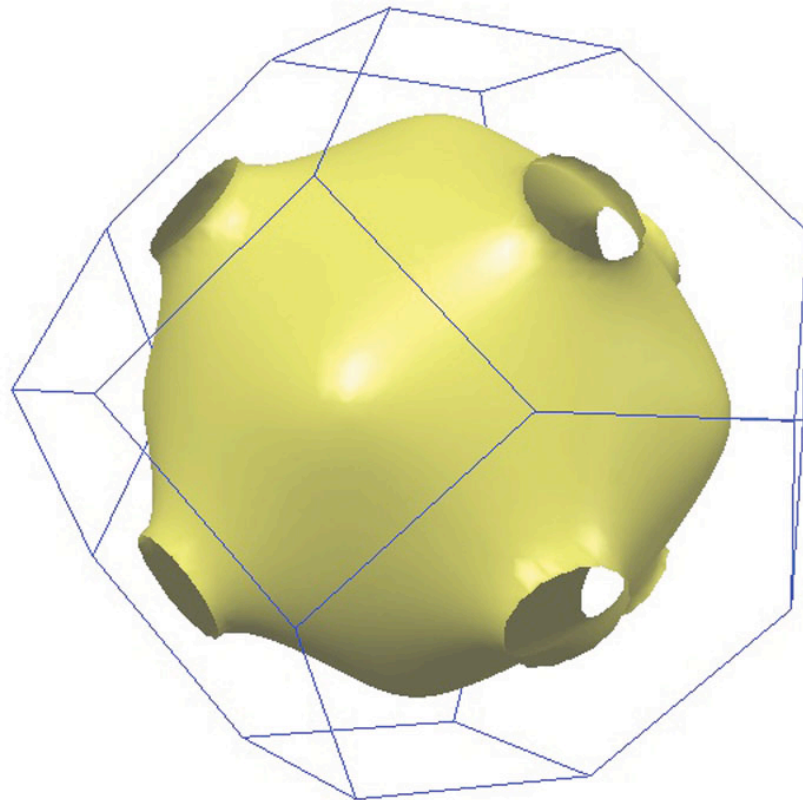
$$g(E) = \frac{1}{L^3} \frac{dN}{dE} = \frac{dn}{dE} = \frac{1}{6\pi^2} \frac{d}{dE} \left(\frac{2mE}{\hbar^2}\right)^{3/2} = \frac{(2m)^{3/2}}{4\pi^2 \hbar^3} E^{1/2}$$

- **Total energy density**:

$$\frac{E_{\text{tot}}}{L^3} = \frac{1}{L^3} \int_0^{k_F} \frac{4\pi k^2 dk}{(2\pi/L)^3} \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{20\pi^2 m} k_F^5 \quad (6\pi^2 n)^{5/3} = \frac{3}{5} n E_F$$

Example I: Free electron-like metals

- e.g. Near-spherical fermi surface of Copper.



Recap: Identical particles

- In quantum mechanics, all elementary particles are classified as fermions and bosons.
 - ① Particles with half-integer spin are described by fermionic wavefunctions, and are antisymmetric under particle exchange.
 - ② Particles with integer spin (including zero) are described by bosonic wavefunctions, and are symmetric under exchange.
- Exchange symmetry leads to development of **(ferro)magnetic spin correlations** in Fermi systems even when Hamiltonian is spin independent.
- Also leads to **Pauli exclusion principle for fermions** – manifest in phenomenon of **degeneracy pressure**.
- For an ideal gas of fermions, the ground state is defined by a filled Fermi sea of particles with an energy density

$$\frac{E_{\text{tot}}}{L^3} = \frac{\hbar^2}{20\pi^2 m} (6\pi^2 n)^{5/3}$$

Example II: Degeneracy pressure

- Cold stars are prevented from collapse by the pressure exerted by “squeezed” fermions.



Crab pulsar

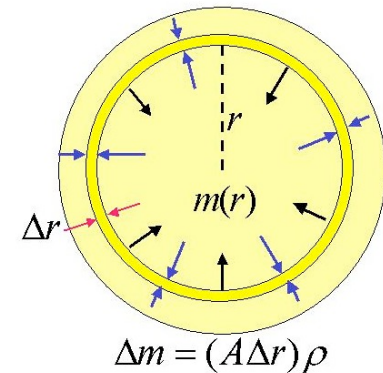
- **White dwarfs** are supported by electron-degenerate matter, and **neutron stars** are held up by neutrons in a much smaller box.

Example II: Degeneracy pressure

- From thermodynamics, $dE = \mathbf{F} \cdot d\mathbf{s} = -PdV$, i.e. pressure

$$P = -\partial_V E_{\text{tot}}$$

- To determine point of star collapse, we must compare this to the pressure exerted by gravity:



- With density ρ , gravitational energy,

$$E_G = - \int \frac{GMdm}{r} = - \int_0^R \frac{G(\frac{4}{3}\pi r^3 \rho)4\pi r^2 dr \rho}{r} = -\frac{3GM^2}{5R}$$

- Since mass of star dominated by nucleons, $M \simeq NM_N$,
 $E_G \simeq -\frac{3}{5}G(NM_N)^2\left(\frac{4\pi}{3V}\right)^{\frac{1}{3}}$, and gravitational pressure,

$$P_G = -\partial_V E_G = -\frac{1}{5}G(NM_N)^2 \left(\frac{4\pi}{3}\right)^{1/3} V^{-4/3}$$

Example II: Degeneracy pressure

$$P_G = -\partial_V E_G = -\frac{1}{5} G(NM_N)^2 \left(\frac{4\pi}{3}\right)^{1/3} V^{-4/3}$$

- At point of instability, P_G balanced by degeneracy pressure. Since fermi gas has energy density $\frac{E_{\text{tot}}}{L^3} = \frac{\hbar^2}{20\pi^2 m} (6\pi^2 n)^{5/3}$, with $n = \frac{N_e}{V}$,

$$E_{\text{WD}} = \frac{\hbar^2}{20\pi^2 m_e} (6\pi^2 N_e)^{5/3} V^{-2/3}$$

- From this expression, obtain degeneracy pressure

$$P_{\text{WD}} = -\partial_V E_{\text{WD}} = \frac{\hbar^2}{60\pi^2 m_e} (6\pi^2 N_e)^{5/3} V^{-5/3}$$

- Leads to critical radius of white dwarf:

$$R_{\text{white dwarf}} \approx \frac{\hbar^2 N_e^{5/3}}{Gm_e M_N^2 N^2} \simeq 7,000\text{km}$$

Example II: Degeneracy pressure

- White dwarf is remnant of a normal star which has exhausted its fuel fusing light elements into heavier ones (mostly ${}^6\text{C}$ and ${}^8\text{O}$).
- If white dwarf acquires more mass, E_F rises until electrons and protons abruptly combine to form neutrons and neutrinos – supernova – leaving behind neutron star supported by degeneracy.



- From $R_{\text{white dwarf}} \approx \frac{\hbar^2 N_e^{5/3}}{G m_e M_N^2 N^2}$ we can estimate the critical radius for a neutron star (since $N_N \sim N_e \sim N$),

$$\frac{R_{\text{neutron}}}{R_{\text{white dwarf}}} \simeq \frac{m_e}{M_N} \simeq 10^{-3}, \quad \text{i.e.} \quad R_{\text{neutron}} \simeq 10\text{km}$$

- If the pressure at the center of a neutron star becomes too great, it collapses forming a **black hole**.

Ideal quantum gases: fermions

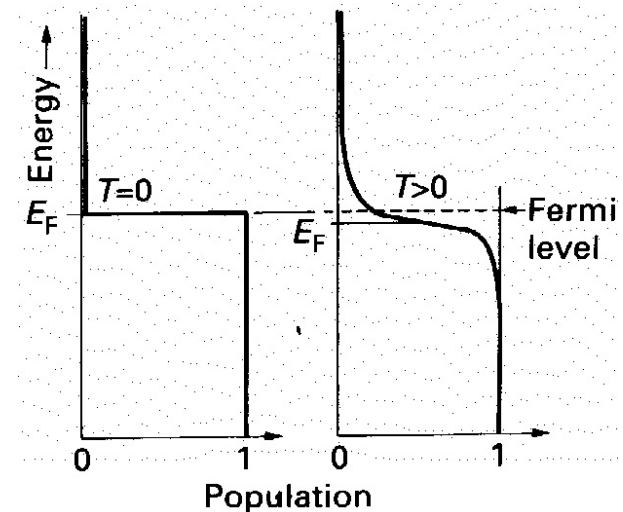
- For a system of identical non-interacting fermions, at non-zero temperature, the **partition function** is given by

$$\mathcal{Z} = \sum_{\{n_{\mathbf{k}}=0,1\}} \exp \left[- \sum_{\mathbf{k}} \frac{(\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}}}{k_{\text{B}} T} \right] = e^{-F/k_{\text{B}} T}$$

with chemical potential μ (coincides with Fermi energy at $T = 0$).

- The average state occupancy given by **Fermi-Dirac distribution**,

$$\bar{n}(\epsilon_{\mathbf{q}}) = \frac{1}{e^{(\epsilon_{\mathbf{q}} - \mu)/k_{\text{B}} T} + 1}$$



Ideal quantum gases: bosons

- In a system of N spinless non-interacting bosons, ground state of many-body system involves wavefunction in which all particles occupy lowest single-particle state, $\psi_B(\mathbf{r}_1, \mathbf{r}_2, \dots) = \prod_{i=1}^N \phi_{\mathbf{k}=0}(\mathbf{r}_i)$.
- At non-zero temperature, partition function given by

$$\mathcal{Z} = \sum_{\{n_{\mathbf{k}}=0,1,2,\dots\}} \exp \left[- \sum_{\mathbf{k}} \frac{(\epsilon_{\mathbf{k}} - \mu) n_{\mathbf{k}}}{k_B T} \right] = \prod_{\mathbf{k}} \frac{1}{1 - e^{-(\epsilon_{\mathbf{k}} - \mu)/k_B T}}$$

- The average state occupancy is given by the **Bose-Einstein distribution**,

$$\bar{n}(\epsilon_{\mathbf{q}}) = \frac{1}{e^{(\epsilon_{\mathbf{q}} - \mu)/k_B T} - 1}$$

Ideal quantum gases: bosons

$$\bar{n}(\epsilon_{\mathbf{k}}) = \frac{1}{e^{(\epsilon_{\mathbf{k}} - \mu)/k_B T} - 1}$$

- The chemical potential μ is fixed by the condition $N = \sum_{\mathbf{k}} \bar{n}(\epsilon_{\mathbf{k}})$. In a three-dimensional system, for N large, we may approximate the sum by an integral $\sum_{\mathbf{k}} \mapsto \left(\frac{L}{2\pi}\right)^3 \int d^3k$, and

$$\frac{N}{L^3} = n = \frac{1}{(2\pi)^3} \int d^3k \frac{1}{e^{(\epsilon_{\mathbf{k}} - \mu)/k_B T} - 1}$$

- For free particle system, $\epsilon_{\mathbf{k}} = \hbar^2 \mathbf{k}^2 / 2m$,

$$n = \frac{1}{\lambda_T^3} \text{Li}_{3/2}(\mu/k_B T), \quad \text{Li}_n(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^n}$$

where $\lambda_T = \left(\frac{\hbar^2}{2\pi m k_B T}\right)^{1/2}$ denotes **thermal wavelength**.

Ideal quantum gases: bosons

$$n = \frac{1}{\lambda_T^3} \text{Li}_{3/2}(\mu/k_B T), \quad \lambda_T = \left(\frac{h^2}{2\pi m k_B T} \right)^{1/2}$$

- As density increases, or temperature falls, μ increases from negative values until, at $n_c = \lambda_T^{-3} \zeta(3/2)$, μ becomes zero, i.e. $n_c \lambda_T^3 \sim 1$.
- Equivalently, inverting, this occurs at a temperature,

$$k_B T_c = \alpha \frac{\hbar^2}{m} n^{2/3}, \quad \alpha = \frac{2\pi}{\zeta^{2/3}(3/2)}$$

- Since Bose-Einstein distribution,

$$\bar{n}(\epsilon_{\mathbf{k}}) = \frac{1}{e^{(\epsilon_{\mathbf{k}} - \mu)/k_B T} - 1}$$

only makes sense for $\mu < 0$, what happens at T_c ?

Ideal quantum gases: bosons

- Consider first what happens at $T = 0$: Since particles are bosons, ground state consists of every particle in lowest energy state ($\mathbf{k} = 0$).
But such a singular distribution is inconsistent with our replacement of the sum \sum_k by an integral.
- If, at $T < T_c$, a fraction $f(T)$ of particles occupy $\mathbf{k} = 0$ state, then μ remains “pinned” to zero and

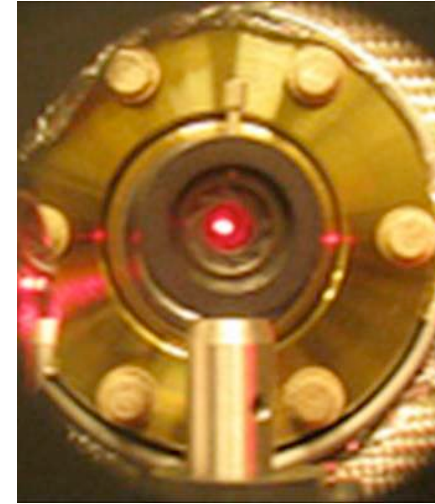
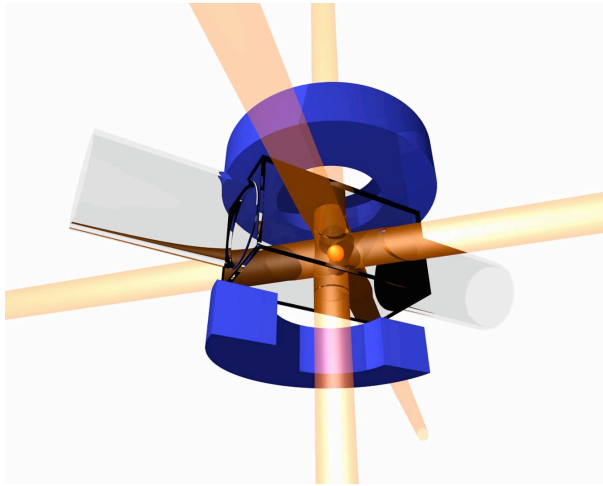
$$n = \sum_{\mathbf{k} \neq 0} \bar{n}(\epsilon_{\mathbf{k}}) + f(T)n = \frac{1}{\lambda_T^3} \zeta(3/2) + f(T)n$$

- Since $n = \frac{1}{\lambda_{T_c}^3} \zeta(3/2)$, we have

$$f(T) = 1 - \left(\frac{\lambda_{T_c}}{\lambda_T} \right)^3 = 1 - \left(\frac{T}{T_c} \right)^{3/2}$$

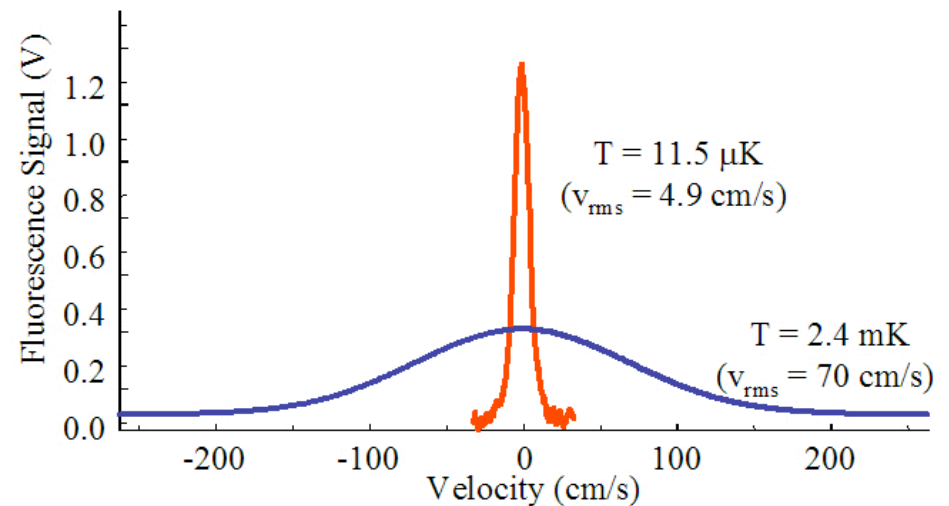
- The remarkable, highly quantum degenerate state emerging below T_c is known as a **Bose-Einstein condensate (BEC)**.

Example III: Ultracold atomic gases



- In recent years, ultracold atomic gases have emerged as a platform to explore many-body phenomena at quantum degeneracy.
Most focus on neutral alkali atoms, e.g. ${}^6\text{Li}$, ${}^7\text{Li}$, ${}^{40}\text{K}$, etc.
- Field has developed through technological breakthroughs which allow atomic vapours to be cooled to temperatures of ca. 100 nK.
- ca. 10^4 to 10^7 atoms are confined to a potential of magnetic or optical origin, with peak densities at the centre of the trap ranging from 10^{13} cm^{-3} to 10^{15} cm^{-3} – low density inhibits collapse into (equilibrium) solid state.

Example III: Ultracold atomic gases



- The development of quantum phenomena (such as BEC) requires phase-space density of $O(1)$, or $n\lambda_T^3 \sim 1$, i.e.

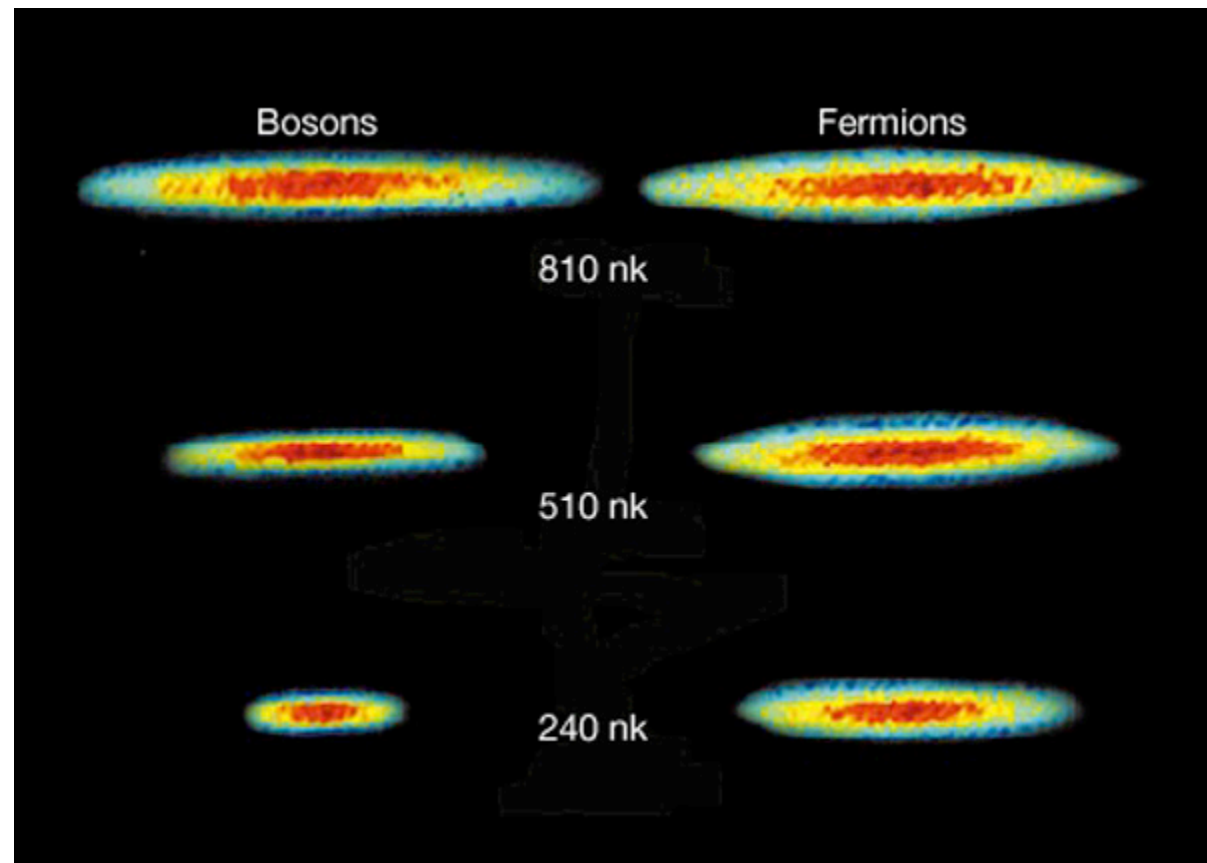
$$T \sim \frac{\hbar^2 n^{2/3}}{mk_B} \sim 100\text{nK to a few } \mu\text{K}$$

- At these temperatures atoms move at speeds $\sqrt{\frac{k_B T}{m}} \sim 1 \text{ cm s}^{-1}$, cf. 500 ms^{-1} for molecules at room temperature, and $\sim 10^6 \text{ ms}^{-1}$ for electrons in a metal at zero temperature.

Degeneracy pressure in cold atoms

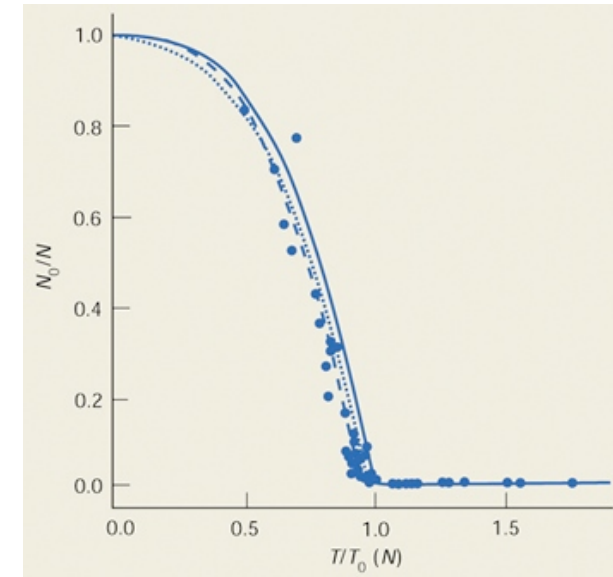
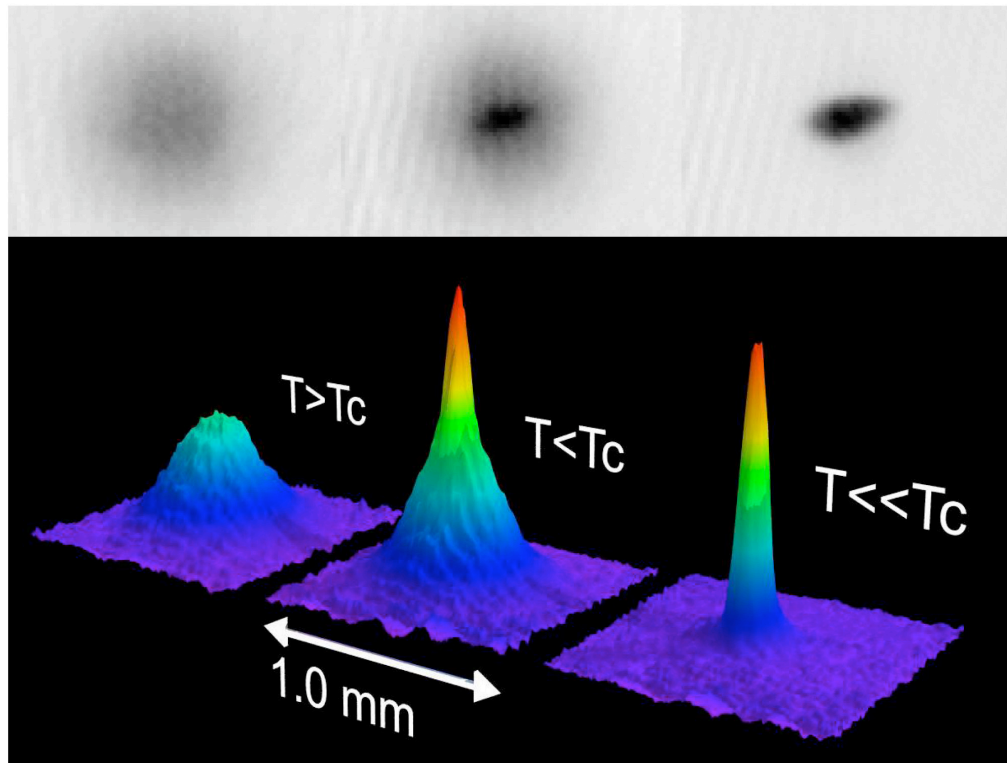
- Since alkalis have odd **atomic number**, Z , neutral atoms with odd/even **mass number**, $Z + N$, are bosons/fermions.

e.g. ${}^7\text{Lithium}$ is a boson and ${}^6\text{Lithium}$ is a fermion.



Bose-Einstein condensation

- Appearance of Bose-Einstein condensate can be observed in ballistic expansion following release of atomic trap.



$$f(T) = 1 - \left(\frac{T}{T_c} \right)^{3/2}$$

- Condensate observed as a second component of cloud, that expands with a lower velocity than thermal component.

Identical particles: summary

- In quantum mechanics, all elementary particles are classified as fermions and bosons.
 - ① Particles with half-integer spin are described by fermionic wavefunctions, and are antisymmetric under particle exchange.
 - ② Particles with integer spin (including zero) are described by bosonic wavefunctions, and are symmetric under exchange.
- The conditions on wavefunction antisymmetry imply spin-dependent correlations even where Hamiltonian is spin-independent, and leads to numerous physical manifestations.
- Resolving and realising the plethora of phase behaviours provides the inspiration for much of the basic research in modern condensed matter and ultracold atomic physics.