6. CONDENSAZIONE DI BOSE-EINSTEIN E SUPERFLUIDITA'

SUPERFLUIDS AND BOSE-EINSTEIN CONDENSATION

1908 Liquefaction of ^4He at 4.2K, H.K. Onnes
Beginning of Low Temperature Physics
1911 Discovery of Superconductivity
1925 Bose-Einstein Condensation predicted
1927 λ transition found in ^4He at 2.2K (Superfluidity)
1933 Meissner effect - SC expels magnetic field
1938 Demonstration of Superfluidity in ^4He
1950 Ginzburg - Landau theory of SC
1957 Bardeen-Cooper-Schrieffer theory of SC
1957 Abrikosov flux lattice - Type II SC
1962 Josephson effect
1963 Anderson - Higgs mechanism
1971 Superfluidity found in ^3He at 2.8 mK
1986 High T_c superconductivity 30-165K
Other compounds A_3C_{60} ; MgB_2 etc
1995 BEC achieved in atomic gases - 0.5 μK
2015 New high T_c SC H_3S ; $T_c = 203K$

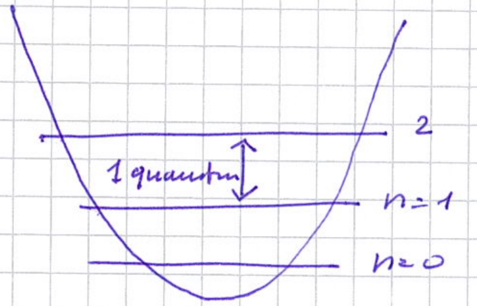
BEC - superconductivity - superfluidity

Macroscopic quantum effects
Usually quantum effects appear at very small scale atomic or subatomic
Here they are macroscopic but very small temperature
[Hopefully also medium T]

Simplest concept: BEC

Bose-Einstein Statistics

Planck black body radiation formula



Photons - only take discrete levels of energy
Analogous to phonons

These two examples - photons and phonons - look more like the quantisation of an amplitude (energy) rather than real particles.

In 1924 S.N. Bose new method to derive the Planck Black Body formula - The light quanta could be considered as particles of light - the photons (like the phonons).
Einstein extended the method beyond light, also for an ~~ided~~ ideal gas of particles with mass. First generalization (quantum) of Maxwell Boltzmann statistics

Bosons: photons - phonons - ^4He atoms.
↳ Counting quantum states for identical particles.

N_s = identical Bose particles

M_s = quantum states

Configuration to distribute the particles

$$W = \frac{(N_s + M_s - 1)!}{N_s!\,(M_s - 1)!}$$

particles and states are indistinguishable -

$$S = k_B \ln W$$

W = number of available microstates with energy (total) = E

S = shell in k space with same energy

$$W = \prod_s W_s = \prod_s \frac{(N_s + M_s - 1)!}{N_s!\,(M_s - 1)!}$$

Stirling $\ln N! \sim N \ln N - N$; $N_s, M_s \gg 1$

$$S = k_B \ln W = k_B \sum_s \left[(N_s + M_s) \ln (N_s + M_s) - N_s \ln N_s - M_s \ln M_s \right]$$

In thermal equilibrium maximize total entropy

$$N = \sum_s N_s \qquad ; \quad U = \sum_s \varepsilon_s N_s$$

Maximize the entropy with the constraint of fixed N and U

Lagrange multipliers ($k_B \beta$ and $-k_B \beta \mu$)

$$\frac{\partial S}{\partial N_s} - k_B \beta \frac{\partial U}{\partial N_s} + k_B \beta \mu \frac{\partial N}{\partial N_s} = 0$$

This leads to

$$\ln (N_s + M_s) - \ln N_s - \beta \varepsilon_s + \beta \mu = 0$$

which leads to

$$N_s = \frac{1}{e^{\beta(\varepsilon_s - \mu)} - 1} M_s \longrightarrow \text{Bose Einstein result}$$

The average number of particles occupying any single quantum state is N_s/M_s → average occupation number

$$\boxed{f_{BE}(\varepsilon) = \frac{1}{e^{\beta(\varepsilon - \mu)} - 1}}$$

Interpretation of β and μ (Lagrange multipliers)

Ist law of thermodynamics for N particles

$$dU = TdS - PdV + \mu dN$$

$$dS = \frac{1}{T}(dU + PdV - \mu dN)$$

$$dS = \sum_s \frac{\partial S}{\partial N_s} dN_s = K_B \beta \sum_s' \left(\frac{\partial U}{\partial N_s} - \mu \frac{\partial N}{\partial N_s}\right) dN_s =$$

$$= K_B \beta (dU - \mu dN)$$

So we can identify $\beta = \frac{1}{K_B T}$

and μ as the chemical potential of the gas.

(This is the microcanonical ensemble, N fixed, U fixed)
OK for fixed amount of atoms - gas in a magnetic trap.

The basic difference with respect to Planck photons or phonons is that in the "real particle" perspective of the B-E statistics we can have a fixed number of particles N.

For photons or phonons this is not the case but we are going to see that if N is fixed something very interesting occurs: the B.E. condensation at a finite temperature.

Usually for $V \to \infty$ with $n = N/V$ fixed is convenient the Grand Canonical in which energy and number can fluctuate

Equilibrium with heat bath, T and chemical potential μ.

BOSE-EINSTEIN CONDENSATION

B-E gas: phase transition for a gas of non-interacting particles (!)

≠ Fermi Dirac and ≠ photons and phonons.

Below T_c the gas of BE particles coexists with condensed particles.

Analogy to liquid-gas phase transition - droplets -

<u>But</u> here the condensed particles are not separated in space from the others. The separation is in <u>momentum space</u>

$$N = \sum_k \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1}$$

$$V \to \infty \qquad \sum_k \to \int \frac{V}{(2\pi)^3} d^3k$$

particle density

$$n = \frac{N}{V} = \frac{1}{(2\pi)^3} \int \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1} d^3k = \int_0^\infty \frac{1}{e^{\beta(\varepsilon_k - \mu)} - 1} g(\varepsilon) d\varepsilon$$

Density of states (3-d free particles)

$$g(\varepsilon) = \frac{m^{3/2}}{\sqrt{2}\pi^2 \hbar^3} \varepsilon^{1/2}$$

dimensionless $z = e^{\beta\mu}$ (fugacity) and $x = \beta\varepsilon$

$$n = \frac{(m k_B T)^{3/2}}{\sqrt{2}\pi^2\hbar^3} \int_0^\infty \frac{z e^{-x}}{1 - z e^{-x}} x^{1/2} dx$$

$$\frac{z e^{-x}}{1 - z e^{-x}} = z e^{-x}(1 + z e^{-x} + z^2 e^{-2x} + \dots) = \sum_{p=1}^\infty z^p e^{-px}$$

which is convergent for $z < 1$

Then the integral becomes

$$\int_0^\infty e^{-px} x^{1/2} dx = \frac{1}{p^{3/2}} \int_0^\infty e^{-y} y^{1/2} dy = \frac{1}{p^{3/2}} \frac{\sqrt{\pi}}{2}$$

[NB: special case of Gamma function
$$\Gamma(t) = \int_0^\infty y^{t-1} e^{-y} dy$$] $\Gamma(3/2) = \frac{\sqrt{\pi}}{2}$

Then the particle density can be expressed in terms of the fugacity

$$n = \left(\frac{m k_B T}{2\pi \hbar^2}\right)^{3/2} g_{3/2}(z)$$

$$g_{3/2}(z) = \sum_{p=1}^\infty \frac{z^p}{p^{3/2}}$$

This series converges when $|z| < 1$ but diverges for $|z| > 1$

At $z = 1$ is just convergent

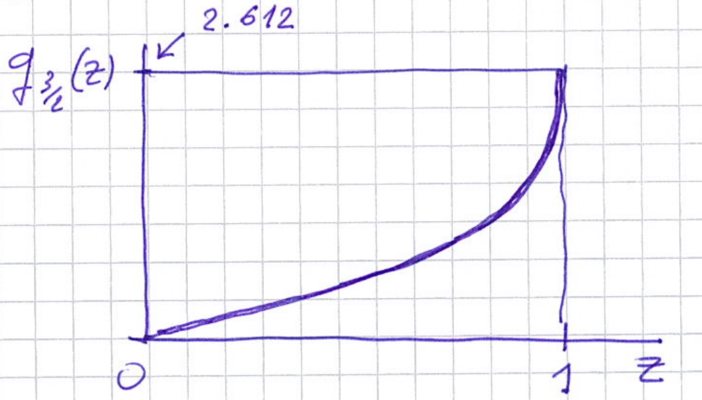
$$g_{3/2}(1) = \sum_{p=1}^\infty \frac{1}{p^{3/2}} = \zeta(3/2) = 2.612$$

$\zeta(s) = \sum_{p=1}^\infty \frac{1}{p^s}$ is the Riemann zeta function

In addition the function has infinite derivative at $z = 1$

$$\frac{d g_{3/2}(z)}{dz} = \frac{1}{z} \sum_{p=1}^\infty \frac{z^p}{p^{1/2}}$$

which diverges at $z = 1$



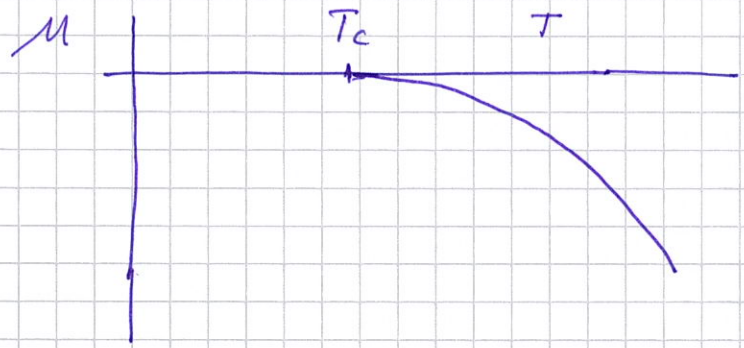
From the relation between n and $g_{3/2}(z)$ we can derive the value of z and μ corresponding to n

$$g_{3/2}(e^{\beta\mu}) = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2} n$$

At high T or low density n, the r.h.s. is small so we can expand $g_{3/2}(z) \simeq z + \cdots$ to obtain

$$\mu \simeq -\frac{3}{2} k_BT \ln\left(\frac{mk_BT}{2\pi\hbar^2 n^{2/3}}\right)$$

which gives a negative chemical potential



On cooling the gas (low T) the value of z increases until it equals one. At this point the chemical potential μ, becomes zero. ($g_{3/2}(1) = 2.612$ maximum value).
The temperature where this happens - for a fixed density n - defines the critical temperature

$$\boxed{T_c = \frac{2\pi\hbar^2}{k_Bm}\left(\frac{n}{2.612}\right)^{2/3}}$$

BEC TEMPERATURE

What about $T<T_c$
Einstein realised that if $\mu=0$ the number of particles in the lowest quantum state is infinite.

More precisely out of a total N particles in the gas, a macroscopic number N_0 occupy the quantum state $\varepsilon_k = 0$.
A finite fraction N_0/N of all particles is in this state.
In the thermodynamic limit $V \to \infty$ the occupation of the $\varepsilon_k = 0$ state is

$$N_0 = \frac{1}{e^{-\beta\mu} - 1} \quad \longrightarrow \mu = -k_B T \ln\left(1 + \frac{1}{N_0}\right) \simeq -k_B T \frac{1}{N_0}$$

If a finite fraction of particles is in this state then
$V \to \infty$; $N_0 \to \infty$; $\mu \to 0$. So below T_c μ is effectively zero as shown before.
Below T_c we must take the $k=0$ point separately

$$N = N_0 + \sum_{k \neq 0} \frac{1}{e^{\beta \varepsilon_k} - 1} \qquad \text{where } \mu = 0$$

$$n = n_0 + \frac{(m k_B T)^{3/2}}{\sqrt{2}\,\pi^2 \hbar^3} \int_{(0)}^{\infty} \frac{e^{-x}}{1 - e^{-x}} x^{1/2} dx$$

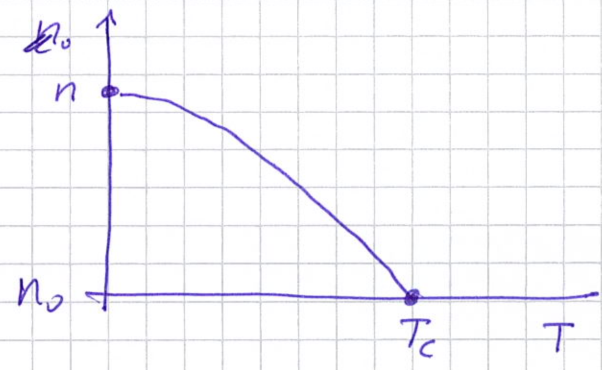
The integral can be evaluated as before and is equal to $\Gamma(3/2)\,\zeta(3/2)$ and we finally obtain for $T < T_c$

$$n = n_0 + 2.612 \left(\frac{m k_B T}{2\pi \hbar^2}\right)^{3/2}$$

The particle density is then divided into a condensate density n_0 and the normal density n_n

$$n = n_0 + n_n$$

$$\frac{n_0}{n} = \left(1 - \frac{T}{T_c}\right)^{3/2}$$



At $T=0$ all particles are condensated.

Other thermodynamical quantities of Bose gas.
Internal energy:

$$U = V\int_0^\infty \frac{\varepsilon}{e^{\beta(\varepsilon-\mu)}-1}\, g(\varepsilon)\, d\varepsilon =$$

$$= V(k_BT)^{5/2}\frac{m^{3/2}}{\sqrt{2}\,\pi^2\hbar^3}\int_0^\infty \frac{z e^{-x}}{1-ze^{-x}}\, x^{3/2}\, dx$$

$$u = \frac{U}{N} = \frac{3}{2}k_BT\,\frac{g_{5/2}(z)}{g_{3/2}(z)} \qquad \text{for } T > T_c$$

and for $T < T_c$ $\qquad \left[\, g_{5/2}(z) = \sum_{p=1}^{\infty}\frac{z^p}{p^{5/2}} \,\right]$

$$u = \frac{3}{2}k_B\frac{T^{5/2}}{T_c^{3/2}}\,\frac{g_{5/2}(1)}{g_{3/2}(1)}$$

where $g_{5/2}(1) = \zeta(5/2) = 1.342$.

For $T \gg T_c$ we have a normal Bose gas

$$u \simeq \frac{3}{2}k_BT$$

(since $g_{5/2}(z) \simeq z$ and $g_{3/2}(z) \simeq z$ for z small)

So Bose Einstein statistics becomes irrelevant for $T \gg T_c$.

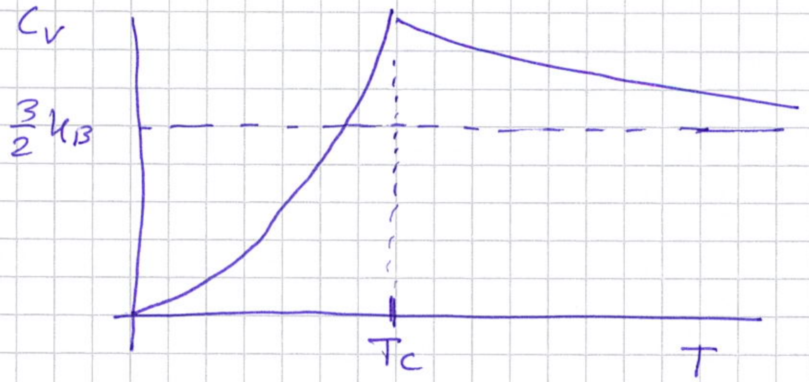
From the heat capacity we can see that T_c represents a real phase transition.

$$C_v = \frac{\partial u}{\partial T} \quad \text{with fixed } n$$

For $T \gg T_c$ we have $C_v \simeq \frac{3k_B}{2}$

and

$$C_V = \frac{15}{4} \frac{g_{5/2}(1)}{g_{3/2}(1)} \left(\frac{T}{T_c}\right)^{3/2} k_B \qquad (\text{for } T < T_c)$$



Cusp or discontinuity in the slope. → Free energy is not analytic → real phase transition. (thermodynamic).

<u>Problem</u>: $\sum_k \to \int dk$ but then realise that $k=0$ is special but the rest is still treated as a continuum.

Consider the occupation number of the first states in a cubic box L.

$k \simeq 2\pi/L \to \varepsilon_k \simeq \hbar^2/mL^2 = V^{-2/3}\hbar^2/m$

The occupation of these states is

$$N_1 = \frac{1}{e^{\beta(\varepsilon_k-\mu)}-1} \sim \frac{1}{e^{\beta V^{-2/3}\hbar^2/m}-1} \underset{V\to\infty}{=} O(V^{2/3})$$

So, while the occupations of the finite k states grow with V, they grow more slowly than the value of N_0; i.e $N_1/N_0 = O(V^{1/3}) \to 0$

So the continuum approximation is OK.

BEC IN COLD ATOMIC GASES

Soon after Einstein's prediction of BEC (130) it was discovered that liquid ^4He becomes a superfluid below the λ point at 2.2K.

^4He atom: 2 electrons; 2 protons; 2 neutrons → total spin zero → Boson

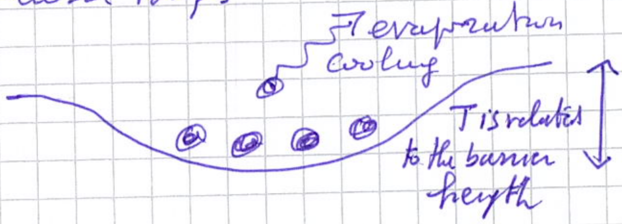
If one uses the density of ^4He, $\rho = 145\ kg/m^3$ and $m = 4m_p$ to find the particle density $n = \rho/m$ from the BEC formula one gets $T_c = 3.1K$.

But this is to some extent a coincidence because BEC theory is for the ideal gas and neglects any interaction between the particles. But in liquid ^4He the density is high and these interactions are important. So superfluidity is not exactly a manifestation of BEC.

In 1995 real physical examples of BEC have been realised with very dilute gases of alkali metal atoms by trapping and cooling atoms in magnetic and laser traps

$\rho \simeq 10^{11} - 10^{15}\ cm^{-3}$

$[\rho_{^4He} = 2\times10^{22}\ cm^{-3}]$



For ^{87}Rb (heavy) we expect from BEC $T_c \sim 10^{-6} - 10^{-8}$
[10 nK – 1 μK]

These incredibly low temperatures can actually be realised and controlled.

How can a large Alkali atom like ^{87}Rb be a Boson?
Alkali atoms have a single valence electron

$2s$ for Li ; $3s$ for Na ; $4s$ for K ; $5s$ for Rb.

The other electrons ~~are~~ into complete shells with total angular momentum and total spin zero.
Other contribution is from the nuclear spin. If we have an odd number of protons and neutrons it will have a net half-integer spin ^{7}Li ; ^{23}Na ; ^{87}Rb all have $S = 3/2$ nuclei.
Note that adding two spins S_1 and S_2 leads to the possible values of the total spin

$$S = |S_1 - S_2| \, ; \, |S_1 - S_2| + 1 \, ; \, \cdots ; \, S_1 + S_2 - 1 \, ; \, S_1 + S_2$$

Spin $S = 3/2$ nucleus and $S = 1/2$ of valence electrons spin combine to give states with a total spin of ~~an~~ either $S = 2$ or $S = 1$. Usually the gas is a mixture of different type of Bosons.
Also cold atoms interact to some extent - short distance repulsion + Van der Waals attraction. These in principle would lead to clusters. But this happens at a slow rate.
In two body collisions are elastic and no binding takes place.
Rate of 3-body collisions is low (depends on the density) and there is time (seconds or minutes) to make experiments.
Interaction:

$$V(r_1 - r_2) \simeq g \, \delta(r_1 - r_2) \quad \text{point like}$$

and single parameter g.

From scattering theory - two body scattering s-wave scattering length a_s

$$g = \frac{4\pi a_s \hbar^2}{m}$$

g and a_s are positive $\rightarrow$ net repulsion

On average this can be described as an additional average potential

$$V_{eff}(r) = g \cdot n(r)$$

where $n(r)$ is the density of atoms at point r in the trap

Effective - non linear Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_{trap}(r) + V_{eff}(r) \right] \psi_i(r) = \varepsilon_i \cdot \psi_i(r)$$

$$n(r) = \sum_i \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1} |\psi_i(r)|^2$$

ε_i are the different energy levels.

The chemical potential μ is determined by the constant total number of atoms N

$$N = \int n(r) d^3 r = \sum_i \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1}$$

This set of equations are closed and must be solved self-consistently. At $T = 0K$ all particles are in the condensate and

$$n(r) = N |\psi_0(r)|^2$$

where ψ_0 is the ground state wave function

(Gross-Pitaevskii equations) - Solution is numerical -

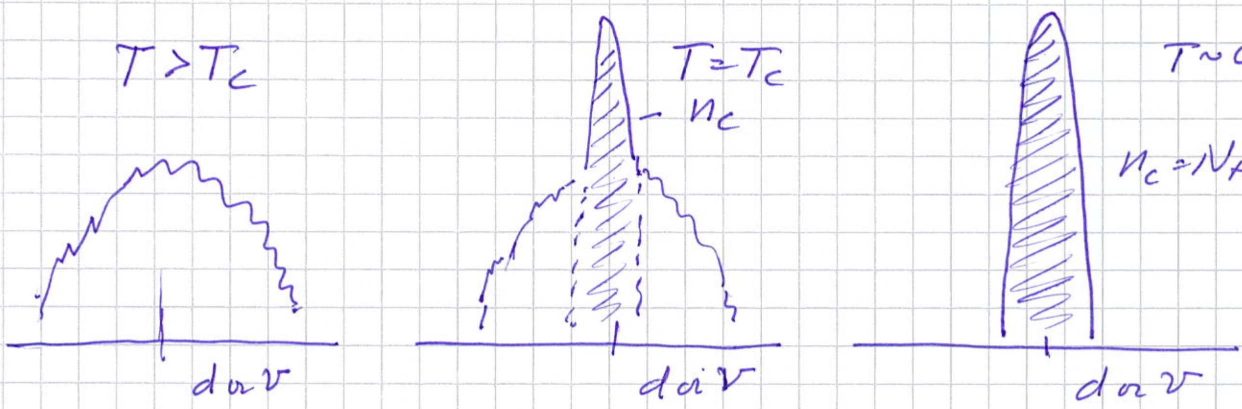
The solution shows a form of BEC. If E_0 is the lowest energy at some T_c the occupation of this state suddenly increases to a value of order N – Thermodynamic limit $N \to \infty$

In the trap $N \sim 10^4 - 10^6 \approx$ OK.

Result of experiment of cold atoms:

Velocity distribution of the atoms in the trap.

Velocity is measured by turning off the trap and observing the velocity. – Spatial distrib. of light ~~p~~ absorbed shows the position – velocity of the atoms at the moment the trap was eliminated



The condensate peak has some width because of

$V_{trap} + V_{eff}$ – The condensate occurs in the g-state wavefunction $\Psi_0(r)$ which has a finite width momentum distributions

$$\Psi_0(r) = \frac{1}{(2\pi)^3} \int A_k \, e^{ikr} d^3k$$

This finite width is due to the indetermination principle

$$\Delta p \sim \hbar / \Delta x$$

where Δx is the effective width of the g-state wavefunction in the trap.

The background can be estimated from Maxwell-Boltzmann

$$\frac{1}{2} m \langle v_x^2 \rangle = \frac{1}{2} k_B T$$

$$\Delta v \sim \left(\frac{k_B T}{m}\right)^{1/2} \longrightarrow \text{normal component}$$

$$\Delta v \sim \left(\frac{\hbar}{m \Delta x}\right) \longrightarrow \text{condensate peak}$$

One can also cool Fermionic atoms and one does not see the BEC phenomenology.
Strictly speaking one observes <u>weakly interacting Bosons</u> not really perfect Bose gas. Interaction is important.
In particular it can be shown that an <u>ideal ~~Bo~~ BEC is not a superfluid</u>. When there are no interactions the critical velocity of the superfluid flow is zero.
Finite interactions are needed to sustain a true superfluid state.
In the real BEC observed these are indeed true superfluids.
Persistent currents have been observed.

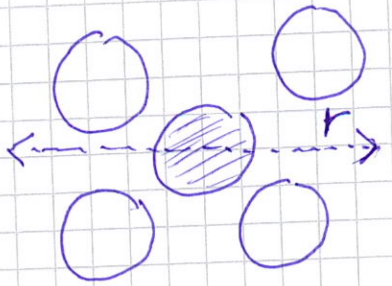
SUPERFLUID ^4He

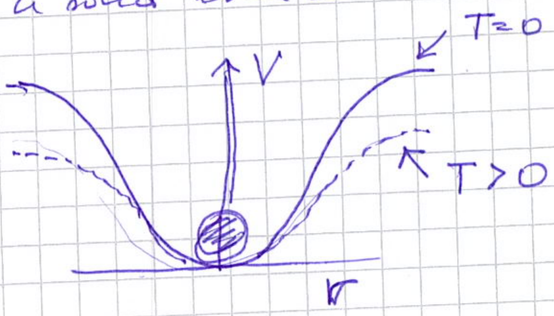
The only superfluids which can be studied in the lab. are ^4He and ^3He. They are unique because they remain in the liquid state even at $T=0$.
All other systems become solids at low T. Hydrogen in principle would be better (lighter) but it is very reactive and it makes H_2 or other compounds. The search for metallic H at low T and very high pressure has been very active but no conclusive results up to now.
However, recently it was found that H_3S under high pressure is SC with $T_c = 203K$ but this is another story.
Back to He. ^4He is a spin zero Boson while ^3He is a spin 1/2 Fermion. In 1930 ^4He was shown to be superfluid at 2.17K while superfluidity of ^3He was shown in 1972 at 2 mK.

Basic concepts for ^4He are the macroscopic wavefunction, or off diagonal long range order $\rightarrow$ link to BEC and Landau quasiparticle theory of ^4He which shows the importance of particle-particle interaction.
The problem of ^4He is therefore much more difficult than simple BEC.
For ^3He the situation is more similar to exotic superconductors and we will not treat it in this course.

The stability of the solid phase

Here we consider the problem of the self-consistent criteria of stability of the solid state. These ideas can be used for the melting transition but also to understand why ^4He does not go into a solid even at $T=0K$.





In a solid an atom is localised by the potential due to the other atoms. When these vibrate effectively the potential which localises the atom (all atoms) becomes softer.

Quasi harmonic approximation - analogous to the Debye Waller factor. The effective force constant at a finite temperature is given by

$$\tilde{K}(T) = K_0 e^{-\lambda \langle u^2 \rangle_T}$$

where $\langle u^2 \rangle_T$ is the mean square displacement of a typical atom at temperature T.

$$\tilde{K}(T) = \langle \nabla\nabla V(r) \rangle_T$$

[If $V(r) \sim \mathrm{Re}\, e^{iqr}$ $\sim \cos qr$ Debye Waller]

$$\langle u^2 \rangle = \sum_s \frac{\hbar}{2NM\omega_s} (2\bar{n}_s + 1) \underset{(T\to 0)}{\simeq} \sum_s \frac{\hbar}{2NM\omega_s}$$

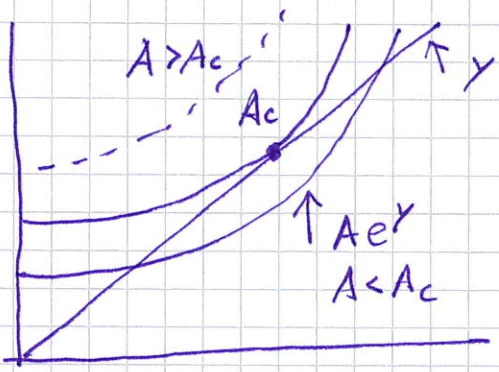
$\langle u^2 \rangle \approx \frac{3\hbar}{2M\omega}$; $\omega = \sqrt{\frac{K}{M}}$

$$\langle u^2 \rangle = \frac{3\hbar}{2\sqrt{MK_0}} e^{\lambda \langle u^2 \rangle}$$

$y = \lambda \langle u^2 \rangle$ $\qquad y = A e^{y}$ $\qquad \begin{cases} A_c = e^{-1} \\ y_c = 1 \end{cases}$

$$A = \frac{3\hbar\lambda}{2\sqrt{MK_0}}$$

Condition for $\exists$ of a solution



$$\boxed{\frac{3\hbar\lambda}{2\sqrt{MK_0}} < e^{-1}}$$

$\lambda = A r_0^{-2}$ $\qquad r_0 = \frac{\hbar^2}{me^2}$

$K_0 = B \frac{e^2}{r_0^2}$

$$\frac{3A\hbar r_0^{-2}}{2\sqrt{MB\, e^2/r_0^3}} = \frac{3A}{2\sqrt{B}} \frac{\hbar}{\sqrt{Me^2 r_0}} = \frac{3A}{2\sqrt{B}} \sqrt{\frac{m}{M}} \frac{\cancel{\hbar}}{\sqrt{\frac{\cancel{e^2}\cancel{\hbar^2}}{\cancel{e^2}}}}$$

$$\boxed{\sqrt{\frac{m}{M}} < \frac{1}{e} \frac{2\sqrt{B}}{3A}}$$

For ^4He

$\hookrightarrow \sqrt{\frac{m_e}{m_p}} < 10^{-2}$

close to real values.

For thermal fluctuations (T large → melting)

$$\ddot{u}_n + 2\tilde{\kappa}\, u_n = 0$$

$$\tilde{\kappa} = \kappa_0\, e^{-2\lambda \langle u_n^2 \rangle}$$

Equipartition $\quad \frac{1}{2} k_B T = \frac{1}{2}\, 2\tilde{\kappa} \langle u_n^2 \rangle$

Selfconsistent relation

$$\langle u_n^2 \rangle = \frac{k_B T}{2\kappa_0}\, e^{2\lambda \langle u_n^2 \rangle}$$

$$\left.\begin{aligned} y &= 2\lambda \langle u_n^2 \rangle \\ \tau &= \frac{k_B T}{\kappa_0}\lambda \end{aligned}\right\} \rightarrow y = \tau e^{y}$$

$$\tau_B = e^{-1} = 0.368$$

$$y_B = 1$$

$$\kappa_B = \kappa_0 e^{-1}$$

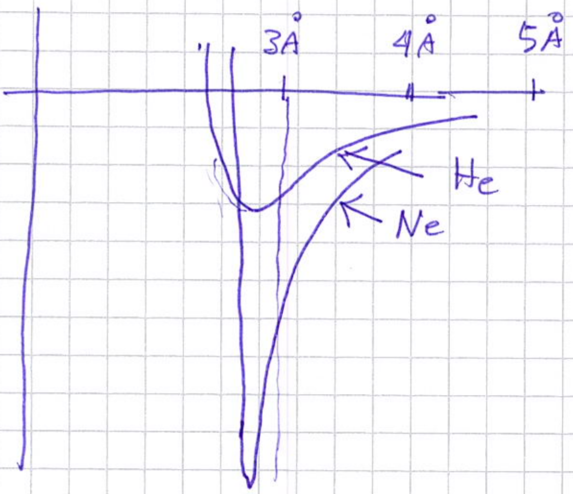
$$\langle u_n^2 \rangle_{T_M} = \frac{1}{2\lambda}$$

Classical and Quantum Fluids

Classical F. → Quantum mechanics is not relevant
Quantum F → QM is important.

<u>How to decide if QM is important?</u>

Consider a single component gas of particles - like rare gases of mass m.
Short range repulsion & long range weak attraction



$$V(r) \simeq a e^{-br} - \frac{c}{r^6}$$

or near the minimum

$$V(r) = \varepsilon_0 \left(\frac{d^{12}}{r^{12}} - 2\frac{d^6}{r^6} \right)$$

Van der Waals

(quantum) He : $\varepsilon_0 = 1.03$ meV at $d = 2.65$ Å $m = 4u$
(classical) Ne : $\varepsilon_0 = 3.94$ meV at $d = 2.96$ Å $m = 20u$

Classical Hamiltonian

$$H(p_1 \cdots p_N; r_1 \cdots r_N) = \sum_{i=1,N} \frac{p_i^2}{2m} + \frac{1}{2}\sum_{i \neq j} V(r_i - r_j)$$

at T $\quad P(p_1, \cdots p_N, r_1, \cdots r_N) = \frac{1}{Z_N} e^{-\beta H} \qquad (\beta = 1/k_B T)$

Classical partition function

$$Z_N = \frac{1}{N!} \int d^3p_1 \cdots d^3p_N d^3r_1 \cdots d^3r_N \, e^{-\beta H}$$

because particles are indistinguishable

Maxwell Boltzmann distribution - We can factorise

$$Z_N = \left(\prod_i \int e^{-p_i^2/2mk_BT} d^3p_i\right) Q_N = (2\pi m k_B T)^{3N/2} \cdot Q_N$$

$$Q_N = \frac{1}{N!}\int d^3r_1 \cdots d^3r_N \exp\left(-\frac{1}{2}\beta\sum_{i\neq j} V(r_i - r_j)\right)$$

The fact that the momentum expression is factorised implies that momenta are statistically independent.
Prob. that a particle has momentum in the region d^3p is

$$P(\mathbf{p})\,d^3p = \frac{1}{(2\pi m k_B T)^{3/2}} e^{-p^2/2mk_BT} d^3p$$

and the fraction of particles with $\mathbf{p}$ between p and $p+dp$

$$P_{MB}(p)\,dp = \frac{4\pi p^2}{(\quad\cdot\quad)^{3/2}} e^{(---)} dp$$

This is true for any chemical system, gas, liquid or solid and arbitrary interaction $V(r)$ - not just for an ideal gas.
So a typical particle has momentum

$$p = (2m k_B T)^{1/2}$$

corresponding to the maximum of P_{MB} -
Quantum mechanics → De Broglie Wavelength → (thermal)

$$\lambda = \hbar/p \qquad \lambda_{DB} = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{1/2}$$

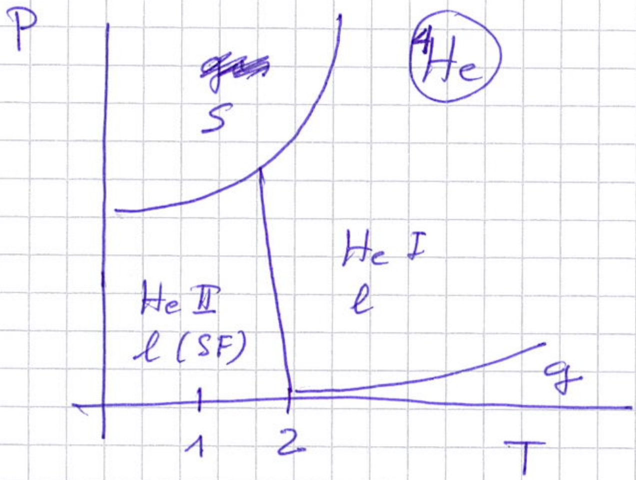
Quantum effects are important when ~~these~~ this wavelength ~~are comparable~~ (~~[illegible]~~) ?
is comparable to other characteristic scales of the system

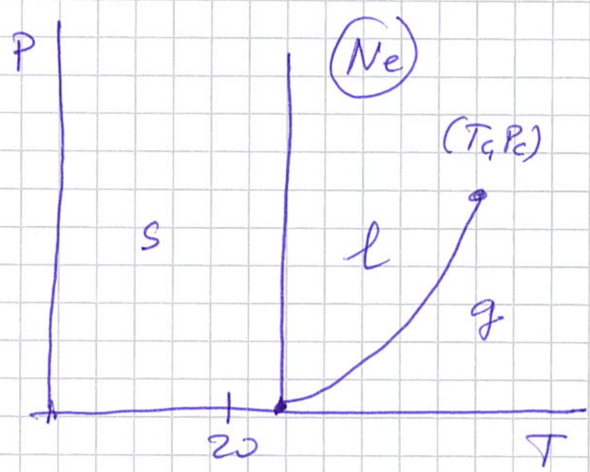
$\boxed{Ne}$: liquid at 27K and solid at 24K at $P=0$ _

$\lambda_{DB} = 0.7$ Å but minimum of potential is at $d = 3.0$ Å so QM is not very important _

$\boxed{He}$: liquid at 4K $\rightarrow$ $\lambda_{DB} \simeq 4.0$ Å which is larger than the interatomic distance $d = 2.7$ Å so QM effects are always important

This has a strong influence on the phase diagram





The phase diagram of ^3He is similar to ^4He but the superfluid phase occurs only at 2mK - Their phase diagram is drastically different with respect to normal atoms like ~~He~~ Ne -

The problem, as we have seen is zero point motion -

$$E_0 = \frac{3}{2}\hbar\omega_0 \quad ; \quad \omega_0 = \sqrt{\frac{4K}{m}}$$

$$K = \frac{1}{2}\frac{d^2V(r)}{dr^2} = \frac{36\,\varepsilon_0}{r_0^2}$$

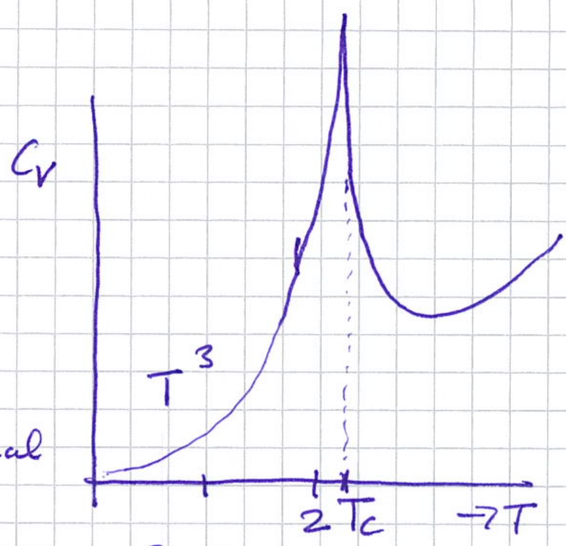
From Lennard Jones parameters of He $E_0 \simeq 7$ meV equivalent to a thermal motion of 70K, which prevents the stabilization of the solid phase - without pressure

~~Bla~~ For Ne we would have $E_0 \approx 4$ meV comparable to thermal motion at melting point $T_M = 24$ K.

The Macroscopic Wavefunction

He I : normal phase

He II : superfluid



λ type transition ≠ BEC

SF: zero viscosity; infinite thermal conductivity etc

At low T $\quad C_V \sim T^3 \quad \left[C_V^{BEC} \sim T^{3/2} \right]$

C_V is singular (not cusp like as in BEC) with a weak power law behavior

$$C_V = \begin{cases} C(T) + A_+ |T-T_c|^{-\alpha} & (T > T_c) \\ C(T) + A_- |T-T_c|^{-\alpha} & (T < T_c) \end{cases}$$

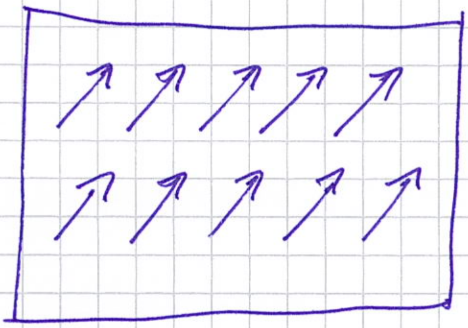
α = critical exponent $\qquad \alpha = -0.009$

In very good agreement with universality class of X-Y model

Order parameter described by 2-d unit vector

$$n(r) = (n_x, n_y) = (\cos\theta, \sin\theta)$$

So, in this respect the order in ~~SH~~ SF ^{4}He is like that of a magnet



Above T_c $n(r)$ is spatially random.

Physical interpretation → macroscopic wave-function
Problem analogous to Gross - Pitaevskii but structure of $V(r)$ is strong and cannot be treated as single mean field.

$$n_0 = |\Psi_0(r)|^2$$

$$N_0 = n_0 V = \int |\Psi_0(r)|^2 d^3r$$ particles in the condensate

Wave function is complex and its ~~angle~~ phase $\theta(r)$ corresponds to the angle in the X-Y model

$$\Psi_0(r) = \sqrt{n_0(r)}\, e^{i\theta(r)}$$

θ is a natural and ~~re~~ real physical parameter of the system.

In BEC g-state wavefunction is $\frac{1}{\sqrt{V}} e^{ik\cdot r}$ for $k=0$
In this case the wavef. is just constant $\frac{1}{\sqrt{V}}$ or one define a phase θ → $e^{i\theta}\frac{1}{\sqrt{V}}$

Now we consider that θ can vary in space $\theta(r)$, → superflow.
Superflow arises when θ vary in space
Particle flow:

$$J_0 = \frac{\hbar}{2mi}\left[\Psi_0^*(r)\nabla\Psi_0(r) - \Psi_0(r)\nabla\Psi_0^*(r)\right]$$

is the number of particles flowing per unit area per second in the condensate. No current because of no charge.

$$\Psi_0(r) = \sqrt{n_0}\, e^{i\theta}$$

leads to

$$\nabla \psi(r) = e^{i\theta} \nabla \sqrt{n_0} + i\sqrt{n_0}\, e^{i\theta} \nabla \theta$$

$$\nabla \psi^*(r) = e^{-i\theta} \nabla \sqrt{n_0} - i\sqrt{n_0}\, e^{-i\theta} \nabla \theta$$

Therefore

$$J_0 = \frac{\hbar}{m}\, n_0 \nabla \theta$$

So the condensate flows with a velocity

$$\boxed{V_S = \frac{\hbar}{m} \nabla \theta}$$ superfluid velocity

So the condensate contributes to the flow with $J_0 = n_0 V_s$ which has no dissipation

Key experiments in the '30

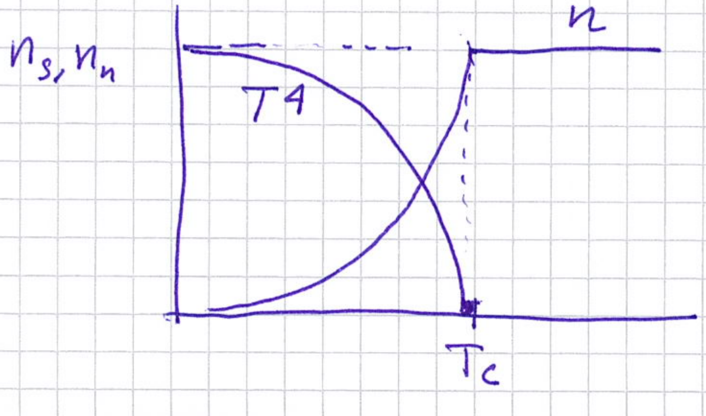
Kapitza : flow through a capillary without resistence (viscosity)

Normally the flow would depend on viscosity η, $\Delta P = P_2 - P_1$ and length and diameter of the tube.

But other experiments seemed to show a finite viscosity i.e. oscillating cylinder in a fluid

Two fluid model

$$n = n_s + n_n \quad ; \quad \rho_s = m \cdot n_s$$



$$n_s(T) \simeq n - A T^4$$

Near T_c

$$n_s \sim \begin{cases} B(T_c - T)^{\nu} & T < T_c \\ 0 & T > T_c \end{cases}$$

$$\nu \simeq 0.67$$

OK with XY model

Move to two fluid hydrodynamics. Different velocities for the two fluids.

$$J = J_s + J_n \quad ; \quad J_s = n_s v_s \quad ; \quad J_n = n_n v_n$$

Normal fluid → entropy
Quantum fluid → single many body quantum state
Flow of heat → only by the normal component
Heat current density

$$Q = T \underset{\uparrow}{S} v_n$$

entropy per unit volume

Unusual thermomechanical effect

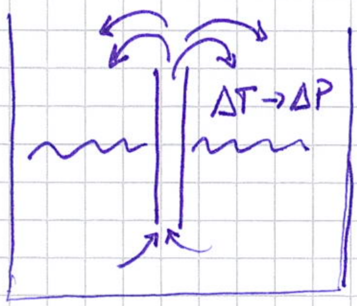
* Connecting two volumes of SF by a (SF) capillary the temperature does not equilibrate. $T_1 \neq T_2$ in equilibrium. But particle flow implies $\mu_1 = \mu_2$

$$G = \mu N \qquad G = U - TS + PV$$

$$dG = -SdT + VdP$$

Therefore ΔT is accompanied by $\Delta P = s\Delta T$

* <u>Fountain effect</u>



Flow quantisation and vortices

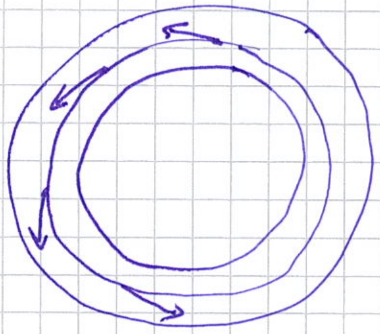
Macroscopic wavefunction → quantisation of the superflow

$$v_s = \frac{\hbar}{m}\nabla\theta \qquad \text{(potential flow)}$$

Taking the curl

$$\nabla \times v_s = 0 \qquad \text{(irrotational)}$$

Consider flow along a closed tube



flow circulation

$$\kappa = \oint v_s \cdot dr$$

This value is independent on the path

$$\kappa = \frac{\hbar}{m}\oint \nabla\theta \cdot dr = \frac{\hbar}{m}\Delta\theta$$ ← change in phase around the tube

but if $\psi_0(r) = \sqrt{n_0}\, e^{i\theta(r)}$ is single valued

we must have

$$\psi(r) = \psi(r)\, e^{i\Delta\theta} \rightarrow \boxed{\Delta\theta = 2\pi n}$$

Circulation of the flow is quantised in units of quantum

$$\kappa = \frac{\hbar}{m}\cdot n.$$

Winding number for the phase around the tube

Experiment: rotate a ring → normal fluid rotates but not the SF
Cooling more normal becomes SF and transfer angular momentum - This is discretised.

The momentum distribution

Hard spheres at small distance

^{4}He is a strongly interacting quantum liquid

$$\hat{H} = \sum_{i=1,N} -\frac{\hbar^2}{2m}\nabla_i^2 + \frac{1}{2}\sum_{i\neq j} V(r_i - r_j)$$

Bosons - symmetric

$$\Psi(\dots r_i \dots r_j \dots) = \Psi(\dots r_j \dots r_i \dots)$$

Energy levels $E_n^{(N)}$ $n = 0, 1, 2 \dots$

$$P_n = \frac{1}{Z_N} e^{-E_n^{(N)}/k_BT} \qquad Z_N = \sum_n e^{-E_n^{(N)}/k_BT}$$

Quantum MonteCarlo methods - numerical

Realistic SF models show a condensate of atoms in the ground state

One particle density matrix

$$\rho_1(|r_1 - r_1'|) = N\int \Psi_0^*(r_1, r_2, \dots r_N)\Psi_0(r_1', r_2, \dots r_N)\, d^3r_2 \dots d^3r_N$$

correlation function. The average is taken on all the other particles in the system except the first one (or any one).

For a non interacting Bose gas at $T=0$ all particles are in $\psi_0(r)$

$$\Psi_0^*(r_1, r_2 \dots r_N) = \psi_0(r_1)\psi_0(r_2)\dots\psi_0(r_N)$$

$$\rho(|r_1 - r_1'|) = N\psi_0^*(r_1)\psi_0(r_1')\int |\psi_0(r_2)|^2 \dots |\psi_0(r_N)|^2 d^3r_2 \dots d^3r_N =$$

$$= N\psi_0^*(r_1)\psi_0(r_1')$$

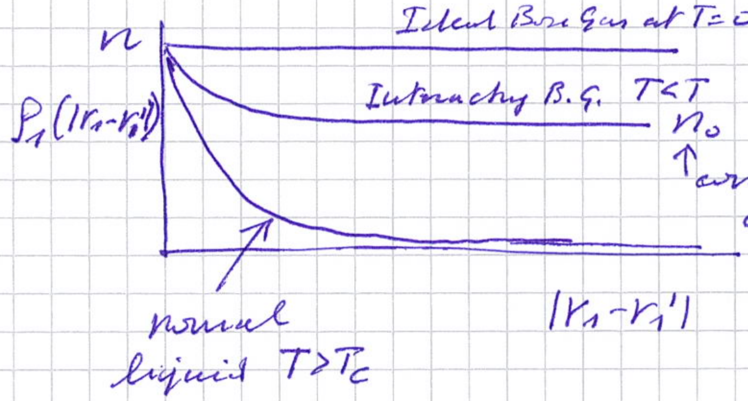
$$\psi_0(r) = \frac{1}{\sqrt{V}} e^{ik\cdot r} = \frac{1}{\sqrt{V}} \qquad (k=0)$$

→ [quantum system in a mixed state]

Therefore the density matrix for a non interacting Bose gas is a constant equal to the particle density

$$\rho_1(|r_1 - r_1'|) = \frac{N}{V} = n \quad \text{at } T=0 \text{ -}$$

In liquid ^4He the density matrix can be computed by Quantum Monte Carlo - Quantum interaction ≃ matrix element between $\Psi(r)$ and $\Psi(r')$. Short term repulsive effect



↑ correct definition of the condensate energy -

This defines an effective single particle macroscopic wavefunction

$$\rho_1(|r_1 - r_1'|) \simeq \Psi_0^*(r_1)\Psi_0(r_1')$$

in the large distance limit

$$|\Psi_0(r)|^2 = n_0$$

Experimental confirmation is given by the momentum distribution. For a quantum fluid at $T=0$

$$P(p)\,d^3p = \frac{V\,d^3p}{(2\pi\hbar)^3}\langle \Psi | n_k | \Psi \rangle \quad ; \quad p = \hbar k$$

The expectation value can be found from the one-body density matrix with a Fourier transform.

$$n_k = \langle \Psi | n_k | \Psi \rangle = \int \rho_1(r)\, e^{ikr}\, d^3r$$

$$\left(\Psi^*(r) \rightarrow a^+ e^{-ikr} \right)$$

For $T < T_c$

$$\rho_1(r) = n_0 + \Delta\rho_1(r)$$

where $\Delta\rho_1(r)$ goes to zero at large r.

$$n_k = \int n_0 e^{ikr} d^3r + \int \Delta\rho_1(r) e^{ikr} d^3r =$$

$$= n_0 V \delta_{k,0} + f(k)$$

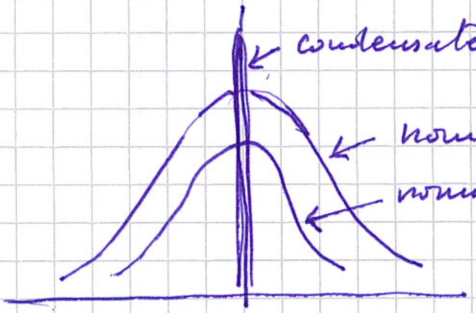
↑ smooth function of k near k=0

Momentum distribution

$$P(p) = n_0 V \delta(p) + \frac{V}{(2\pi\hbar)^3} f(p/\hbar)$$

↑ delta function from the condensate ($N_0 = n_0 V$ particles in $k=0$)

Second contribution from the remaining $N - N_0$ particles. It is a smooth function genuine line (apparently similar to MB distribution) due to quantum zero point motion. Present also at $T=0$



Momentum distribution can be measured by neutron scattering $P(p)$. Quantitative agreement with QMC.
For Liquid ^4He at $T=0$ the condensate part is only about 10% of the total fluid

$$T=0 \quad n_0 \simeq 0.1\, n$$

Quasiparticle excitations

{ Condensate density n_0 For non interacting Bose gas
{ Superfluid density n_s $n_0 = n_s = n$

The condensate density refers to the g-state - particles in the $k=0$ state.
Superfluid density arises from the two fluid model of superflow from the equation for particle current

$$J_s = n_s v_s = n_s \hbar \nabla\theta / m$$

At $T=0$ all particles participate in the superflow even if only a fraction is in the condensate

$$n_s = n \quad ; \quad n_0 \simeq 0.1 n.$$

Galilean invariance

$$r' = r - vt \quad ; \quad p' = p - mv \quad ; \quad E' = E - p.v + \tfrac{1}{2} m v^2$$

in Q.M. $p \to i\hbar\nabla$
Construct a wavefunction for the moving superflow.

$\Psi_0(r_1 \cdots r_N)$ g.s. at rest

when it moves each particle has additional momentum mv
$\hbar q = mv \to$ extra factor $e^{iq\cdot r}$

$$\Psi(r_1 \cdots r_N) = e^{iq(r_1 + r_2 + \cdots r_N)} \Psi_0(r_1 \cdots r_N)$$

For the moving fluid

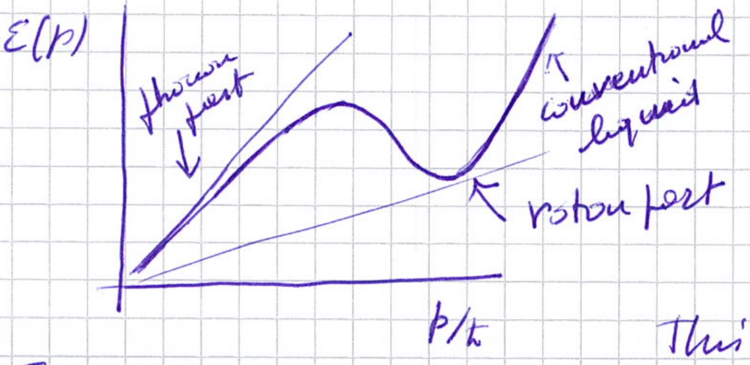
$$\langle P \rangle = N\hbar q \quad ; \quad P = p_1 + p_2 + \cdots p_N$$

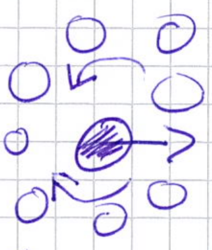
$$\langle H\rangle \approx E_0 + N\frac{\hbar q^2}{2m} = E_0 + \frac{1}{2M}\langle P\rangle^2$$

NB: The superfluid has zero net momentum in the moving reference frame. These are the classical macroscopic equations for an object of mass M and momentum $\langle P\rangle$ moving with velocity

$$V_s = \frac{1}{M}\langle P\rangle = \frac{\hbar q}{m}$$

At $T=0$ the whole mass of the fluid contributes to the superflow and not just the fraction in the zero momentum condensate. Rigidity of the g. state wavefunction.
An observer in a Galilean frame moving with the fluid would see the same wavefunction as a stationary observer would see with a fluid at rest. Every particle contributes to the superflow so $n_s = n$ at $T=0$.
Landau: consider the scattering with the walls of the tube.
For a normal energy spectrum there would be scattering in the normal but also in the SF state.
In ~~order~~ order to have real superfluidity the energy spectrum $E(p)$ must be different in the superfluid.





Complex many body motion

This spectrum explains the absence of viscosity — for small V_s —

First sound and second sound