



BAYERISCHE AKADEMIE DER WISSENSCHAFTEN Technische Universität München

Superconductivity and Low Temperature Physics II



Lecture Notes Summer Semester 2022

R. Gross © Walther-Meißner-Institut

Chapter 1

Quantum Liquids



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I.1 Foundations and General Properties

- Satyendranath Bose (1924)
 - letter to Einstein: proposes new method to derive Planck's law for spectral density of electromagnetic radiation emitted by a black body
 - Bose describes the radiation emitted by a black body in thermal equilibrium by a gas on non-interacting identical particles
 → photons
 - description is in perfect agreement with Einstein's explanation of the photoelectric effect
 - Einstein immediately recognized that this description can be transferred to many other systems:
 (i) gases of identical particles with finite mass,
 (ii) phonons
 - Einstein strongly supported the publication of Bose's results, he translated the paper to German

Satyendranath Bose: <u>Plancks Gesetz und Lichtquantenhypothese</u>. In: Zeitschrift für Physik. 26 (1924), S. 178-181.



Satyendranath Bose (around 1926)



What happens if you cool down a gas of noninteracting bosons ?

Below a certain temperature the particles feel each other due to their finite de Broglie wavelength, although they are non-interacting !

phase transition driven by statistics of particles (not by their interactions)

Bose-Einstein Condensation

thermodynamic phase transition in a gas of non-interacting particles: driven by statistics of particles and not by interactions

I.1 Foundations and General Properties

- 1924: prediction of Bose-Einstein Condensation (BEC) by Einstein
- 1995: first observation of BEC on alkali atoms by



Nobel Prize in Physics 2001

"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"

Eric A. Cornell

Wolfgang Ketterle

Carl E. Wieman

→ long period between theoretical prediction and experimental realization: high density, ultra-cold gas of non-interacting atoms required

 \rightarrow problem: gas liquefies or solidifies due to finite interactions

 \rightarrow more simple to realize:

interacting quantum gas, e.g. superfluid ⁴He

nomenclature

 system of non-interacting particles: 	classical gas	e.g. classical ideal gas
 if quantum fluctuations dominate: 	quantum gas	e.g. Bose-Einstein Condensate, Fermi gas
 system of interacting particles: 	classical liquid	e.g. water, liquid helium-4
 if quantum fluctuations dominate: 	quantum liquid	e.g. superfluid helium-4, Fermi liquid





quantum liquids & condensates show fascinating properties -> discussed in this lecture



- classical liquids and solids characteristic energy scales:
 - (1) average interaction energy: $\langle V \rangle$ or $\langle E_{\text{pot}} \rangle$ characteristic energies: (2) thermal (kinetic) energy: $k_{\rm B}T$ or $\langle E_{\rm kin} \rangle$
 - criterion for liquid/solid: *liquid*: $k_{\rm B}T \gg \langle V \rangle$ $k_{\rm B}T \ll \langle V \rangle$ solid:
- characteristic length scales in a gas:
 - particle distance:
- $d = n^{-1/3}$
 - interaction range: $r_0 \simeq a$
 - de Broglie wavelength:

$$\lambda_{\rm T} = \sqrt{\frac{h^2}{2\pi m k_{\rm B} T}} = \sqrt{\frac{2\pi \hbar^2}{m k_{\rm B} T}}$$

(scattering length *a*)



classical non-interacting gas: $d \gg r_0$, since atoms interact only during collisions

calculation of the average thermal wavelength of a statistical ensemble (1)

we consider a classical gas of N particles:

 \rightarrow probability for a specific particular configuration at temperature T is given by Boltzmann distribution

$$P(\mathbf{p}_1, \dots, \mathbf{p}_N, \mathbf{r}_1, \dots, \mathbf{r}_N) = \frac{1}{Z_N} \exp(-\beta \mathcal{H}) \qquad \beta = 1/k_{\rm B}T, \mathcal{H} = \text{Hamiltonian}$$

$$Z_N = \frac{1}{N!} \int d^3 p_1, \dots, d^3 p_N d^3 r_1, \dots, d^3 r_N \exp(-\beta \mathcal{H})$$

classical partion function, $\frac{1}{N!}$ results from fact that particles cannot be distinguished

potential energy contribution

partition function can be factorized into two terms (related to kinetic and potential energy)

$$Z_N = \frac{1}{N!} \prod_i \int d^3 p_i \exp\left(-p_i^2/2mk_{\rm B}T\right) \cdot \int d^3 r_1, \dots, d^3 r_N \exp\left(-\frac{1}{2}\beta \sum_{i\neq j} V(\mathbf{r}_i - \mathbf{r}_j)\right)$$

kinetic energy contribution product of independent factors

 $[(2\pi m k_{\rm B} T)^{3/2}]^{N}$

(momenta of particles are statistically independent)

- supplementary material

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• calculation of the average thermal wavelength of a statistical ensemble (2)

probability that particle has momentum in volume d^3p of phase space

$$P(\mathbf{p})d^{3}p = (2\pi mk_{\rm B}T)^{3/2} \exp(-p_{i}^{2}/2mk_{\rm B}T)d^{3}p$$

fraction of particles with momentum between p and p + dp

$$P_{\rm MB}(p)dp = \frac{4\pi p^2}{(2\pi mk_{\rm B}T)^{3/2}} \exp(-p^2/2mk_{\rm B}T) dp$$
 Maxwell-Boltzmann distribution

the most likely momentum of the particles is $p=\sqrt{2mk_{\rm B}T}$, the average momentum is $\bar{p}~=\sqrt{8mk_{\rm B}T/\pi}$

→ typical value of the thermal de Broglie wavelength

$$\lambda_{\rm T} = \frac{h}{p_{\rm T}} = \sqrt{\frac{h^2}{2\pi m k_{\rm B} T}} = \sqrt{\frac{2\pi\hbar^2}{m k_{\rm B} T}}$$

• calculation of the average thermal wavelength of a statistical ensemble (3)

the wave number k is given by

$$p_{\rm T} = \int_{-\infty}^{\infty} \mathrm{d}p \exp\left(-\frac{p^2/2m}{k_{\rm B}T}\right)$$

$$p_{\rm T} = \sqrt{2\pi m k_{\rm B} T}$$

• cooling down a classical gas $\rightarrow \lambda_{\rm T} = \sqrt{\frac{h^2}{2\pi m k_{\rm B} T}}$ increases and we can distinguish three regimes

(1) classical regime: $\lambda_{\rm T} \ll r_0 \ll d$

(2) quantum collisions: $r_0 \ll \lambda_{\rm T} \ll d$

collissions can no longer be treated classically

(3) quantum degeneracy: $r_0 \ll d \le \lambda_{\mathrm{T}}$

all degrees of freedom of the gas must be treated quantum mechanically



• define new energy scale related to $d = \lambda_{\rm T}$

(3) zero-point energy E_{zp}

with - particle density n = N/V, $d = n^{-1/3}$ - de Broglie wavelength $\lambda_{\rm T} = d$

 \rightarrow momentum uncertainty

$$\Delta p = \hbar \Delta k = \frac{h}{\lambda_{\rm T}} = \frac{h}{d} = h n^{1/3}$$

→ zero-point energy

$$E_{zp} = \frac{\Delta p^2}{2m} = \frac{h^2}{2md^2} = \frac{h^2 n^{2/3}}{2m} = \pi k_{\rm B} T_{zp}$$
 characteristic temperature

for an ideal gas the energy $E = \pi k_{\rm B}T$ is assumed; the factor π results from the partition function

• classification of liquids (interacting liquids with $\langle V \rangle > 0$):

(a) classical liquid: $T_{zp} \ll T_{melting} \ll T$ (quantum fluctuation play no role)(b) quantum liquid: $T_{melting} < T < T_{zp}$ (quantum fluctuation dominate)VVproportional to $\langle V \rangle$ or $\langle E_{pot} \rangle$

quantum liquid:

 $\Lambda > 1$

quantum parameter:



classical liquid:

 $\Lambda < 1$

• classification of liquids (non-interacting liquids: $\langle V \rangle = 0$):

(a) classical liquid: (b) quantum liquid:

$$T_{zp} < T$$

 $T < T_{zp}$

$$T_{\rm zp} = \frac{h^2 n^{2/3}}{2\pi m k_{\rm B}} = \frac{h^2}{2\pi m k_{\rm B} d^2} \qquad \qquad \qquad T = \frac{h^2}{2\pi m k_{\rm B} \lambda_{\rm T}^2}$$

(a) classical liquid:
$$\lambda_{\rm T} \leq n^{-1/3} \simeq d \rightarrow n \cdot \lambda_{\rm T}^3 \leq 1$$

(a) quantum liquid: $\lambda_{\rm T} \geq n^{-1/3} \simeq d \rightarrow n \cdot \lambda_{\rm T}^3 \geq 1$
average particle distance
e.g. electrons @ 300 K: $\lambda_{\rm T} = 4.2$ nm, $d \simeq 0.2$ nm for Cu ($n \simeq 8.5 \times 10^{28}$ m⁻³)

\rightarrow particles become indistinguishable \rightarrow degenerate quantum liquid

• cooling down a classical gas $\rightarrow \lambda_{\rm T} = \sqrt{\frac{h^2}{2\pi m k_{\rm B} T}}$ increases and we can distinguish three regimes

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collissions can no longer be treated classically

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T(K)



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I.1.1 **Quantum Fluids**

quantum statistics:

•

photons, mesons, ⁴ He-atoms,	integral spin	$S=0,\hbar,2\hbar,3\hbar,$	
electrons, nucleons, ³ He-atoms,	half-integral spin	$S = \hbar/2, 3\hbar/2, 5\hbar/2,$	

indistinguishability of identical particles:

symmetry of many-particle wavefunction with respect to particle exchange

$$\begin{split} \wp \ \Psi(1,2) &\equiv \Psi(2,1) = e^{\iota \alpha} \quad \Psi(1,2) \\ \wp \ \Psi(2,1) &\equiv \Psi(1,2) = (e^{\iota \alpha})^2 \ \Psi(1,2) \end{split} \qquad \blacksquare \qquad e^{\iota \alpha} = \pm 1 \end{split}$$

• **bosons** (integral spin)

bosons (integral spin)
$$\Psi_{AB}(1,2) = \frac{1}{\sqrt{2}} [\Psi_A(1)\Psi_B(2) + \Psi_A(2)\Psi_B(1)]$$
fermions (semi-integral spin)
$$\Psi_{AB}(1,2) = \frac{1}{\sqrt{2}} [\Psi_A(1)\Psi_B(2) - \Psi_A(2)\Psi_B(1)]$$

• Pauli principle: two fermions cannot occupy the same quantum state

I.1.1 Quantum Fluids

classical:

4 possibilities

• example: two particles (1,2) in quantum states A and B:

	double-occupancy ratio: 1/2	A(1)B(2)	B(1)A(2)	
bosons:	3 possibilities double-occupancy ratio: 2/3	A(1)A(2) $\frac{1}{\sqrt{2}} \{A(1)B(2)$ B(1)B(2)) + A(2)B(1)}	
fermions:	1 possibility double-occupancy ratio: 0	$\frac{1}{\sqrt{2}} \left\{ A(1)B(2) \right\}$	2) – <i>A</i> (2) <i>B</i> (1)}	
bosons: fermions:	tendency to occupy the same quantum state multiple occupancy of the same quantum state is forbidden			

A(1)A(2)

B(1)B(2)

Quantum Fluids



Bose-Einstein, **Fermi-Dirac** and **Maxwell-Boltzmann distributions** as a function of normalized energy. For the Bose-Einstein distribution we assumed $\mu = 0$, for the Fermi-Dirac distribution $\mu = 5k_BT$ (for a metal μ is several eV corresponding to temperatures of several 10 000 K). For the Maxwell-Boltzmann distributions we also assumed $\mu = 0$ und $5k_BT$ so that the classical distribution coincides with the quantum mechanical distributions for large $\varepsilon \gg k_BT$.

WM

I.1.1

Quantum Fluids



WMI

I.1.1

Quantum Fluids



WMI

I.1.1

- well-known quantum fluids:
 - *liquid helium:* 1.

- small mass and d
- small $\langle V \rangle$
- ⁴He: spin 0
- \rightarrow high T_{zp} (a few K)
 - \rightarrow liquid down to T = 0
 - \rightarrow Bose liquid
- 3 He: spin $\frac{1}{2}$ \rightarrow Fermi liquid
- *electrons in metals:* "non-interacting" electron gas 2. - very small electron mass, higher density as for He \rightarrow very high T_{zp} (a few 10⁴ K) $\rightarrow T_{zp} \gg T_{melting}$ \rightarrow Fermi liquid - spin $\frac{1}{2}$ nuclear matter: - fermions in nuclei, neutron stars, ... - very high density \rightarrow very high T_{zp} (a few 10¹² K)
 - \rightarrow Fermi liquid - spin $\frac{1}{2}$

3.

I.1.1 Quantum Fluids

	mass (kg)	<i>n</i> (m⁻³)	<i>Т_{zp}</i> (К)	statistics
³ He	5.01 x 10 ⁻²⁷	1.63 x 10 ²⁸	6.50	Fermi
⁴He	6.65 x 10 ⁻²⁷	2.18 x 10 ²⁸	5.93	Bose
electrons in Na	9.11 x 10 ⁻³¹	2.65 x 10 ²⁸	4.94 x 10 ⁴	Fermi
nuclear matter	1.67 x 10 ⁻²⁷	1.95 x 10 ³⁸	1 x 10 ¹²	Fermi

$$E_{zp} = \frac{\Delta p^2}{2m} = \frac{h^2}{2md^2} = \frac{h^2 n^{2/3}}{2m} = \pi k_{\rm B} T_{zp}$$



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application of ⁴He in low temperature physics

- soon after discovery on earth, race for the liquefaction of He
 - → main opponents: *Heike Kamerlingh Onnes* and *James Dewar*
 - → Onnes extracted 360 l of He gas out of Monazit sand from North Carolina
- **1908**: first liquefaction: July 10, 1908
- 1925: first liquefaction of He in Germany (March 7, 1925: 4.2 K, 200 ml)
 by *Walther Meißner*, 3rd system world-wide besides Leiden and Toronto
- 1932: Linde supplies first industrial He liequfier to University of Charkov, Ukraine
- **1947**: first commercial liquefier by *S.C. Collins*



Heike Kamerlingh Onnes * 21. 09. 1853 † 21. 02. 1926



James Dewar * 20. 09. 1842 † 27.03.1923

I.1.2 Helium



SIR JAMES DEWAR

Sir James Dewar, (1842-1923) was a chemist and physicist, best known for his work with low-temperature phenomena. Dewar was born in Kincardine, Scotland, and educated at the University of Edinburgh. He was professor of experimental natural philosophy at the University of Cambridge, England, in 1875 and professor of chemistry at the Royal Institution of Great Britain in 1877, where he was appointed director of the Davy-Faraday Research Laboratory.

Dewar developed structural formulas for benzene (1867). He studied the specific heat of hydrogen and was the first person to produce hydrogen in liquid form (1898) and to solidify it (1899). He constructed a machine for producing liquid oxygen in quantity (1891). He invented the Dewar flask or thermos (1892) and co-invented cordite (1889), a smokeless gunpowder, with Sir Frederick Abel. His discovery (1905) that cooled charcoal can be used to help create high vacuums later proved useful in atomic physics. Dewar was knighted in 1904.

The Dewar flask or vacuum flask/bottle is a container for storing hot or cold substances, i.e. liquid air. It consists of two flasks, one inside the other, separated by a vacuum. The vacuum greatly reduces the transfer of heat, preventing a temperature change. The walls are usually made of glass because it is a poor conductor of heat; its surfaces are usually lined with a reflective metal to reduce the transfer of heat by radiation. Dewar used silver. The whole fragile flask rests on a shock-absorbing spring within a metal or plastic container, and the

air between the flask and the container provides further insulation. The common thermos bottle is an adaptation of the Dewar flask. Dewar invented the Dewar flask in 1892 to aid him in his work with liquid gases.

The vacuum flask was not manufactured for commercial/home use until 1904, when two German glass blowers formed Thermos GmbH. They held a contest to rename the vacuum flask and a resident of Munich submitted "Thermos", which came from the Greek word "Therme" meaning "hot."



- history: ³He
 - 1933: discovery by *Oliphant, Kinsey* and *Rutherford* (they believed that ³He is unstable, disproven by *Alvarez* and *Cornog* in 1939)
 - **1947**: first experiments with gaseous ³He
 - **1949**: first condensation of ³He gas (*Sydorniak and Co.*)
 - 1956: theory of Fermi liquids (L.D. Landau, Nobel Prize in Physics 1962)
 - 1960s: first experiments with the Fermi liquid ³He (various groups)
 - **1963**: first theory of superfluid ³He (*Anderson and Morel, Balian and Werthamer*)
 - 1971: discovery of superfluid phase transition at 2 mK (*Lee, Osheroff, Richardson,* Nobel Prize in Physics 1996)
 - 1975: extension of BCS theory to triplet pairing (*Leggett*, Nobel Prize in Physics 2003)
 - 1977: first experiments on superfluid ³He in Germany at WMI (*Eska, Schuberth, Uhlig*)



- *He isotops: ⁴He* and ³*He*
 - ⁴He: obtained out of natural gas (e.g. sources in USA, Poland, Algeria contain up to 10%)

-L = 0, S = 0, nuclear spin $I = 0 \rightarrow boson$

• **³He:** - natural amount of ³He in ⁴He is only 0.14 ppm

- artificial generation of ³He by nuclear reaction

 ${}_{3}^{6}\text{Li} + {}^{1}\text{n} \rightarrow {}_{1}^{3}\text{T} + {}_{1}^{4}\text{He} \qquad {}_{1}^{3}\text{T} \rightarrow {}_{2}^{3}\text{He} + e^{-} + \overline{\nu}_{e} \qquad (12.5 \text{ years})$

- ³He is very expensive, several 1000 € per liter

- L = 0, S = 0, nuclear spin $I = \frac{1}{2}$ \rightarrow fermion

- despite their simple electronic structure, the liquids of both He isotopes show
 - a rich variety of exotic phenomena
 - pronounced differences due to different quantum statistics





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Lecture No. 2 05 May 2022

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I.1.3 Van der Waals Bonding

- **neutral atom**, average dipole moment vanishes: $\langle \mathbf{p}_A \rangle = \mathbf{0}$
 - $\textbf{\textbf{\rightarrow}}$ dipole moment induced by electric field: $p_{A}^{ind} \propto E$

proportionality constant is **polarizability** α_A of atom A:

$$\mathbf{p}_A^{\text{ind}} = \alpha_A \mathbf{E}$$



$$|\mathbf{p}_{A}\rangle = \mathbf{0}$$

• assumption:

E-field is generated by charge $q_{\rm B}$ of ion B at distance R

$$\mathbf{p}_{\mathrm{A}}^{\mathrm{ind}} = \alpha_{\mathrm{A}} \mathbf{E}_{\mathrm{B,ion}} = \alpha_{\mathrm{A}} \frac{q_{B}}{4\pi\epsilon_{0}R} \ \widehat{\mathbf{R}}$$

• potential energy of atom A

$$E_{\text{pot}} = -\mathbf{p}_{\text{A}}^{\text{ind}} \cdot \mathbf{E}_{\text{B,ion}} = -(\alpha_A \mathbf{E}_{\text{B,ion}}) \cdot \mathbf{E}_{\text{B,ion}} \propto \mathbf{E}_{\text{B,ion}}^2$$



I.1.3 Van der Waals Bonding

- assumption:
 - field $\mathbf{E}(\mathbf{p}_B)$ at position of atom A is generated by atom B with dipole moment \mathbf{p}_B
 - $\mathbf{E}(\mathbf{p}_B)$ induces dipole moment \mathbf{p}_A of atom A, which in turn generates field $\mathbf{E}(\mathbf{p}_A)$ at position of atom B

$$\mathbf{E}(\mathbf{p}_{B}) = \mathbf{E}(\mathbf{p}_{B}) = \mathbf{E}_{B} + \mathbf{P}_{A} + \mathbf{P}_{A} + \mathbf{E}(\mathbf{p}_{A}) = \frac{1}{4\pi\epsilon_{0}R^{3}}(3p_{B}\cos\vartheta_{B}\ \hat{\mathbf{R}} - \mathbf{p}_{B}) + \mathbf{E}_{B} + \mathbf{E}_{A} + \mathbf{$$





Van der Waals (right) and Heike Kamerlingh Onnes in Leiden with the helium 'liquefactor' (1908)



Johannes Diderik Van der Waals (1837 - 1923) Nobel Prize in Physics (1910)

"for his work on the equation of state for gases and liquids"



I.1.3 Van der Waals Bonding

• interaction potential with short range repulsion due to Pauli principle:

 $E_{\text{pot}}(R) = 4\epsilon \left[\left(\frac{\sigma}{R} \right)^{12} - \left(\frac{\sigma}{R} \right)^{6} \right]$

Lennard-Jones potential



	Ne	Ar	Kr	Xe
ϵ (eV)	0.0031	0.0104	0.0141	0.0200
σ (Å)	2.74	3.40	3.65	3.98
R_0/σ	1.14	1.11	1.10	1.09

11.6 K ⇔ 1 meV

→ Van der Waals bonding is very weak !!
I.1.3 Van der Waals Bonding

determination of *equilibrium distance* of atoms in lattice: → minimize total potential energy

$$U_{\text{tot}} = \frac{N}{2} \sum_{i \neq j} 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^{6} \right]$$

 $U_{\text{tot}}(R) = 2N\epsilon \left[A_{12} \left(\frac{\sigma}{-} \right)^{12} - A_{\epsilon} \left(\frac{\sigma}{-} \right)^{6} \right]$

we rewrite

with
$$A_k = \sum_{i \neq j} \frac{1}{\alpha_{ij}^k}$$
, $k = 6, 12$ (lattice sum)

equilibrium distance: $\partial U_{tot}(R)/\partial R = 0$

$$R_0 = \left(2\frac{A_{12}}{A_6}\right)^{1/6} \cdot \sigma \qquad \qquad R_0 = 1.09 \cdot \sigma$$

 Σ = binding energy of a single atom *j* with all other atoms *i*. Total binding energy is obtained by multiplication with *N*/2.

R: nearest neighbor distance

 $r_{ij} = \alpha_{ij}R$ k: number of nearest neighbors

	Kristallstruktur	A ₆	A ₁₂	
	fcc	14.4539	12.1319	
	hcp	14.4549	12.1323	
	bcc	12.253	9.114	
	$U_{\text{tot}}(R_0) = -N\epsilon \begin{cases} 8.61016 & \text{fcc} - \text{structure} \\ 8.61107 & \text{hcp} - \text{structure} \end{cases}$			

hcp has lowest energy but fcc is found experimentally for nobel gases

→ effect of zero point fluctuations

→ more detailed band structure calculation is required

(modification of Van der Waals binding energy due to overlap of excited atomic states with neighboring atoms in crystal structure)

estimate of *zero-point fluctuation amplitude* for harmonic oscillator:

$$E_{\rm tot} = E_{\rm kin} + E_{\rm pot}$$

• for
$$x = x_{\max}$$
:

$$E_{\rm kin} = 0$$
, $E_{\rm pot} = \frac{1}{2}kx_{\rm max}^2 = \frac{1}{2}M\omega^2 x_{\rm max}^2$



spring constant k is given by second derivative of the interaction potential

• by equating $\frac{1}{2}kx_{\text{max}}^2$ with the ground state energy $\frac{1}{2}\hbar\omega$ of the harmonic oscillator, we obtain

$$\implies x_{\max}^2 = \frac{\hbar}{M\omega} = \frac{\hbar}{\sqrt{kM}}$$

for He: $x_{\max} \approx 0.3 - 0.4$ times the lattice constant a $a \approx \left(\frac{V_{mol}}{N_A}\right)^{1/3}$ V_{mol} = mole volume, N_A = Avogadro number

(*Lindeman* criterion for melting of solid: $x_{\text{max}} \approx 0.3 \cdot a$)

→ Helium stays liquid even at T = 0 due to large zero point fluctuations caused by (i) weak Van der Waals forces (small k) (ii) small mass M

• we can use uncertainty relation to estimate the *kinetic energy* due to zero point fluctuations:

$$\Delta p \cdot \Delta x \simeq \hbar \quad \Rightarrow \quad \Delta p \sim \frac{\hbar}{\Delta x} \approx \frac{\hbar}{0.3 a} \approx \frac{h}{a} \qquad a = \text{lattice constant}$$

$$E_{\rm zp} = \frac{\Delta p^2}{2m} \approx \frac{h^2}{2Ma^2} \approx 18 \ {\rm K}$$

- \rightarrow large quantum mechanical zero-point energy due to small mass M
- ➔ kinetic energy due to zero point fluctuations is comparable to potential energy due to Van der Waals interaction

due to strong influence of quantum fluctuations, helium stays liquid down to temperatures, where $\lambda_T \ge d \simeq a$

➔ Helium becomes a quantum liquid

• total potential energy for solid and liquid He



solid: regular lattice

→ same distance between atoms → $E_{\text{pot}}(R) \approx \text{potential } U_{\text{tot}}(R)$

liquid: disordered system

 \rightarrow varying distance between atoms

 $\rightarrow E_{pot}$ is smeared out due to averaging over various distances

 \rightarrow reduced depth and increased width of $E_{\text{pot}}(\langle R \rangle)$

Why does He not become solid at low T ??

zero point fluctuations play a crucial role

for liquid helium:



contribution of E_{zp} smaller due to broadened E_{pot}



- without quantum fluctuations: ⁴He would be solid at a molar volume of **10 cm³**
- with quantum fluctuations: ⁴He stays liquid with molar volume of 28 cm³



Comparison of *ab initio* potential energies for Ne, Ar, Kr, Xe (symbols) with SAAP calculations (solid lines)

U. K. Deiters et al., J. Chem. Phys. 150, 134504 (2019) https://doi.org/10.1063/1.5085420

comparison of ⁴He and Ne:

	Не	Ne
potential minimum ε	1.03 meV	3.94 meV
interatomic distance R_0	0.265 nm	0.296 nm
	$1 m_0 V - 11 C V$	

 $\frac{36\varepsilon}{R_0^2}$

(for fcc)



 $\Lambda > 1$



quantum parameter:

liquid	Хе	Kr	Ar	Ne	H ₂	⁴He	³ He
Λ	0.06	0.10	0.19	0.59	1.73	2.64	3.05

Large E_{zp} , identical E_{pot} , but also large E_{pot}

mass of ³He smaller than of ⁴He

- → even stronger effect of quantum fluctuations
- → larger quantum parameter
- → larger molar volume
 - ³He: **40 cm³/mole**, ⁴He: **28 cm³/mole**

I.1.6 pT phase diagram of ⁴He

general nomenclature, definitions



https://commons.wikimedia.org/wiki/File:Phase-diag2.svg

I.1.5 Helium under Pressure



WM

I.1.6 pT phase diagram of ⁴He



Phase diagram of ⁴He at low temperatures. ⁴He remains liquid at zero temperature if the pressure is below 2.5 MPa (approximately 25 atmospheres) \rightarrow *no triple point*.

The liquid has a phase transition to a *superfluid phase*, also known as He-II, at the temperature of 2.17 K (at vapor pressure). The solid phase has either hexagonal close packed (hcp) or body centered cubic (bcc) symmetry.

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I.1.6 pT phase diagram of ³He



big difference in value of **T**_{sf}

- normal/superfluid transition dominated by quantum effects
- quantum statistics matters!!
 (bosons vs. Fermions)
- nature of superfluid phase in
 ⁴He and ³He is different

- phase diagram of ³He: note the logarithmic temperature scale. There are *two superfluid phases of ³He, A and B*.
- the line within the solid phase indicates a transition between spin-ordered and spin disordered structures (at low and high temperatures, respectively).

I.1.6 pT phase diagram of ³He





 $\frac{\partial p_m}{\partial T} = \frac{\Delta S_m}{\Delta V_m} < 0$

since volume of liquid state is larger, the entropy of the liquid state must be smaller

 → more ordered liquid state!?
 → explanation follows later: ordering in momentum space





Characteristic Properties of Helium Isotopes

	³ He	⁴He
boiling point T_b (K) (@ p = 1 bar)	3.19	4.21
critical temperature $T_{\rm c}$ (K)	3.32	5.20
critical pressure p _c (bar)	1.16	2.29
superfluid transition temperature $T_{\rm s}$ (K)	0.0025	2.177
density ρ (g/cm ³) (for T \rightarrow 0 K)	0.076	0.145
density ρ (g/cm³) (@ boiling point)	0.055	0.125
classical molar volume V _m (cm ³ /mole) (@ saturated vapor pressure and T = 0 K)	12	12
actual molar volume V_m (cm ³ /mole) (@ saturated vapor pressure and $T = 0$ K)	36.84	27.58
melting pressure p _m (bar) (@ T = 0 K)	34.39	25.36

strong difference between superfluid properties of ⁴He and ³He

➔ different nuclear spin ➔ different quantum statistics

Characteristic Properties of Helium Isotopes



Condensation of Pairs of HE - 3 Atoms

Condensation of Pairs (Cooper Pairs) of

Electrons in a Lattice of Positive Ions

Condensation of

Single HE - 4 Atoms

WM

I.1.7

I.1.8 Specific Heat of ⁴He – Lambda Point

- first measurements by *Dana* and *Kamerlingh Onnes* in 1923
 - anomalous increase of C_p at about $T_\lambda=2.177~{
 m K}$
 - in publication (1926) some data points were omitted, since they were believed to result from exp. artefacts
- confirmation by *Clusius* and *Keesom* in 1932 (introduced denotion He I and He II → phase transition)
 - He I: normal fluid, He II: superfluid



Buckingham, M. J. and Fairbank, W. M., "The Nature of the Lambda Transition", in Progress in Low Temperature Physics III, 1961.

I.1.8 Specific Heat of ⁴He – Lambda Point

comparison of specific heat of ⁴He and that of an ideal Bose-Einstein condensate



2nd order phase transition is expected for ideal Bose-Einstein condensate

 \rightarrow no divergence of C_V at $T = T_{\lambda}$

measured behavior of ⁴He near T_{λ} is more complicated

(detailed discussion follows later)



Specific Heat of ⁴He – Precision Measurement



- specific heat is measured with very high temperature resolution (≈ nK)
- extreme purity of liquid He is important
 - → model system for testing physics of phase transitions
- experimental problem:
 → hydrostatic pressure
 → space experiments





Specific heat of liquid helium in zero gravity very near the lambda point J. A. Lipa et al., Phys. Rev. B 68, 174518 (2003)

→ key result: second order phase transition with logarithmic singularity

I.1.8 Specific Heat of ³He



$C_V(T)$ similar to a metallic superconductor

- $T > T_c$: linear $C_V(T)$ of Fermi liquid

> $C_V(T) = \gamma T$ $\gamma = \frac{3}{2} \frac{n}{E_F} \frac{\pi^2}{3} k_B^2 \qquad \text{(Sommerfeld, 1927)}$

 $-T = T_c$

jump due to superfluid transition

 $- T < T_c$:

reduction of C_V due to condensation of Fermions (similar to superconductors)

Source:

Greywall, Phys. Rev. B 33, 7520 (1986) ³He specific heat and thermometry at millikelvin temperatures



- specific heat of ⁴He is large: $C_V \approx 1 \text{ J/g K}$ (compared to about 10⁻⁵ J/g K of Cu, $C_V \propto n \cdot T/T_F$)
- Iatent heat of evaporation of ⁴He is small (20.59 J/g), but large compared to specific heat of other materials
 → application as cooling liquid
- strong anomaly of specific heat at T_{λ} , origin unknown for more than 30 years \rightarrow originates from *Bose-Einstein condensation* (bosonic character of ⁴He, interacting bosonic system)
- shape of anomaly resembles greek letter $\lambda \rightarrow Lambda \ point$
- below T_{λ} entropy and specific heat decrease rapidly with decreasing T \rightarrow condensation in momentum space
- for ⁴He temperature variation of C_V below T_λ determined by collective excitations in superfluid (*phonons, rotons* discussion later)

I.1 Summary of Experimental Observations

- for ⁴He phase transition at $T_{\lambda} \rightarrow$ Lambda point is due to **bosonic character of** ⁴He
 - → no such transition was expected for ³He due to nuclear spin I = 1/2 (fermionic character of ³He)
- only after the development of BCS theory in 1957 (condensation of Cooper pairs into macroscopic quantum state), the search for the superfluid phase of ³He has been intensified
- 1963: Theory of superfluid ³He (Anderson and Morel, Balian and Werthamer)
- 1971: after the temperature regime below 5 mK has been accessed, the superfluid phase of ³He has been found by Osheroff, Richardsen and Lee in NMR experiment
 D.D. Osheroff, R.C. Richardsen, D.M. Lee,
 Phys. Rev. Lett. 28, 885 (1972)
- there is not only a single superfluid phase, but three, depending on temperature, pressure and applied magnetic field
- 1977: first experiment with ³He in Germany at WMI (Eska, Schuberth, Uhlig,)





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I.4 Vortices

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I.5 ³He

- I.5.1 normal fluid ³He
- I.5.2 solid ³He and Pomeranchuk effect
- I.5.3 superfluid ³He
- I.6 ³He / ⁴He mixtures



basic assumption

⁴He is treated as a non-interacting gas of bosons

we already have learnt that there are Van der Waals interactions

- → treatment of ⁴He as an ideal bosonic gas is only a *first order approximation*
- → interactions lead to devitations from behavior of ideal gas of non-interacting bosons



• high temperatures:

average distance \overline{R} of atoms in gas is large compared to **de Broglie wavelength** $\lambda_T = h/p \propto 1/\sqrt{T}$ \rightarrow classical gas with Maxwell-Boltzmann statistics

thermal de Broglie wave length:

$$\lambda_{\rm T} = \sqrt{\frac{h^2}{2\pi m k_{\rm B} T}} = \sqrt{\frac{2\pi\hbar^2}{m k_{\rm B} T}}$$

compare I.1.1

• low temperatures:

- quantum mechanical description, as soon as average particle distance $\bar{R} = \lambda_{\rm T}$
- classical gas of distiguishable particles turns into quantum soup of indistinguishable identical particles
 - → quantum gas with Bose or Fermi statistics
 - → Bose-Einstein condensation for bosons





Bose -Einstein Condensation

- phase transition occurs for *interactionless bosonic particles*
- originates from the *indistinguishability of identical particles*



Albert Einstein und Satyendranath Bose

proposed in 1924 that below a characteristic temperature T_B a macroscopic number of bosons can condense into the state of lowest energy

experimental confirmation in 1995



Eric A. Cornell

Wolfgang Ketterle



Nobel Prize in Physics 2001 "for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"

Carl E. Wieman



Bose-Einstein Condensation

m

SITZUNGSBERICHTE DER PREUSSISCHEN

AKADEMIE DER WISSENSCHAFTEN.

Sitzung der physikalisch-mathematischen Klasse vom 8. Janua

Quantentheorie des einatomigen idealen Gases. Zwetts Ahhandleng. Von A. Enstres.

1925 SITZUNGSBERICHTE DER PREUSSISCHEN AKADEMIE DER WISSENSCHAFTEN

Staong der physikalisch-mathematischen Klasse vom 29. Januar

Zur Quantentheorie des idealen Gases. Von A. Esserius.

A. Einstein. Quantentheorie des einatomigen Gases. SITZUNGSBERICHTE DER PREUSSICHEN AKADEMIE DER WISSENSCHAFTEN PHYSIKALISCH-MATHEMATISCHE KLASSE 3, 1925.

Quantentheorie des einatomigen idealen Gases.

1925

1

Von A. EINSTEIN.

Quantentheorie des einatomigen idealen Gases.

Zweite Abhandlung.

Von A. EINSTEIN.

Line von willkürlichen Ansätzen freie Quantentheorie des einatomigen idealen Gases existiert bis heute noch nicht. Diese Lücke soll im folgenden ausgefüllt werden auf Grund einer neuen, von Hrn. D. Bose erdachten Betrachtungsweise, auf welche dieser Autor eine höchst beachtenswerte Ableitung der PLANCKschen Strahlungsformel gegründet hat¹.

Der im folgenden im Anschluß an Bosz einzuschlagende Weg läßt sich so charakterisieren. Der Phasenraum eines Elementargebildes (hier eines einatomigen Moleküls) in bezug auf ein gegebenes (dreidimensionales) Volumen wird in «Zellen« von der Ausdehnung h3 eingeteilt. Sind viele Elementargebilde vorhanden, so ist deren für die Thermodynamik in Betracht kommende (mikroskopische) Verteilung durch die Art und Weise charakterisiert, wie die Elementargebilde über diese Zellen verteilt sind. Die »Wahrscheinlichkeit« eines makroskopisch definierten Zustandes (im PLANCKSchen Sinne) ist gleich der Anzahl der verschiedenen mikroskopischen Zustände, durch welche der makroskopische Zustand realisiert gedacht werden kann. Die Entropie des makroskopischen Zustandes und damit das statistische und thermodynamische Verhalten des Systems wird dann durch den BOLTZMANNSchen Satz bestimmt.

In einer neulich in diesen Berichten (XXII 1924, S. 261) erschienenen Abhandlung wurde unter Anwendung einer von Hrn. D. Bose zur Ableitung der PLANCKSchen Strahlungsformel erdachten Methode eine Theorie der »Entartung« idealer Gase angegeben. Das Interesse dieser Theorie liegt darin, daß sie auf die Hypothese einer weitgehenden formalen Verwandtschaft zwischen Strahlung und Gas gegründet ist. Nach dieser Theorie weicht das entartete Gas von dem Gas der mechanischen Statistik in analoger Weise ab wie die Strahlung gemäß dem Planckschen Gesetze von der Strahlung gemäß dem Wienschen Gesetze. Wenn die Bosesche Ableitung der PLANCKSchen Strahlungsformel ernst genommen wird, so wird man auch an dieser Theorie des idealen Gases nicht vorbeigehen dürfen; denn wenn es gerechtfertigt ist, die Strahlung als Quantengas aufzufassen, so muß die Analogie zwischen Quantengas und Molekülgas eine vollständige sein. Im folgenden sollen die früheren Überlegungen durch einige neue ergänzt werden, die mir das Interesse an dem



Pauli exclusion principle

does not allow further compression of fermions in momentum space at low T

- degenerate multiparticle system: Bosons and Fermions (cf. I.1.1)
 - at given density *n*: particle occupies cube with $d = 1/n^{1/3}$
 - classical liquid: $\lambda_{\rm T} \leq d$

particles are distinguishable

• quantum liquid: $\lambda_{\mathrm{T}} \geq d$

→ degenerate quantum liquid

• *Bosons*: (⁴He,)

→ Bose-Einstein condensation

- *Fermions*: (³He, e, p, n,)
 - ➔ Fermi sea



• cooling down atoms

	temperature	density (1/cm³)	phase space density
atomic oven	500 K	10-1	10 ⁻¹³
Laser cooling	50 μΚ	10 ¹¹	10 ⁻⁶
evaporation cooling	500 nK	10 ¹⁴	2.612
Bose-Einstein condensation		10 ¹⁵	107

 $\lambda_{\rm T} = \sqrt{\frac{h^2}{2\pi m k_{\rm B} T}} = \sqrt{\frac{2\pi \hbar^2}{m k_{\rm B} T}} \propto \frac{1}{\sqrt{mT}}$

 $\lambda_{\rm T}^3/d^3$

I.2.1.1 Laser Cooling

• Laser cooling:

techniques in which atomic and molecular samples are cooled down to near absolute zero through the interaction with one or more laser fields

- Laser cooling techniques
 - Doppler cooling (Schawlow, Hänsch)

T.W. Hänsch, and A.L. Schawlow, Cooling of gases by laser radiation, Optics Communications, 13, 68 (1975)

- other techniques
 - Sisyphus cooling
 - Resolved sideband cooling
 - Velocity selective coherent population trapping (VSCPT)
 - Anti-Stokes inelastic light scattering (typically in the form of fluorescence or Raman scattering)
 - Cavity mediated cooling
 - Sympathetic cooling
- Nobel Price in Physics 1997:

"for the development of methods to cool and trap atoms with laser light" for Steven Chu, Claude Cohen-Tannoudji und William D. Phillips

- in **Doppler cooling**, the frequency of *light is tuned slightly below an electronic transition in the atom*
- because the light is detuned to the "red" (i.e., at lower frequency) of the transition, the atoms will absorb more photons if they move towards the light source, due to the Doppler effect
 - a stationary atom sees the laser neither red- nor blueshifted and does not absorb the photon
 - an atom moving away from the laser sees it red-shifted and does not absorb the photon
 - an atom moving towards the laser sees it blue-shifted and absorbs the photon, slowing the atom
 - the photon excites the atom, moving an electron to a higher quantum state.
 - the atom re-emits a photon,
 as its direction is random, there is no net change in
 momentum over many absorption-emission cycles





• **Doppler shift** (how does the moving atom see the laser frequency)



atom = observer (O) fixed position



$$f_0 = \frac{f_S}{1 - \frac{\mathbf{v}_S \cdot \mathbf{e}_{SO}}{c}}$$

laser frequency seen by the atom is blue-shifted, if laser and atom move towards each other

→ red detuned laser light becomes resonant if atom moves towards the laser

• momentum/velocity change of atom due to photon absorption

$$\frac{\Delta p}{p} = \frac{\hbar k_{ph}}{mv} = \frac{\Delta v}{v} \qquad \Rightarrow \quad \Delta v = \frac{\hbar k_{ph}}{m}$$

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• atom-laser detuning with atom at rest:

$$\delta_0 = \omega_{atom} - \omega_{laser}$$

• atom-laser detuning with atom moving at velocity v:

$$\delta_{\text{Doppler}} = 2\pi (f_0 - f_S) = 2\pi f_0 \frac{\mathbf{v} \cdot \mathbf{e}_{SO}}{c} = 2\pi f_0 \frac{\hbar \mathbf{k} \cdot \mathbf{v}}{\hbar \omega_0} = \mathbf{k} \cdot \mathbf{v} \qquad \qquad \mathbf{f}_0 = \frac{f_S}{1 - \frac{\mathbf{v}_S \cdot \mathbf{e}_{SO}}{c}}$$

effective detuning between atom and laser

$$\delta_{\rm eff} = \delta_0 - \delta_{\rm Doppler} = \delta_0 - \mathbf{k} \cdot \mathbf{v}$$

• force acting on the atom:

$$\mathbf{F} = \hbar \mathbf{k} \, \gamma = \hbar \mathbf{k} \frac{\Gamma}{2} \frac{(I/I_0)}{1 + \frac{I}{I_0} + \left(\frac{2\delta_{\text{eff}}}{\Gamma}\right)^2}$$

large intensity $I \gg I_0$:

- γ = absorption rate
- $\Gamma =$ line width of atom transition,

we use:

 $p = \frac{E}{c}, \qquad c = \frac{E}{p} = \frac{\hbar\omega}{mv} = \frac{\hbar\omega}{\hbar k}$

- spontaneous emisson rate
- I_0 = saturation intensity

www.wmi.badw.de



 velocity distribution of an atom beam before and after (dashed line) the interaction with a laser beam of fixed frequency

 velocity distribution of an atom beam before and after (dashed line) the interaction with a laser beam of continuously decreasing frequency

- achievable minimum temperature in Doppler cooling:
 - spontaneous absorption and emission are random processes
 - \rightarrow the average force acting on the atoms is statistically fluctuating
 - \rightarrow Brownian motion in phase space
 - minimum temperature is given by the compensation of heating effect due to the random absorption and emission processes and maximum cooling rate

$$k_{\rm B}T_{\rm Doppler} = \frac{\hbar\Gamma}{2}$$

- e.g. $T_{\text{Doppler}} = 240 \ \mu$ K for Na corresponding to average velocity of 1 km/h $T_{\text{Doppler}} = 140 \ \mu$ K for Rb
I.2.1.1 Laser Cooling – Optical Molasses

- optical molasses (Steven Chu, 1985)
- an optical molasses consists of 3 pairs of counter-propagating circularly polarized laser beams intersecting in the region where the atoms are present
- while for simple Doppler cooling the minimum temperature for Na atoms is about 250 μK, optical molasses can cool the atoms down to 40 μK, i.e. an order of magnitude colder.





I.2.1.1 Laser Cooling – Optical Molasses

• force acting by two laser with opposite directions

$$\mathbf{F} = +\hbar\mathbf{k}\frac{\Gamma}{2}\frac{(I/I_0)}{1+\frac{I}{I_0} + \left(\frac{2(\delta_0 - \mathbf{k} \cdot \mathbf{v})}{\Gamma}\right)^2} - \hbar\mathbf{k}\frac{\Gamma}{2}\frac{(I/I_0)}{1+\frac{I}{I_0} + \left(\frac{2(\delta_0 + \mathbf{k} \cdot \mathbf{v})}{\Gamma}\right)^2}$$



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BAYERISCHE AKADEMIE DER WISSENSCHAFTEN Technische Universität München

Superconductivity and Low Temperature Physics II



Lecture No. 3 12 May 2022

R. Gross © Walther-Meißner-Institut



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- consider a gas of N (\approx 10²²) bosons of mass m in a cube of volume V = L^3 (\approx 1 cm³), canonical ensemble (given T, V, N)
 - eigen energies:

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 n^2$$
 with $n^2 = n_x^2 + n_y^2 + n_z^2$

- $\Delta \varepsilon / k_B T \le 10^{-14}$
- \rightarrow level spacing small compared to thermal energy (e.g. He @ 10 K) \rightarrow no influence on experimental result
- occupation probability:

y:
$$n_k = \frac{1}{\exp\left(\frac{\varepsilon_k - \mu}{k_B T}\right) - 1}$$

Bose-Einstein distribution

 μ = chemical potential

important note:

- $\mu \leq \varepsilon_k$ for all k to avoid negative occupation probabilities
- usually one sets $\varepsilon_0 = 0$ for the lowest energy state

• energy and particle number:

$$U(T,V,\mu) = \sum_{k} \varepsilon_k n_k$$

$$N(T, V, \mu) = \sum_{k} n_{k}$$

- derivation of Bose-Einstein distribution (1)
 - we use the single spin density of states of free particles in 3D:

$$D(\varepsilon) = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\varepsilon}, \qquad N(\varepsilon) = \frac{D(\varepsilon)}{V}$$

- total entropy of the particle gas: $S = k_B \ln \Omega$ Ω = number of the available states at given total energy *E*
- Ω is determined by the number of possibilities to distribute the N particles on the available states
 - we divide the k-space into spherical shells with the shell s containing M_s states
 - the number of possibilities to put N_s particles on M_s states is given by

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

(we use $M_s = D(\varepsilon)\delta\varepsilon_s$ for the number of available states in the shell *s*)

- the total number Ω of possibilities is obtained by multiplying the numbers Ω_s

$$\Omega = \prod_{s} \Omega_s = \prod_{s} \frac{(N_s + M_s - 1)!}{N_s! (M_s - 1)!}$$

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- derivation of Bose-Einstein distribution (2)
 - we use the Stiring approximation $\ln N! = N \ln N N$ and for N_s , $\Omega_s \gg 1$ we obtain

$$S = k_{\rm B} \ln \Omega = k_{\rm B} \sum_{s} \left[(N_s + M_s) \ln(N_s + M_s) - N_s \ln N_s - M_s \ln M_s \right]$$

- in thermal equilibrium the particles are distributed on the shells to maximize *S* under the boundary conditions $N = \sum_{s} N_{s} = const$. and $U = \sum_{s} \varepsilon_{s} N_{s} = const$.
- we maximize S for N = const. and U = const. we obtain $(dU = TdS + \mu dN)$

$$\frac{\partial S}{\partial N_s} - \frac{1}{T} \frac{\partial U}{\partial N_s} + \frac{\mu}{T} \frac{\partial N}{\partial N_s} = 0 = \frac{\partial S}{\partial N_s} - k_{\rm B} \beta \frac{\partial U}{\partial N_s} + k_{\rm B} \beta \mu \frac{\partial N}{\partial N_s} \qquad \beta = 1/k_{\rm B} T$$

(Lagrangian multipliers)

performing the differentiation we obtain

$$\ln(N_s + M_s) - \ln N_s - \beta \varepsilon_s + \beta \mu = 0 \quad \Rightarrow \quad N_s = \frac{1}{\exp(\beta(\varepsilon_s - \mu)) - 1} \quad M_s$$

average particle number occupying state in shell s

$$n_{\rm BE} = \left[\exp\left(\frac{\varepsilon_s - \mu}{k_{\rm B}T}\right) - 1 \right]^{-1}$$

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• how to get rid of the summation over k?

$$\sum_{k} \dots \Rightarrow \int Z(k) d^{3}k = \frac{V}{(2\pi)^{3}} \int d^{3}k$$
$$\sum_{k} \dots \Rightarrow \int D(\varepsilon) d\varepsilon = \frac{V}{4\pi^{2}} \left(\frac{2m}{\hbar^{2}}\right)^{3/2} \int \sqrt{\varepsilon} d\varepsilon$$

for free bosons with dispersion
$$\varepsilon_k = \frac{\hbar^2 k^2}{2m^2}$$

$$Z(k) = \frac{V}{(2\pi)^3}$$

$$D(\varepsilon) = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \sqrt{\varepsilon}$$

$$U(T, V, \mu) = \sum_{k} \varepsilon_{k} n_{k} \quad \Rightarrow \quad \frac{V}{4\pi^{2}} \left(\frac{2m}{\hbar^{2}}\right)^{3/2} \int \frac{\varepsilon^{3/2}}{\exp\left(\frac{\varepsilon - \mu}{k_{\mathrm{B}}T}\right) - 1} d\varepsilon$$

$$N(T,V,\mu) = \sum_{k} n_{k} \quad \Rightarrow \quad \frac{V}{4\pi^{2}} \left(\frac{2m}{\hbar^{2}}\right)^{3/2} \int \frac{\varepsilon^{1/2}}{\exp\left(\frac{\varepsilon - \mu}{k_{\rm B}T}\right) - 1} d\varepsilon$$

we assume that the states are not degenerate, otherwise we have to multiply with degeneracy g_k

• we assume
$$g_k = 1$$

crucial point: the integral is bounded!! If the particle number *N* is too large of the temperature too low, the equation can no longer be satisfied

• evaluation of the equation for the particle number

$$N(T, V, \mu) = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2}}{\exp\left(\frac{\varepsilon - \mu}{k_{\rm B}T}\right) - 1} d\varepsilon = \frac{V}{4\pi^2} \left(\frac{2mk_{\rm B}T}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\gamma e^{-x}}{1 - \gamma e^{-x}} x^{1/2} dx$$

with $x = \varepsilon/k_{\rm B}T = \beta\varepsilon$ and fugacity $\gamma = \exp\left(\frac{\mu}{k_{\rm B}T}\right)$

Gamma function: $\Gamma(t) = \int_0^\infty e^{-y} y^{t-1} dy$

to solve the integral we use the series development

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

plugging in this expression we can perform the integration by using

$$\int_{0}^{\infty} e^{-px} x^{1/2} dx = \frac{1}{p^{3/2}} \int_{0}^{\infty} e^{-y} y^{1/2} dy = \frac{1}{p^{3/2}} \frac{\sqrt{\pi}}{\sum_{\Gamma(3/2)}^{\infty}} \Rightarrow \int_{0}^{\infty} \frac{\gamma e^{-x}}{1 - \gamma e^{-x}} x^{1/2} dx = \frac{\sqrt{\pi}}{2} \sum_{\substack{p=1\\p_{3/2}\\p_{3/2}(\gamma)}}^{\infty} \frac{\gamma^{p}}{p^{3/2}}$$
Gamma function: $\Gamma(t) = \int_{0}^{\infty} e^{-y} y^{t-1} dy$

$$N(T, V, \mu) = V \left(\frac{mk_{\rm B}T}{2\pi\hbar^2} \right)^{3/2} g_{3/2}(\gamma) = \frac{V}{\lambda_T^3} g_{3/2}(\gamma)$$

$$n(T,\mu) \lambda_T^3 = g_{3/2}(\gamma)$$

 $\langle k_{\rm B}T \rangle$

• analysis of the function $g_{3/2}(\gamma)$

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

i. $|\gamma| < 1$: the series converges ii. $|\gamma| > 1$: the series diverges

iii. $|\gamma| = 1$: the series converges and has the value $g_{3/2}(1)$



what happens with decreasing T?

 $-\lambda_T$ increases $\propto 1/\sqrt{T} \rightarrow g_{3/2}(\gamma)$ has to increase to keep $n(T,\mu) = \frac{1}{\lambda_T^3} g_{3/2}(\gamma)$ constant

• problem:

 $g_{3/2}(\gamma)$ has maximum value $g_{3/2}(1) = \zeta(3/2) = 2.61$ for $\gamma = 1$, resp. $\mu = 0$,

→ $g_{3/2}(\gamma = 1)$ is related to maximum value $\lambda_T = \lambda_{T,\text{BEC}}$,

resp. to minimum temperature $T_{\rm BEC}$

$$\lambda_{T,\text{BEC}}^3 \cdot n = g_{3/2}(\gamma = 1) = \zeta(3/2) = 2.61237 \dots$$

defines the characteristic temperature T_{BEC} :

for $T < T_{\text{BEC}}$ it is not possible to satisfy the equation $n(T, \mu) = \frac{1}{\lambda_m^3} g_{3/2}(\gamma)$



• with $\lambda_{T,\text{BEC}} = h/\sqrt{2\pi m k_{\text{B}} T_{\text{BEC}}}$, we obtain:

$$n = 2.612 \left(\frac{mk_{\rm B}T_{\rm BEC}}{2\pi\hbar^2}\right)^{3/2} \implies T_{\rm BEC} = \frac{2\pi\hbar^2}{mk_{\rm B}} \left(\frac{n}{2.612}\right)^{2/3}$$

Bose-Einstein condensation temperature

 \succ $\lambda_{T,BEC}^3 \cdot n \simeq O(1)$ → criterion for the importance of quantum effects or degeneracy

- how to solve the problem ?
 - physical solution of the problem that we cannot satisfy the equation $n(T, \mu) = \frac{1}{\lambda_T^3} g_{3/2}(\gamma)$ below T_{BEC}
 - \rightarrow we have to put a significant number N_0 of the particles in the ground state k = 0
 - → this is in agreement with the Bose-Einstein distribution
 - → setting $\varepsilon(k = 0) = \varepsilon_0 = 0$, the number of bosons in the ground state is

$$N_0(T,\mu) = \frac{1}{\exp\left(\frac{0-\mu}{k_{\rm B}T}\right) - 1} \simeq \frac{1}{1 - \frac{\mu}{k_{\rm B}T} - 1} = \frac{k_{\rm B}T}{|\mu|} \to \infty \text{ for } |\mu| = |\varepsilon_0 - \mu| \to 0$$



if $|\varepsilon_0 - \mu| = |0 - \mu| = |\mu| \rightarrow 0$, the occupation number $N_0 = n(k = 0)$ of the ground state $\varepsilon_0 = 0$ strongly increases



• calculation of $N_0(T) = N(\varepsilon_0, T)$ for $(\varepsilon_0 - \mu) = (0 - \mu) = -\mu \rightarrow 0$:

$$N_0(T,\mu) = \frac{1}{\exp\left(\frac{\varepsilon_0 - \mu}{k_{\rm B}T}\right) - 1} \simeq \frac{1}{1 + \frac{\varepsilon_0 - \mu}{k_{\rm B}T} - 1} = \frac{k_{\rm B}T}{\varepsilon_0 - \mu} \to \infty \text{ for } \varepsilon_0 - \mu \to 0$$

→
$$N_0(T,\mu)$$
 grows dramtically for $(\varepsilon_0 - \mu) \rightarrow 0$, that is, for $\mu \rightarrow 0$

Note:

$$\varepsilon_0 - \mu = k_{\rm B}T \ln\left(1 + \frac{1}{N_0}\right) \simeq \frac{k_{\rm B}T}{N_0}$$

 \Rightarrow difference between ground
state and chemical potential is
much smaller than $k_{\rm B}T$



detailed analysis of the chemical potential •

$$n(T,\mu) = \frac{N(T,V,\mu)}{V} = \left(\frac{mk_{\rm B}T}{2\pi\hbar^2}\right)^{3/2} g_{3/2}(\gamma) = \frac{1}{\lambda_T^3} g_{3/2}(\gamma) \implies g_{3/2}(\gamma) = \left(\frac{2\pi\hbar^2}{mk_{\rm B}T}\right)^{3/2} n(T,\mu)$$

- for high temperatures T and/or small particle density n we can use the approximation $g_{3/2}(\gamma) \simeq \gamma + \cdots \simeq e^{\beta \mu} + \cdots$

$$\Rightarrow e^{\beta\mu} = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2} n(T,\mu) \implies \mu \simeq -\frac{3}{2}k_BT \ln\left(\frac{mk_BT}{2\pi\hbar^2 n^{2/3}}\right)$$

$$\varsigma_{3/2} = 2.61237 \dots$$
• for $T \to \infty$:
 $\lambda_T \to 0, \mu \to -\infty, \gamma \to 0, \ln \gamma \to -\infty$ and therefore $g_{3/2}(\gamma) \to 0$
• for decreasing T :
 λ_T increases, μ/k_BT increases $\to 0, \gamma$ increases $\to 1$ and therefore $g_{3/2}(\gamma) \to 2.61$
 $g_{3/2}(\gamma) \to 2.61$

for d

Chapter 1/RG 91

- what happens if we decrease T to values below T_{BEC} ?
 - for $T < T_{\text{BEC}}$, there is no solution of equation $n(T, \mu) = \frac{1}{\lambda_T^3} g_{3/2}(\gamma)$ as $g_{3/2}(\gamma)$ has maximum value $g_{3/2}(1)$ for $\gamma \to 1$
 - → for $T < T_{\text{BEC}}$, the particle number N_0 in the ground quantum state ($\varepsilon_0 = 0$) must become large (first recognized by Einstein)

occupation of the ground state
$$\varepsilon_0 = 0$$
: $N_0 = \frac{1}{\exp(-\mu/k_B T) - 1} \Rightarrow \mu = -k_B T \ln\left(1 + \frac{1}{N_0}\right) \simeq -k_B T \frac{1}{N_0}$

- from the total particle number N a macroscopically large number N_0 has to be placed in ground state ε_0
- macroscopically large means that N_0 is proportional to system volume V
- if the fraction of particles in the ground state becomes finite at $T = T_{BEC}$, then in the thermodynamic limit $V \rightarrow \infty$ the particle number $N_0 \rightarrow \infty$ and hence the chemical potential $\mu \rightarrow 0$

→ $\mu = 0$ for $T \le T_{\text{BEC}}$

as μ corresponds to the average energy required to add a particle to the systems, the result is evident: we are adding particles only to the ground state $\varepsilon_0 = 0$



• for $T \leq T_{BEC}$: how are the *N* particles distributed among the available states ?

$$- N = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\sqrt{\varepsilon}}{\exp\left(\frac{\varepsilon-\mu}{k_BT}\right) - 1} d\varepsilon \text{ yields } \mu \to 0 \text{ for } T \to T_{\text{BEC}}$$
$$- \text{ for } \mu \to 0 \text{ } (T \to T_{\text{BEC}}) \text{, we obtain } N_0 = \frac{1}{\exp\left(\frac{\varepsilon_0 - \mu}{k_BT}\right) - 1} \simeq \frac{k_BT}{|\mu|} \to \infty$$
$$\varepsilon_0 = \frac{\hbar^2}{2m} \left(\frac{\pi}{L}\right)^2 \propto \frac{1}{V^{2/3}} \propto \frac{1}{N^{2/3}} \to 0 \quad \text{for } N \to \infty \text{ (thermodynamic limit)}$$

below $T_{\rm BEC}$: macroscopic occupation $N_0 \gg 1$ of the ground state is required

- key result:
 - at $T \leq T_{BEC}$ a finite fraction of all particles occupies the ground state
 - this phenomenon is called *Bose-Einstein condensation*
 - the name *"condensation"* is used since in analogy to the gaseous-liqud transition the condensed particles do no longer contribute to the pressure (see discussion below)

• for $T \leq T_{BEC}$: occupation of the first excited state

for $\mu \rightarrow 0$ and $T \sim 1$ K: level spacing for 10^{22} atoms in a box with L = 1 cm: $\Delta \varepsilon / k_B T = \varepsilon_1 / k_B T \le 10^{-14}$

$$\implies n_1(T) = \frac{1}{1 + \exp\left(\frac{\epsilon_1 - \mu}{k_{\rm B}T}\right) - 1} \simeq \frac{1}{1 + \frac{\varepsilon_1 - \mu}{k_{\rm B}T} - 1} \simeq \frac{k_{\rm B}T}{\varepsilon_1 - \mu} \approx 10^{14}$$

 n_1 and all $n_{k>1}$ are small compared to N_0 and the total particle number $N = 10^{22}$

(justifies why only the ground state was singled out in the calculation of T_{BEC})

- more detailed calculation: $n_1/N_0 \propto N^{-1/3}$, i.e. $n_1/N_0 \rightarrow 0$ for $N \rightarrow \infty$

$$\frac{n_1}{N_0} = \frac{k_{\rm B}T}{\varepsilon_1 - \mu} \cdot \frac{\varepsilon_0 - \mu}{k_{\rm B}T} = -\frac{\mu}{\varepsilon_1 - \mu} \simeq -\frac{\mu}{\varepsilon_1} \simeq \frac{k_{\rm B}T}{N_0\varepsilon_1} \qquad \text{we use} \quad N_0(T,\mu) \simeq \frac{k_{\rm B}T}{\varepsilon_0 - \mu} = \frac{k_{\rm B}T}{-\mu}$$

for $T < T_{\rm BEC}/2$ we can use the crude approximations $N_0 \simeq N$, $T \simeq T_{\rm BEC} \propto N^{2/3}$:

$$\frac{n_1}{N_0} \propto \frac{1}{N^{1/3}} \propto \frac{1}{V^{1/3}} \quad \Rightarrow \text{ already at } T \simeq T_{\text{BEC}}/2 \text{, we have } N_0 \gg n_1, n_{k>1}$$

- for $T \to 0$: $\varepsilon_{k>0}/k_{\rm B}T \to \infty$ and hence $n_{k>0} \to 0$, $\mu/k_{\rm B}T = 1/N_0 \simeq 0$: all bosons occupy ground state

• for $T < T_{\rm BEC}$ we have to treat the ground state ε_0 separately

$$N = \sum_{\mathbf{k}} \frac{1}{\exp\left(\frac{\varepsilon_{\mathbf{k}} - \mu}{k_{B}T}\right) - 1} = N_{0} + N_{ex} = N_{0} + \sum_{\mathbf{k} \neq 0} \left[\exp\left(\frac{\varepsilon_{\mathbf{k}}}{k_{B}T}\right) - 1\right]^{-1} = N_{0} + \int_{0}^{\infty} D(\varepsilon)n(\varepsilon) d\varepsilon$$

$$particles in$$
ground state
particles in
excited states

• we obtain for **free bosons**:

$$N_{ex} = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\varepsilon^{1/2}}{\exp\left(\frac{\varepsilon - \mu}{k_B T}\right) - 1} d\varepsilon = \frac{V}{4\pi^2} \left(\frac{2mk_B T}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\gamma e^{-x}}{1 - \gamma e^{-x}} x^{1/2} dx \qquad \text{with } x = \beta \varepsilon \text{ and} \\ fugacity \ \gamma = \exp\left(\frac{\mu}{k_B T}\right) = 1$$

$$\implies n = n_0 + n_{ex} = n_0 + 2.612 \left(\frac{mk_B T}{2\pi\hbar^2}\right)^{3/2} \implies \frac{n_0}{n} = 1 - \left(\frac{T}{T_{BEC}}\right)^{3/2} \qquad n_0: \text{ condensate density} \\ n_{ex}: \text{ normal fluid density}$$

$$T_{BEC} = \frac{2\pi\hbar^2}{mk_B} \left(\frac{n}{2.612}\right)^{2/3} \Rightarrow n = 2.612 \left(\frac{2\pi\hbar^2}{mk_B T_{BEC}}\right)^{3/2}$$

• Summary: temperature dependence of N₀ and N_{ex}

we assume constant particle number: $N = N_0(T) + N_{ex}(T) = \text{const.}$

-
$$T > T_{\text{BEC}}$$
: $N_0 = O(1)$ \rightarrow can be neglected

 \rightarrow

$$N = N_{ex} = \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\sqrt{\varepsilon}}{\exp\left(\frac{\varepsilon - \mu}{k_{\rm B}T}\right) - 1} d\varepsilon \qquad \text{is valid}$$

$$- T = T_{\text{BEC}}: \quad \mu \to 0, \quad \lambda_{T,\text{BEC}}^3 \cdot n = 2.612 \quad \Rightarrow \quad N = N_{ex} = 2.612 \cdot \frac{V}{\lambda_{T,\text{BEC}}^3}$$

$$- T \leq T_{BEC}: \quad \mu = 0, \qquad N = N_0 + N_{ex} = N_0 + 2.612 \cdot \frac{V}{\lambda_T^3} = N_0 + 2.612 \cdot \frac{V}{\lambda_T^3} \cdot \frac{\lambda_{T,BEC}^3}{\lambda_{T,BEC}^3}$$
$$N = N_0 + 2.612 \cdot \frac{V}{\lambda_{T,BEC}^3} \cdot \left(\frac{T}{T_{BEC}}\right)^{3/2} = N_0 + N \cdot \left(\frac{T}{T_{BEC}}\right)^{3/2}$$

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_{\text{BEC}}}\right)^{3/2} \qquad \frac{N_{ex}}{N} = \left(\frac{T}{T_{\text{BEC}}}\right)^{3/2}$$

• normal fluid density ($T < T_{BEC}$)

 $\frac{N_{ex}}{N} = \left(\frac{T}{T_{\rm BEC}}\right)^{3/2}$

• superfluid or condensate density

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_{\text{BEC}}}\right)^{3/2}$$

$$T_{\text{BEC}} = \frac{2\pi\hbar^2}{mk_B} \left(\frac{n}{2.612}\right)^{2/3}$$
$$\lambda_T^3 = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{3/2}$$



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Total number N (inset) and ground-state fraction N_0/N as a function of T/T_{BEC} .

The solid (dotted) line shows the infinite (finite) *N* theory curves. At the transition, the cloud consists of 40 000 ⁸⁷Rb atoms at 280 nK.

Bose-Einstein Condensation in a Dilute Gas: Measurement of Energy and Ground-State Occupation J. R. Ensher, D. S. Jin, M. R. Matthews, C. E. Wieman, and E. A. Cornell Phys. Rev. Lett. 77, 4984 (1996)





- Bose-Einstein condensation can be viewed as condensation of gas in momentum space
 - → all atoms have the same momentum
- Bose-Einstein condensation corresponds to order-disorder phase transition (first order phase transition)



decrease *T* at $\mu = const$. decrease μ at T = const. 16 24 $\boldsymbol{\varepsilon}_{\mathbf{0}} = \mathbf{0}$ $\boldsymbol{\varepsilon}_{\mathbf{0}}=\mathbf{0}$ $\mu = -0.1 \Delta \varepsilon$ $\Delta \varepsilon/k_{\rm B}T = 0.2$ 12 18 $\Delta \varepsilon / k_{\rm B} T = 0.1$ $D(\varepsilon) n(\varepsilon)$ $\mu = -0.01\Delta\varepsilon$ D(ɛ) n(ɛ) 8 12 $\Delta \varepsilon / k_{\rm B} T = 0.2$ $= -0.1\Delta\varepsilon$ 4 6 $-\Delta\varepsilon$ $\Delta \varepsilon / k_{\rm B} T = 1$ $\boldsymbol{u} =$ 0 5 3 0 4 6 1 2 3 0 4 $\varepsilon / \Delta \varepsilon$ $\varepsilon / \Delta \varepsilon$

we defined the Bose-Einstein temperature T_{BEC} as the temperature, where $N_{ex}/N = 1$:

 $T > T_{BEC}$ $0 < T < T_{BEC}$ T = 03 3 3 OC 000 $\mathbf{0}$ ОС 000000 $\mathbf{O} \mathbf{O} \mathbf{O}$ ---- $\mathbf{O}\mathbf{C}$ 00000000000



condensate

• thermodynamic properties of ideal Bose gas: inner energy U

$$U = \sum_{k} \varepsilon_{k} n_{k} \quad \Rightarrow \quad U = \int D(\varepsilon)\varepsilon \, d\varepsilon = \frac{V}{4\pi^{2}} \left(\frac{2m}{\hbar^{2}}\right)^{3/2} \int \frac{\varepsilon^{3/2}}{\exp\left(\frac{\varepsilon - \mu}{k_{\rm B}T}\right) - 1} d\varepsilon$$

$$U = \frac{V}{4\pi^2} k_{\rm B} T \left(\frac{2mk_{\rm B}T}{\hbar^2}\right)^{3/2} \int_0^\infty \frac{\gamma {\rm e}^{-x}}{1 - \gamma {\rm e}^{-x}} x^{3/2} dx \qquad \text{with } x = \varepsilon/k_{\rm B}T = \beta\varepsilon \text{ and } fugacity \ \gamma = \exp\left(\frac{\mu}{k_{\rm B}T}\right)$$

we use again
$$\frac{\gamma e^{-x}}{1 - \gamma e^{-x}} = \gamma e^{-x} (1 + \gamma e^{-x} + \gamma^2 e^{-2x} + \cdots) = \sum_{p=1}^{\infty} \gamma^p e^{-px}$$
 and $\int_0^\infty e^{-px} x^{3/2} dx = \frac{1}{p^{5/2}} \underbrace{\int_0^\infty e^{-y} y^{3/2} dy}_{\Gamma(t) = \int_0^\infty e^{-y} y^{t-1} dy} = \frac{1}{p^{5/2}} \underbrace{\frac{3\sqrt{\pi}}{4}}_{\Gamma(5/2)} \underbrace{\int_0^\infty e^{-y} y^{t-1} dy}_{\Gamma(t) = \int_0^\infty e^{-y} y^{t-1} dy} = \frac{1}{p^{5/2}} \underbrace{\int_0^\infty e^{-y} y^{t-1} dy}_{\Gamma(t) = \int_0^\infty e^{-y} y^{t-1} dy} = \frac{1}{p^{5/2}} \underbrace{\int_0^\infty e^{-y} y^{t-1} dy}_{\Gamma(t) = \int_0^\infty e^{-y} y^{t-1} dy} = \frac{1}{p^{5/2}} \underbrace{\int_0^\infty e^{-y} y^{t-1} dy}_{\Gamma(t) = \int_0^\infty e^{-y} y^{t-1} dy} = \frac{1}{p^{5/2}} \underbrace{\int_0^\infty e^{-y} y^{t-1} dy}_{\Gamma(t) = \int_0^\infty e^{-y} y^{t-1} dy}$

$$\Rightarrow \int_{0}^{\infty} \frac{\gamma e^{-x}}{1 - \gamma e^{-x}} x^{3/2} dx = \frac{3\sqrt{\pi}}{\frac{4}{\Gamma(5/2)}} \sum_{\substack{p=1\\g_{5/2}(\gamma)}}^{\infty} \frac{\gamma^{p}}{p^{5/2}} = \Gamma(5/2) g_{5/2}(\gamma) \qquad \implies U = V \frac{3}{2} k_{\rm B} T \left(\frac{mk_{\rm B}T}{2\pi\hbar^{2}}\right)^{3/2} g_{5/2}(\gamma)$$

with $V = N\lambda_T^3 / g_{3/2}(\gamma)$, resp. $V = N\lambda_{T,BEC}^3 / g_{3/2}(1)$ we obtain

$$U = \frac{3}{2} N k_{\rm B} T \frac{g_{5/2}(\gamma)}{g_{3/2}(\gamma)} \qquad \qquad U = \frac{3}{2} N k_{\rm B} T \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{g_{5/2}(\gamma)}{g_{3/2}(1)}$$

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free bosons:

 $\varepsilon_{k} = \frac{\hbar^{2}k^{2}}{2m}$ $D(\varepsilon) = \frac{V}{4\pi^{2}} \left(\frac{2m}{\hbar^{2}}\right)^{3/2} \sqrt{\varepsilon}$

Ideal Bose Gas I.2.2

> thermodynamic properties of ideal Bose gas: inner energy Ulacksquare

> > $T \gg T_{BEC}$: it is sufficient to use only the first term in the series evolution of g:

 $g_{5/2}(\gamma) = \sum_{p=1}^{\infty} \frac{\gamma^p}{p^{5/2}} \simeq \gamma; \quad g_{3/2}(\gamma) = \sum_{p=1}^{\infty} \frac{\gamma^p}{p^{3/2}} \simeq \gamma \text{ since } \gamma \to 1$

i.
$$T > T_{BEC}$$
: $U(T) = \frac{3}{2}Nk_{B}T\frac{g_{5/2}(\gamma)}{g_{3/2}(\gamma)}$

α	$\Gamma(\alpha)$	$\zeta_{\alpha}(\gamma=1)$
1	1	∞
1.5	$\sqrt{\pi}/2 = 0.886$	2.612
2	_ 1	$\pi^2/6 = 1.645$
2.5	$3\sqrt{\pi}/4 = 1.329$	1.341
3	2 0 000	1.202
3.5	$15\sqrt{\pi/8} = 3.323$	1.127
4	6	$\pi^{*}/90 = 1.082$

 $\Gamma = Gamma function$ ζ = Riemann Zeta function

 $U(T) = \frac{3}{2}Nk_{\rm B}T$

result for gas of classical non-interacting particles (quantum statistics does not play any role at high T)

iii.
$$T < T_{\text{BEC}}$$
: $U(T) = \frac{3}{2}Nk_{\text{B}}T\frac{g_{5/2}(1)}{g_{3/2}(1)}$ $g_{5/2}(1) = \zeta\left(\frac{5}{2}\right) = 1.341, \quad g_{3/2}(1) = \zeta\left(\frac{3}{2}\right) = 2.612$

$$U(T) = \frac{3}{2} N_{ex} k_{\rm B} T \frac{g_{5/2}(1)}{g_{3/2}(1)} = \frac{3}{2} N \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} k_{\rm B} T \frac{g_{5/2}(1)}{g_{3/2}(1)} = 0.770 \ N \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} k_{\rm B} T$$

we use $\frac{N_0}{N} = 1 - \left(\frac{T}{T_{\rm BEC}}\right)^{\frac{3}{2}} \Rightarrow N_{ex} = N - N_0 = N \left(\frac{T}{T_{\rm BEC}}\right)^{3/2}$ particles in ground state $\varepsilon_0 = 0$ do not contributed

ibute!

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ii.





• thermodynamic properties of ideal Bose gas: specific heat: $C_V(T) = \left(\frac{\partial U}{\partial T}\right)_{V,N}$

I.2.2 Ideal Bose Gas

i. $T > T_{BEC}$: $\mu < 0, \gamma < 1, g_{5/2}(\gamma)$ and $g_{3/2}(\gamma)$ are functions of T and n = N/V

with $V = N\lambda_T^3 / g_{3/2}(\gamma)$, resp. $V = N\lambda_{T,BEC}^3 / g_{3/2}(1)$ we obtain

$$U(T) = \frac{3}{2} N k_{\rm B} T \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{g_{5/2}(\gamma)}{g_{3/2}(1)} = \frac{3}{2} N k_{\rm B} T \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{g_{5/2}(\gamma)}{\zeta(3/2)}$$

$$g_{3/2}(1) = \zeta(3/2)$$

$$C_V(T) = \left(\frac{\partial U}{\partial T}\right)_{V,N} = \frac{15}{4} N k_{\rm B} \frac{g_{5/2}(\gamma)}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} + \frac{3}{2} N k_{\rm B} \frac{T}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{\partial g_{5/2}(\gamma)}{\partial \gamma} \left(\frac{\partial \gamma}{\partial T}\right)_{N}$$
to derive $\left(\frac{\partial \gamma}{\partial T}\right)_N$ we use $\lambda_T^3 \cdot \frac{N}{V} = \lambda_T^3 \cdot n = g_{3/2}(\gamma) \Rightarrow 1 = \frac{g_{3/2}(\gamma)}{\lambda_T^3 \cdot n} = \frac{g_{3/2}(\gamma)}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2}$
temperature derivative yields: $0 = \frac{3}{2T} \frac{g_{3/2}(\gamma)}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} + \frac{1}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{\partial g_{3/2}(\gamma)}{\partial \gamma} \left(\frac{\partial \gamma}{\partial T}\right)_N = \frac{3}{2T} g_{3/2}(\gamma) + \gamma^{-1} g_{1/2}(\gamma) \left(\frac{\partial \gamma}{\partial T}\right)_N$

 $U(T) = \frac{3}{2} N k_{\rm B} T \frac{g_{5/2}(\gamma)}{g_{5/2}(\gamma)}$

 $\Rightarrow \left(\frac{\partial \gamma}{\partial T}\right)_{N} = -\frac{3\gamma}{2T} \frac{g_{3/2}(\gamma)}{g_{1/2}(\gamma)}$

- $\left(\frac{\partial U}{\partial T}\right)_{V,N}$ thermodynamic properties of ideal Bose gas: specific heat: $C_V(T) =$
- $T > T_{BEC}$: i.

4

 $\langle T_{\rm BEC} \rangle$

$$C_{V}(T) = \left(\frac{\partial U}{\partial T}\right)_{V,N} = \frac{15}{4} N k_{\rm B} \frac{g_{5/2}(\gamma)}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} + \frac{3}{2} N k_{\rm B} \frac{T}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{\partial g_{5/2}(\gamma)}{\frac{\partial \gamma}{\sqrt{-1}}} \left(\frac{\partial \gamma}{\partial T}\right)_{N}$$

$$C_{V}(T) = \frac{15}{10} N k_{\rm B} \frac{g_{5/2}(\gamma)}{\tau(2/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} + \frac{3}{2} N k_{\rm B} \frac{T}{\tau(2/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{g_{3/2}(\gamma)}{(T_{\rm BEC})} \left(-\frac{3\gamma}{2\pi} \frac{g_{3/2}(\gamma)}{(T_{\rm BEC})}\right)$$

 $g_{1/2}(\gamma)$

$$\left(\frac{\partial\gamma}{\partial T}\right)_{N} = -\frac{3\gamma}{2T}\frac{g_{3/2}(\gamma)}{g_{1/2}(\gamma)}$$

$$S_{V}(T) = \frac{15}{4} N k_{\rm B} \frac{g_{5/2}(\gamma)}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} + \frac{3}{2} N k_{\rm B} \frac{T}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{g_{3/2}(\gamma)}{\gamma} \left(-\frac{3\gamma}{2T} \frac{g_{3/2}(\gamma)}{g_{1/2}(\gamma)}\right)^{3/2}$$

4

$$C_{V}(T) = Nk_{\rm B} \frac{g_{5/2}(\gamma)}{\zeta(3/2)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \left[\frac{15}{4} - \frac{9}{4} \frac{g_{3/2}(\gamma)}{g_{5/2}(\gamma)} \frac{g_{3/2}(\gamma)}{g_{1/2}(\gamma)}\right]$$
$$C_{V}(T) = Nk_{\rm B} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \left[\frac{15}{4} \frac{g_{5/2}(\gamma)}{\zeta(3/2)} - \frac{9}{4} \frac{g_{3/2}(\gamma)}{\zeta(3/2)} \frac{g_{3/2}(\gamma)}{g_{1/2}(\gamma)}\right]$$
$$C_{V}(T) = \frac{15}{4} Nk_{\rm B} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} \frac{g_{5/2}(\gamma)}{\zeta(3/2)} - \frac{9}{4} Nk_{\rm B} \frac{g_{3/2}(\gamma)}{g_{1/2}(\gamma)}\right]$$

we use
$$\lambda_T^3 \cdot \frac{N}{V} = \lambda_T^3 \cdot n = g_{3/2}(\gamma) \implies 1 = \frac{g_{3/2}(\gamma)}{\lambda_T^3 \cdot n} = \frac{g_{3/2}(\gamma)}{\zeta(3/2)} \left(\frac{T}{T_{\text{BEC}}}\right)^{3/2}$$

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- thermodynamic properties of ideal Bose gas: specific heat: $C_V(T) = \left(\frac{\partial U}{\partial T}\right)_{V.N}$
 - ii. $T \gg T_{\text{BEC}}$:

$$C_V(T) = \frac{3}{2}Nk_{\rm B}, \qquad C_V^{\rm mol}(T) = \frac{3}{2}N_Ak_{\rm B} = \frac{3}{2}R$$

result for classical gas of non-interacting particles

$$U(T) = \frac{3}{2}Nk_{\rm B}T$$

(quantum statistics does not play any role at high T)

iii. $T < T_{BEC}$:

$$C_V(T) = \frac{15}{4} N k_{\rm B} \frac{\zeta_{5/2}(1)}{\zeta_{3/2}(1)} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2} = 1.925 \cdot N k_{\rm B} \left(\frac{T}{T_{\rm BEC}}\right)^{3/2}$$

$$U(T) = \frac{3}{2} N \left(\frac{T}{T_{\text{BEC}}}\right)^{3/2} k_{\text{B}} T \frac{g_{5/2}(1)}{g_{3/2}(1)}$$
$$g_{5/2}(1) = \zeta(5/2) \qquad g_{3/2}(1) = \zeta(3/2)$$

interpretation: all
$$N_{\text{ex}} = N \left(\frac{T}{T_{\text{BEC}}}\right)^{3/2}$$
 non-condensed particles contribute $O(k_{\text{B}})$ to the specific heat

• thermodynamic properties of ideal Bose gas: specific heat: $C_V(T) = \left(\frac{\partial O}{\partial T}\right)$



$$C_V(T) = \frac{3}{2}Nk_{\rm B}$$

- classical result
- $C_V(T)$ decreases towards lower T since more and more particles condense into the ground state ε_0
- temperature T_{BEC} represents phase transition temperatue
- $C_V(T)$ shows cusp at T_{BEC} , indicating the free energy is not analytical at T_{BEC}
- phase transition is ussually interpreted as 1st order phase transition

- thermodynamic properties of ideal Bose gas: pressure
 - we discuss only the case $T < T_{BEC}$:

$$\boldsymbol{p} = -\left(\frac{\partial F}{\partial V}\right)_{N,T} = \frac{2}{3} \left(\frac{\partial U}{\partial V}\right)_{N,T}$$

F = U - TS $dF = TdS - pdV + \mu dN - TdS - SdT$ $dF = -pdV + \mu dN - SdT$ $\left(\frac{\partial F}{\partial V}\right)_{N,T} = -p, \left(\frac{\partial F}{\partial N}\right)_{V,T} = \mu, \left(\frac{\partial F}{\partial T}\right)_{N,V} = -S$

$$U(T) = \frac{3}{2} N k_{\rm B} T \frac{g_{5/2}(1)}{g_{3/2}(1)}$$
$$F(T) = -\frac{2}{3} U(T)$$

with
$$V = N\lambda_{T,\text{BEC}}^3/g_{3/2}(1)$$
 we obtain

$$U = \frac{3}{2} N k_{\rm B} T \frac{g_{5/2}(1)}{g_{3/2}(1)} = \frac{3}{2} \frac{V}{\lambda_{T,\rm BEC}^3} g_{3/2}(1) k_{\rm B} T \frac{g_{5/2}(1)}{g_{3/2}(1)} = \frac{3}{2} \frac{V}{\lambda_{T,\rm BEC}^3} k_{\rm B} T g_{5/2}(1)$$

$$p = \frac{2}{3} \left(\frac{\partial U}{\partial V} \right)_{N,T} = \frac{k_{\rm B}T}{\lambda_T^3} g_{5/2}(1)$$

pressure of the gas does not depend on V in the BEC regime
→ compressibility of the BEC phase is infinite

 $\left(\frac{\partial F}{\partial V}\right)_{\rm N}$

p =

this pathological behavior is removed by the inclusion of finite interactions

- experimental realization with ultra-cold atomic gases
 - first realization in 1995 with trapped alcali metal atoms, e.g. ⁸⁷Rb (Eric A. Cornell, Carl E. Wieman, Wolfgang Ketterle)
 - − typical densities: $n \simeq 10^{11} 10^{15} \text{ cm}^{-3} \Rightarrow T_{\text{BEC}} \simeq 10 \text{ nK} 1 \mu\text{K}$ due to large atomics mass (compared to ⁴He)
 - ⁸⁷Rb: electron configuration: (Kr)5s¹ ⇒ $J = \frac{1}{2}$, nuclear spin $I = \frac{3}{2}$ ⇒ total spin is even → boson similar behavior: ⁷Li, ²³Na
 - important: alcali metal atoms interact (short length repulsion, attractive Van der Waals interaction)
 - atoms do not cluster since most interactions are elastic two-particle interactions:
 particles cannot bind since they cannot get rid of their kinetic energy

(

- rate for three-particle interactions is very small
- → description of pairwise interactions: $V(\mathbf{r}_1 \mathbf{r}_2) \simeq g \, \delta(\mathbf{r}_1 \mathbf{r}_2)$

g =strenght of the scatterer

$$a_s = \frac{\hbar^2}{mg} = s$$
-wave scattering length

(interactions and effect of trapping potential will be discussed later)



Anderson, M. H.; Ensher, J. R.; Matthews, M. R.; Wieman, C. E.; Cornell, E. A. *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor* Science **269**, 198-201 (1995).

velocity distribution for a gas of rubidium atoms, $n=2.5 \times 10^{12} {\rm ~cm^{-3}}$

The measured distribution confirmed the existence of a Bose-Einstein condensate.

Left: $T > T_{BEC} \simeq 170 \text{ nK}$ Center: $T < T_{BEC}$ Right: nearly pure condensate

experimental technique:

- switch-off the trap potential and let the condensate freely expand
- image the position of the atoms after a specific time by absorption of laser light by atom cloud
- measured spatial distribution is proportional to velocity distribution in condensate
I.2.2 Ideal Bose Gas



velocity distribution for a gas of sodium atoms, $n \sim 10^{14} \ {\rm cm^{-3}}$

the measured distribution confirmed the existence of a Bose-Einstein condensate.

K. B. Davis, M. -O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle **Bose-Einstein Condensation in a Gas of Sodium Atoms** Phys. Rev. Lett. **75**, 3969 (1995)

I.2.2 Ideal Bose Gas

• what determines the width of the central peak associated with the condensate



Anderson, M. H.; Ensher, J. R.; Matthews, M. R.; Wieman, C. E.; Cornell, E. A. *Observation of Bose-Einstein Condensation in a Dilute Atomic Vapor* Science **269**, 198-201 (1995).

expected:

 delta function distribution since condensate atoms occupy the same state

observed:

- finite width Δx of the condensate due to trapping of condensate in trapping potential of finite width Δx
- resulting finite momentum distribution: $\Delta p \simeq \hbar / \Delta x \implies \Delta v \simeq \hbar / m \Delta x$
- width of the normal component:

$$\frac{1}{2}m \langle v_x^2 \rangle = \frac{1}{2}k_{\rm B}T \implies \Delta v \simeq \sqrt{k_{\rm B}T/m}$$





Space Station Experiment (2018)

Changing density of a cloud of rubidium atoms as it is cooled to lower and lower temperatures (going from left to right) approaching absolute zero. The emergence of a sharp peak in the later graphs confirms the formation of a Bose-Einstein condensate occurring here at about $T_{\text{BEC}} = 130 \text{ nK}$

I.2.2 Ideal Bose Gas

- concluding remarks
 - Bose-Einstein condensates have been realized with many different atoms
 - ideal model system, as most parameters can we well controlled and changed
 - it became evident the finite interactions between the particles has an important impact
 - > ideal **non-interacting Bose gas is not a superfluid** that can show frictionless flow
 - ➔ no persistent current of the condensate
 - ➔ no vortices
 - > we will see later that this is due to fact that the Landau critical velocity of the superfluid is zero





BAYERISCHE AKADEMIE DER WISSENSCHAFTEN Technische Universität München

Superconductivity and Low Temperature Physics II



Lecture No. 4 19 May 2022

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- treatment of the finite interaction between particles
 - → description by pairwise interaction: $V(\mathbf{r}_1 \mathbf{r}_2) \simeq g \, \delta(\mathbf{r}_1 \mathbf{r}_2)$
- g = strenght of the scatterer $a_s = \frac{\hbar^2}{mg} = \text{s-wave scattering length}$
- modeling of pairwise interactions by average "mean field" potential seen by every particle due to interaction with all others

 $V_{\rm eff}(\mathbf{r}) \simeq g n(\mathbf{r})$

- \succ in addition, particles see finite trapping potential $V_{trap}(\mathbf{r})$ of e.g. a magnetic trap
- Schrödinger equation for particles in trap:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V_{\text{trap}}(\mathbf{r}) + V_{\text{eff}}(\mathbf{r})\right)\psi_k(\mathbf{r}) = \varepsilon_k\psi_k(\mathbf{r})$$

important:

Schrödinger equation is nonlinear since $V_{eff}(\mathbf{r})$ depends on $n(\mathbf{r})$ and hence on wave function $\psi_k(\mathbf{r})$ itself

→ self-consistent solution: Gross-Pitaevskii equations

particle density and number:

$$n(\mathbf{r}) = \sum_{k} \left[\exp\left(\frac{(\varepsilon_k - \mu)}{k_B T}\right) - 1 \right]^{-1} |\psi_k(\mathbf{r})|^2$$
$$N = \int n(\mathbf{r}) d^3 r = \sum_{k} \left[\exp\left(\frac{(\varepsilon_k - \mu)}{k_B T}\right) - 1 \right]^{-1}$$

• Now: more detailed discussion of finite interactions between particles

assumptions: (i) *weak interactions* (allows pertubative treatment (ii) *repulsive interactions* (attractive interactions may lead to instability)

we will shows: repulsive interactions stabilize the Bose-Einstein condensate (counter-intuitive, as a repulsive interaction is expected to push particles out of a single-particle ground state)

• Gedanken experiment:

we consider two bosons and show that in the presence of a repulsive interaction it is more favorable to put them into the same eigenstate

- bosons = particles in a box described by normalized wave functions $\phi(\mathbf{r}) = \exp(\iota \mathbf{k} \cdot \mathbf{r}), \ \tilde{\phi}(\mathbf{r}) = \exp(\iota \mathbf{k} \cdot \mathbf{r}),$
 - **>** two bosons in the same eigenstate:

 $\psi(\mathbf{r}_1, \mathbf{r}_2) = \phi(\mathbf{r}_1)\phi(\mathbf{r}_2) = \exp(\iota \mathbf{k} \cdot (\mathbf{r}_1 + \mathbf{r}_2))$

symmetric wave function:
$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \psi(\mathbf{r}_2, \mathbf{r}_1)$$

$$\int |\psi(\mathbf{r}_1, \mathbf{r}_2)|^2 d^3 r_1 d^3 r_2 = 1$$

two bosons in different eigenstates:

 $\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \left[\phi(\mathbf{r}_1) \tilde{\phi}(\mathbf{r}_2) + \phi(\mathbf{r}_2) \tilde{\phi}(\mathbf{r}_1) \right]$

symmetric superposion of the two posibilities $\phi(\mathbf{r}_1)\tilde{\phi}(\mathbf{r}_2)$ and $\phi(\mathbf{r}_2)\tilde{\phi}(\mathbf{r}_2)$ $\int |\psi(\mathbf{r}_1,\mathbf{r}_2)|^2 d^3r_1 d^3r_2 = 1$

what happens if we add repulsive potential $V(\mathbf{r}_1 - \mathbf{r}_2)$ between the two bosons?

> energy change for the two bosons in the same eigenstate: $\psi(\mathbf{r}_1, \mathbf{r}_2) = \phi(\mathbf{r}_1)\phi(\mathbf{r}_2) = \exp(\iota \mathbf{k} \cdot (\mathbf{r}_1 + \mathbf{r}_2))$

$$\frac{\delta E}{\delta E} = \int d^3 r_1 d^3 r_2 |\psi(\mathbf{r}_1, \mathbf{r}_2)|^2 V(\mathbf{r}_1 - \mathbf{r}_2) = \int d^3 r_1 d^3 r_2 V(\mathbf{r}_1 - \mathbf{r}_2) = \int d^3 r V(\mathbf{r}) = \frac{E_0}{\delta r_1} > 0$$

we use $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and $d^3 r_1 d^3 r_2 = d^3 R d^3 r_1$

note that $\delta E = \int d^3 r V(\mathbf{r}) = E_0 > 0$ for a purely repulsive potential

> energy change for the two bosons in the same eigenstate: $\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}} \left[\phi(\mathbf{r}_1) \tilde{\phi}(\mathbf{r}_2) + \phi(\mathbf{r}_2) \tilde{\phi}(\mathbf{r}_1) \right]$

$$\delta E = \int d^3 r_1 d^3 r_2 \, |\psi(\mathbf{r}_1, \mathbf{r}_2)|^2 V(\mathbf{r}_1 - \mathbf{r}_2)$$

- $=\frac{1}{2}\int d^{3}r_{1}d^{3}r_{2}\left[|\phi(\mathbf{r}_{1})|^{2}|\tilde{\phi}(\mathbf{r}_{2})|^{2}+|\phi(\mathbf{r}_{2})|^{2}|\tilde{\phi}(\mathbf{r}_{1})|^{2}+\phi(\mathbf{r}_{1})\tilde{\phi}(\mathbf{r}_{2})\phi^{*}(\mathbf{r}_{2})\tilde{\phi}^{*}(\mathbf{r}_{1})+c.c.\right]V(\mathbf{r}_{1}-\mathbf{r}_{2})$
- since $\int d^3r_1 |\phi(\mathbf{r}_1)|^2 = 1$ and $\int d^3r_2 |\phi(\mathbf{r}_2)|^2 = 1$, the first two terms in [] yields the contribution $\int d^3r V(\mathbf{r})$
- the last term in [] comes from the fact that the wave function must be symmetric with respect to the exchange of particles since they are indistinguishable → results in additional exchange energy
- since $\phi(\mathbf{r}_1)\tilde{\phi}(\mathbf{r}_2)\phi^*(\mathbf{r}_2)\tilde{\phi}^*(\mathbf{r}_1) = \exp[\iota(\mathbf{k} \tilde{\mathbf{k}}) \cdot (\mathbf{r}_1 \mathbf{r}_2)]$ last term in [] results in an energy change $V_{\mathbf{k} \tilde{\mathbf{k}}}/2$ with

 $V_{\mathbf{k}-\tilde{\mathbf{k}}} = \int d^3 r \ e^{i(\mathbf{k}-\tilde{\mathbf{k}})\cdot\mathbf{r}} V(\mathbf{r})$ Fourier transform of $V(\mathbf{r})$ (we assume $V(\mathbf{r}) = V(-\mathbf{r})$ so

 $\Rightarrow \delta E = E_0 + V_{\mathbf{k} - \tilde{\mathbf{k}}}$

Fourier transform of $V(\mathbf{r})$ (we assume $V(\mathbf{r}) = V(-\mathbf{r})$ so that the FT is real: $V_{\mathbf{k}}^* = V_{\mathbf{k}} \rightarrow$ the complex conjugate yields the same contribution $V_{\mathbf{k}-\tilde{\mathbf{k}}}/2$)

 $\rightarrow \delta E = 2E_0$ (if we assume two bosons with the same wave number)

due to the bosonic nature of the particles it is energetically favorable to put them into the same quantum state in the presence of a repulsive interaction potential

• description of finite interactions between particles within second quantization formalism

$$\mathcal{H}_{\text{int}} = \frac{V_0}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}}^N \hat{b}_{\mathbf{k}_2 + \mathbf{q}/2}^{\dagger} \hat{b}_{-\mathbf{k}_1 + \mathbf{q}/2}^{\dagger} \hat{b}_{-\mathbf{k}_2 + \mathbf{q}/2} \hat{b}_{\mathbf{k}_1 + \mathbf{q}/2}$$



describes scattering process:

particle $|\mathbf{k}_1 + \mathbf{q}/2\rangle$ is destroyed and $|-\mathbf{k}_1 + \mathbf{q}/2\rangle$ created and particle $|-\mathbf{k}_2 + \mathbf{q}/2\rangle$ is destroyed and $|\mathbf{k}_2 + \mathbf{q}/2\rangle$ created

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• description of finite interactions between particles within second quantization formalism

$$\mathcal{H}_{\text{int}} = \frac{V_0}{2} \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}}^N \hat{b}_{\mathbf{k}_2 + \mathbf{q}/2}^{\dagger} \hat{b}_{-\mathbf{k}_1 + \mathbf{q}/2}^{\dagger} \hat{b}_{-\mathbf{k}_2 + \mathbf{q}/2} \hat{b}_{\mathbf{k}_1 + \mathbf{q}/2}$$

we have made the following simplifying assumptions:

- ➤ we assume a *local interaction* V(r₁ r₂) → Fourier transform V_{k₁,k₂,q} does not depend on k₁ and k₂: $V_{k_1,k_2,q} \simeq V_q$
- \succ since we are at very low T, the involved velocities and hence wavevectors **q** are very small
- ➢ if the interaction range R of the potential is small, $qR \ll 1$, then the FT V_q is essentially independent of **q** and we can use the approximation V_q = V₀
- \succ as above, we assume two bosons with the same wave number $\mathbf{k}_1 = \mathbf{k}_2$ and set it equal to zero
- \succ we describe the two states of the interacting bosons with the bosonic operators \hat{b} and $\hat{ ilde{b}}$

$$\mathcal{H}_{\text{int}} = \frac{V_0}{2} \Big[\hat{b}^\dagger \, \hat{b}^\dagger \hat{b} \hat{b} + \hat{b}^\dagger \, \hat{\tilde{b}}^\dagger \hat{b} \hat{\tilde{b}} + \hat{\tilde{b}}^\dagger \, \hat{b}^\dagger \hat{b} \hat{\tilde{b}} + \hat{b}^\dagger \, \hat{\tilde{b}}^\dagger \hat{\tilde{b}} \hat{b} + \hat{\tilde{b}}^\dagger \, \hat{\tilde{b}}^\dagger \hat{\tilde{b}} \hat{b} + \hat{\tilde{b}}^\dagger \, \hat{\tilde{b}}^\dagger \hat{\tilde{b}} \hat{b} \Big]$$

we do not include terms like $\hat{\hat{b}}^{\dagger} \hat{\hat{b}}^{\dagger} \hat{\hat{b}} \hat{\hat{b}}$, as we do not consider states occupied with two $\hat{\hat{b}}$ bosons

- relevant relations
 - > both states occupied with single boson: $|1,1\rangle = \hat{b}^{\dagger}\hat{\tilde{b}}^{\dagger} |0\rangle$ with $|0\rangle =$ normalized vacuum state
 - $\succ \langle 1,1|1,1 \rangle = \left\langle 0 \left| \hat{\hat{b}} \hat{b} \ \hat{b}^{\dagger} \hat{\hat{b}}^{\dagger} \right| 0 \right\rangle = 1, \qquad \text{as } \hat{\hat{b}} \text{ and } \hat{b} \text{ commute and } \hat{b} \hat{b}^{\dagger} \left| 0 \right\rangle = 0$
 - > one state occupied with two bosons and the other is empty: $|2,0\rangle = \hat{b}^{\dagger}\hat{b}^{\dagger}|0\rangle = (\hat{b}^{\dagger})^{2}|0\rangle$
 - $\langle 2,0|2,0\rangle = \langle 0|bb\hat{b}^{\dagger}\hat{b}^{\dagger}|0\rangle = \langle 0|b(1+\hat{b}^{\dagger}b)\hat{b}^{\dagger}|0\rangle = 2, \quad \text{as } [b,\hat{b}^{\dagger}] = 1 \text{ and } b\hat{b}^{\dagger}|0\rangle = 0$ $\Rightarrow |2,0\rangle = \frac{1}{\sqrt{2}} (\hat{b}^{\dagger})^{2}|0\rangle \quad \text{correctly normalized state}$
 - interaction energy for the states $|1,1\rangle$ and $|2,0\rangle$:

 $|2,0\rangle: \text{ only the first term in } \frac{V_0}{2} \left[\hat{b}^{\dagger} \hat{b}^{\dagger} \hat{b} \hat{b} + \hat{b}^{\dagger} \hat{b}^{\dagger} \hat{b} \hat{b} \right] \text{ contributes} \\ \frac{1}{2} \langle 0 | \hat{b} \hat{b} (\hat{b}^{\dagger} \hat{b}^{\dagger} \hat{b} \hat{b}) \hat{b}^{\dagger} \hat{b}^{\dagger} | 0 \rangle = \frac{1}{2} 2 \langle 0 | \hat{b} \hat{b} (\hat{b}^{\dagger} \hat{b}^{\dagger}) | 0 \rangle = 2 \qquad \rightarrow \langle 2, 0 | \mathcal{H}_{int} | 2, 0 \rangle = V_0 \\ |1,1\rangle: \text{ all four last terms in } \frac{V_0}{2} \left[\hat{b}^{\dagger} \hat{b}^{\dagger} \hat{b} \hat{b} + \hat{b}^{\dagger} \hat{b}^{\dagger} \hat{b} \hat{b} \right] \text{ contribute equally, since } \hat{b} \text{ and } \hat{b} \text{ commute}$

$$4\left\langle 0\left|\hat{\hat{b}}\hat{b}\left(\hat{b}^{\dagger}\hat{\hat{b}}^{\dagger}\hat{b}\hat{\hat{b}}\right)\hat{b}^{\dagger}\hat{\hat{b}}^{\dagger}\right|0\right\rangle = 4\left\langle 0\left|\hat{b}\hat{b}^{\dagger}\hat{b}\hat{b}^{\dagger}\right|0\right\rangle\left\langle 0\left|\hat{\hat{b}}\hat{\hat{b}}^{\dagger}\hat{\hat{b}}\hat{\hat{b}}^{\dagger}\right|0\right\rangle = 4 \quad \rightarrow \langle \mathbf{1},\mathbf{1}|\mathcal{H}_{int}|\mathbf{1},\mathbf{1}\rangle = 2V_{\mathbf{0}}$$

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• generalization to states with N bosons (without calculation)

 $\langle N, 1 | \mathcal{H}_{int} | N, 1 \rangle - \langle N + 1, 0 | \mathcal{H}_{int} | N + 1, 0 \rangle = N V_0$

- it is energetically more favorable to put an additional boson into the same state as occupied by all the others rather than putting it into another state
- > energy difference scales with the particle number N and is therefore an extensive variable

- Bogoliubov theory of weakly interacting Bose gas (N.N Bogoliubov, J. Phys. USSR 11, 23 (1947))
 - starting hypothesis: condensation of a large number of bosons into ground state also exists at finite interactions
 - \succ since ground state k = 0 is occupied by large particle number, we have to deal with large quantum numbers
 - o quantum fluctuations become negligible
 - the value of the commutator $[\hat{b}_0, \hat{b}_0^{\dagger}] = 1$ is small compared to these large values

 \rightarrow we can set $[\hat{b}_0, \hat{b}_0^{\dagger}] = 0$, i.e. the operators commute like classical quantities

- number of bosons in ground state, $N_0 = \langle \hat{b}_0^{\dagger} \hat{b}_0 \rangle \simeq \hat{b}_0^{\dagger} \hat{b}_0$, is large and also the numbers \hat{b}_0^{\dagger} and \hat{b}_0 themselves
- as \hat{b}_0^{\dagger} and \hat{b}_0 are complex conjugate, we can take them real by eliminating an irrelevant phase factor:

 $N_0 = \hat{b}_0^{\dagger} \hat{b}_0 = \hat{b}_0^2$ and $\hat{b}_0^{\dagger} = \hat{b}_0 = \sqrt{N_0}$

– interaction energy:

$$\mathcal{H}_{\text{int}}^{(0)} = \frac{V_0}{2} \left[\underbrace{\hat{b}^{\dagger} \ \hat{b}^{\dagger} \hat{b} \hat{b}}_{\hat{b}_0^2 \hat{b}_0^2 = N_0^2} + \hat{b}^{\dagger} \ \hat{\bar{b}}^{\dagger} \hat{b} \hat{\bar{b}} + \hat{\bar{b}}^{\dagger} \ \hat{\bar{b}}^{\dagger} \hat{b} \hat{\bar{b}} + \hat{\bar{b}}^{\dagger} \ \hat{\bar{b}}^{\dagger} \hat{\bar{b}} \hat{\bar{b}} + \hat{\bar{b}}^{\dagger} \ \hat{\bar{b}} \hat{\bar{b}} \hat{\bar{b}} \right]$$

dominating term is the one with all wave numbers equal and zero

 $E_{\rm int}^{(0)} = \frac{V_0}{2} N_0^2$

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- interaction energy, next order term in powers of \widehat{b}_0 :
 - \rightarrow we cannot have three \hat{b}_0 factors due to momentum conservation
 - ightarrow we have to consider only terms with two \hat{b}_0 factors in the next order
 - → momentum conservation requires that we have factors $\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{\mathbf{k}}$ (4 possibilities), $\hat{b}_{\mathbf{k}}^{\dagger}\hat{b}_{-\mathbf{k}}^{\dagger}$ (1 possibility) and $\hat{b}_{\mathbf{k}}\hat{b}_{-\mathbf{k}}$ (1 possibility)

$$\mathcal{H}_{\text{int}}^{(1)} = \frac{V_0}{2} \hat{b}_0^2 \sum_{\mathbf{k}} \left(4 \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{-\mathbf{k}}^{\dagger} + \hat{b}_{\mathbf{k}} \hat{b}_{-\mathbf{k}} \right)$$

 $\mathcal{H}_{\text{int}}^{(1)}$ contains a contribution $\hat{b}_0^2 \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} = N_0 \sum_{\mathbf{k}} \hat{n}_{\mathbf{k}}$, where $\hat{n}_{\mathbf{k}}$ is the particle number operator for bosons in state \mathbf{k}

 \rightarrow we have to take into account the bosons that are not in the ground state $\mathbf{k} = \mathbf{0}$ (as already done for the non-interacting Bose gas)

$$N = N_0 + \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} \Rightarrow \frac{V_0}{2} \left(\hat{b}_0^2\right)^2 = \frac{V_0}{2} N_0^2 = \frac{V_0}{2} \left(N - \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}\right)^2 \simeq \frac{V_0}{2} \left(N^2 - 2N \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}\right) \simeq \frac{V_0}{2} \frac{V_0}{2} N_0^2 = \frac{V_0}{2} N_0^2 \sum_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}}$$

$$\mathcal{H} = \sum_{\substack{\mathbf{k} \\ \mathbf{k}inetic \, energy}} \varepsilon_{\mathbf{k}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + N \frac{V_0}{2} \sum_{\mathbf{k}} (2\hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + \hat{b}_{\mathbf{k}}^{\dagger} \hat{b}_{-\mathbf{k}}^{\dagger} + \hat{b}_{\mathbf{k}} \hat{b}_{-\mathbf{k}})$$
additional ground state energy

the last two terms do not conservate particle number:

additional states are excited out of the condensate or absorbed into the condensate

- diagonalization of the Hamiltonian by Bogoliubov transformation
 - introduction of new operators being linear combinations of the original bosonic operators

spinors of Bogoliubov operators: $\mathcal{B}_{\mathbf{k}}^{\dagger} = (\alpha_{\mathbf{k}}^{\dagger}, \beta_{-\mathbf{k}}) = \underbrace{\mathcal{C}_{\mathbf{k}}^{\dagger}}_{(\widehat{\mathbf{b}}_{\mathbf{k}}^{\dagger}, \widehat{\mathbf{b}}_{-\mathbf{k}})} \qquad \mathcal{B}_{\mathbf{k}} = (\alpha_{\mathbf{k}}, \beta_{-\mathbf{k}}^{\dagger}) = \underbrace{\mathcal{U}_{\mathbf{k}}^{\dagger}}_{(\widehat{\mathbf{b}}_{\mathbf{k}}, \widehat{\mathbf{b}}_{-\mathbf{k}}^{\dagger})^{T}}$ $\alpha_{\mathbf{k}}^{\dagger} = u_{\mathbf{k}} \widehat{\mathbf{b}}_{\mathbf{k}}^{\dagger} - v_{\mathbf{k}} \widehat{\mathbf{b}}_{-\mathbf{k}} \qquad \alpha_{\mathbf{k}} = u_{\mathbf{k}}^{\star} \widehat{\mathbf{b}}_{\mathbf{k}} - v_{\mathbf{k}}^{\star} \widehat{\mathbf{b}}_{-\mathbf{k}}$ $\beta_{-\mathbf{k}} = v_{\mathbf{k}}^{\star} \widehat{\mathbf{b}}_{\mathbf{k}}^{\dagger} + u_{\mathbf{k}}^{\star} \widehat{\mathbf{b}}_{-\mathbf{k}} \qquad \beta_{-\mathbf{k}}^{\dagger} = v_{\mathbf{k}} \widehat{\mathbf{b}}_{\mathbf{k}} + u_{\mathbf{k}} \widehat{\mathbf{b}}_{-\mathbf{k}}^{\dagger}$

- appropriate unitary matrix to make transformed energy matrix $\tilde{\mathcal{E}}_k = \mathcal{U}_k^{\dagger} \mathcal{E}_k \mathcal{U}_k$ diagonal:

choose $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ such that off-diagonal terms vanish

• diagonalization of the Hamiltonian by Bogoliubov transformation (without detailed calculation)

$$u_{\mathbf{k}} = \sqrt{\frac{1}{2} \frac{(\varepsilon_{\mathbf{k}} + NV_0)}{E_{\mathbf{k}}} + 1} \qquad \qquad v_{\mathbf{k}} = \sqrt{\frac{1}{2} \frac{(\varepsilon_{\mathbf{k}} + NV_0)}{E_{\mathbf{k}}} - 1} \qquad \qquad u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1$$

with
$$E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k}} + NV_0)^2 - (NV_0)^2} = \sqrt{\varepsilon_{\mathbf{k}} (\varepsilon_{\mathbf{k}} + 2NV_0)}$$

resulting Hamiltonian

$$\mathcal{H} = \underbrace{\mathcal{H}_{0}}_{\substack{\text{ground state}\\ \text{energy}}} + \underbrace{\sum_{\mathbf{k}} \{E_{\mathbf{k}} \alpha_{\mathbf{k}}^{\dagger} \alpha_{\mathbf{k}} + E_{\mathbf{k}} \beta_{-\mathbf{k}}^{\dagger} \beta_{-\mathbf{k}} \}}_{elementary \text{ excitations}}$$

elementary excitations of the interacting Bose gas are non-interacting bosonic quasiparticles described by the creation and annihilation operators $\alpha_{\mathbf{k}}^{\dagger}\alpha_{\mathbf{k}}$ and $\beta_{-\mathbf{k}}^{\dagger}\beta_{-\mathbf{k}}$

- nature of excitations
 - large **k**: kinetic energy dominates: $\varepsilon_{\mathbf{k}} \gg NV_0 \Rightarrow E_{\mathbf{k}} \simeq \varepsilon_{\mathbf{k}}, u_{\mathbf{k}} \simeq 1, v_{\mathbf{k}} \simeq 0,$ $\alpha_{\mathbf{k}}^{\dagger} = u_{\mathbf{k}}\hat{\mathbf{b}}_{\mathbf{k}}^{\dagger} - v_{\mathbf{k}}\hat{\mathbf{b}}_{-\mathbf{k}} \simeq \hat{\mathbf{b}}_{\mathbf{k}}^{\dagger}$

excitations are identical to bare bosons

-
$$\mathbf{k} \to \mathbf{0}$$
: kinetic energy vanishes: $\varepsilon_{\mathbf{k}} \ll NV_0 \Rightarrow E_{\mathbf{k}} \simeq \sqrt{2NV_0\varepsilon_{\mathbf{k}}} = \sqrt{NV_0/m} \ \hbar k = \hbar k \ c_s$
 $c_s = \text{sound velocity}$

propagating sound waves are expected for interacting system, correctly described by Bogoliubov theory \rightarrow quantized sound waves: phonons

$$u_{\mathbf{k}}\simeq v_{\mathbf{k}}$$
 with $u_{\mathbf{k}}^2\simeq v_{\mathbf{k}}^2=1/2$

excitations are equal superpositions of $\hat{b}_{\mathbf{k}}^{\dagger}$ and $\hat{b}_{-\mathbf{k}}$ ($\hat{b}_{-\mathbf{k}}^{\dagger}$ and $\hat{b}_{\mathbf{k}}$) both adding (removing) a momentum $\hbar \mathbf{k}$ to the system \rightarrow consistent with excitation of quantized sound waves

- supplementary material

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- What do we already know about ⁴He?
 - ⁴He does no become solid at ambient pressure due to the weak Van der Waals interaction and the large zero-point fluctuations
 - ⁴He is a boson and shows superfluidity
 discovered in 1937 by Pyotr Kapitsa ("Viscosity of Liquid Helium Below the λ-Point", Nature 141, 74 (1938))
 and John F. Allen, and Don Misener ("Flow of Liquid Helium II" Nature 142, 643 (1938))
 - the properties of superfluid ⁴He often deviate from those of an ideal Bose-Einstein condensate
 - $\succ C_V \propto T^3$ instead of $C_V \propto T^{3/2}$ at low T
 - ➢ behavior of C_V around T_{BEC} is different − sharp λ-shaped peak instead of "cusp": ⁴He shows critical behavior consistent with 3D-XY universality class
 - description of superfluid ⁴He by macroscopic wave function $\psi(\mathbf{r})$

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r})e^{i\theta(\mathbf{r})}, \qquad |\psi_0(\mathbf{r})|^2 = n_0(\mathbf{r}), \qquad N_0 = \int |\psi_0(\mathbf{r})|^2 \,\mathrm{d}^3 r$$

• How well does the ideal Bose gas describe the normal-superfluid transition temperature?

$$T_{\rm BEC} = \frac{2\pi\hbar^2}{mk_{\rm B}} \left(\frac{n}{2.612}\right)^{2/3}$$

⁴He is not an ideal Bose gas: *interaction of He atoms*

- ➢ hard core repulsion
- admixture of higher k-states (is equivalent to larger k-uncertainty)
- reduction of particle number in ground state



(is well below normal-superfluid transition temperature)

(agrees only qualitatively with measured $T_{\lambda} = 2.17$ K)

 \succ $T_{\rm BEC} \simeq 0.5$ K by using data of gaseous ⁴He

 \succ $T_{\rm BEC} \simeq 3.1$ K by using data of liquid ⁴He

• superfluid fraction of ⁴He is only about 14% for $T \rightarrow 0$: $n_0(T = 0) \simeq 0.14 n$



experimentra observations

$$T \ll T_{\lambda}$$
: $n_s(T) \simeq n_s(0) - AT^{\alpha}$ with $\alpha \simeq 4$

$$T \sim T_{\text{BEC}}$$
: $n_s(T) \simeq \begin{cases} B(T_\lambda - T)^\beta & \text{for } T < T_\lambda \\ 0 & \text{for } T > T_\lambda \end{cases}$

data obtained from x-ray scattering and neutron scattering

J.S. Brooks and R.J. Donnelly, J. Phys. Chem. Ref. Data 6, 51 (1977).

• superfluid fraction of ⁴He



condensate fraction of superfluid ⁴He as a function of the density. Open circles are experimental results obtained from deep inelastic neutron scattering, squares are HD predictions at the same densities. The star diamond, and hexagonal points correspond to quantumfield hydrodynamics (HD) results using the experimental measures of the static structure factor S(**p**)

Lozovik, Yurii & Kurbakov, I. & Astrakharchik, G. & Boronat, J. (2020). Universal relation between the static structure factor and the condensate fraction.

- superfluid fraction of ⁴He more detailed treatment (1)
 - reduced superfluid fraction is caused by the fact that superfluid ⁴He is a strongly interacting Bose gas described by

$$\mathcal{H} = \sum_{i=1}^{N} \frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{i \neq j} V(\mathbf{r}_i - \mathbf{r}_j)$$

solutions are symmetric N-particle wave functions

$$\psi(\mathbf{r}_1, \dots, \mathbf{r}_i, \dots, \mathbf{r}_j, \dots, \mathbf{r}_N) = \psi(\mathbf{r}_1, \dots, \mathbf{r}_j, \dots, \mathbf{r}_i, \dots, \mathbf{r}_N)$$
$$\mathcal{H}\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E_n\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$$

- occupation probability of eigenstate with energy E_n

$$P_n = \frac{1}{Z_N} \exp(-E_n/k_{\rm B}T)$$
 with partition function $Z_N = \sum_n \exp(-E_n/k_{\rm B}T)$

- if particle number is not fixed (grand canonical ensemble): $Z_N = \sum_{n=N} \exp\left(-\frac{E_n^{(N)}}{k_{\rm B}T} - \mu N\right)$

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- superfluid fraction of ⁴He more detailed treatment (2)
 - for grand canonical ensemble:

 $\Omega(T,\mu) = -k_{\rm B}T \ln Z$ grand canonical potential $\langle N \rangle = k_{\rm B}T \frac{\partial \ln Z}{\partial \mu}$ average particle number

$$U = \langle \mathcal{H} \rangle = \mu \langle N \rangle - k_{\rm B} T \frac{\partial \ln Z}{\partial \beta} \qquad \text{inner energy (with } \beta = 1/k_{\rm B} T)$$

 calculations have to be performed numerically, e.g. by perturbation theory (if interactions are weak) or quantum Monte Carlo simulations in the case of strong interactions (as for superfluid ⁴He)

key result: superfluid ⁴He forms a condensate of He atoms in the ground state, however, not all atoms occupy ground state at T = 0see e.g. D.M. Ceperley, Rev. Mod. Phys. 67, 279-355 (1995)

- superfluid fraction of ⁴He more detailed treatment (3)
 - single particle density matrix:

$$\rho(\mathbf{r}_1 - \mathbf{r}_1') = N \int \psi_0^*(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \psi_0(\mathbf{r}_1', \mathbf{r}_2, \dots, \mathbf{r}_N) d^3 r_2 \dots d^3 r_N$$

- corresponds to correlation function between the many-body wave functions at the coordinates $\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N$ and $\mathbf{r}'_1, \mathbf{r}_2, ..., \mathbf{r}_N$ - by integrating of all coordinates despite \mathbf{r}_1 and \mathbf{r}'_1 , we average over all configurations of the particles despite the first ones

- properties if the single particle density matrix:
 - \blacktriangleright depends only on relative coordinate $\mathbf{r}_1 \mathbf{r}_1'$ due to translational invariance
 - ✓ for **r**₁ = **r**'₁ we obtain: $\int \rho_1(0) d^3 r_1 = \frac{N}{V} = n$
- for ideal non-interacting Bose gas we have $\psi_0(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \psi_0(\mathbf{r}_1)\psi_0(\mathbf{r}_2) ... \psi_0(\mathbf{r}_N)$

$$\rho(\mathbf{r}_1 - \mathbf{r}_1') = N\psi_0^*(\mathbf{r}_1)\psi_0(\mathbf{r}_1')\int |\psi_0(\mathbf{r}_1)|^2 |\psi_0(\mathbf{r}_2)|^2 \dots |\psi_0(\mathbf{r}_N)|^2 \,\mathrm{d}^3 r_2 \dots \mathrm{d}^3 r_N = N\psi_0^*(\mathbf{r}_1)\psi_0(\mathbf{r}_1')$$

$$\rho(\mathbf{r}_1 - \mathbf{r}_1') = \frac{N}{V} = n \quad \text{since } \psi_0(\mathbf{r}) = \frac{1}{\sqrt{V}} \exp(\iota \mathbf{k} \cdot \mathbf{r})$$

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- superfluid fraction of ⁴He more detailed treatment (4)
 - for interacting Bose gas we obtain more complicated result
 - $\succ
 ho(\mathbf{r}_1 \mathbf{r}_1')$ is no longer independent of $\mathbf{r}_1 \mathbf{r}_1'$
 - $\succ \rho(\mathbf{r}_1 \mathbf{r}_1')$ decreases with increasing $\mathbf{r}_1 \mathbf{r}_1'$ and converges towards a constant value at large $\mathbf{r}_1 \mathbf{r}_1'$
 - condensate density:



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superfluid fraction of ⁴He – more detailed treatment (5)

plausibility consideration by considering spatial distribution function



- without interactions particles can be described by plane waves with $k = k_0$

→ $g(\mathbf{r}_1 - \mathbf{r}_2) = 1$, all particles in ground state: $n_0 = n$

- in the presence of interactions, $g(\mathbf{r}_1 \mathbf{r}_2) \neq 1$ for short distances
 - \rightarrow we have to admix states with higher k to describe the situation: spatial localization requires finite Δk
 - → some states with $k > k_0$ are occupied: $n_0 < n$
 - → n_0 becomes smaller, if $g(\mathbf{r}_1 \mathbf{r}_2)$ deviates more strongly from $g(\mathbf{r}_1 \mathbf{r}_2) = 1$, i.e. with increasing interactions

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- nomenclature and history
 - superfluid ⁴He can flow through tiny capillaries without any friction → nomenclature *superfluidity*
 - **discovery of superfluidity** in 1937 by two groups:
- (i) *P. Kapitza, Nature 141, 74 (1938)*
- (ii) J.F. Allen, A.D. Misener, Nature 141, 75 (1938)

- theory of superfluidity:
 - F. London (1938):superfluidity caused by ordered state in momentum spaceF. London, Nature 141, 643 (1938); Phys. Rev. 54, 947 (1938).
 - L. Tisza (1938): two-fluid model: prediction of second sound L. Tisza, Nature 141, 913 (1938).
 - L.D. Landau (1941-47): two-fluid hydrodynamics of superfluid ⁴He → superfluidity as a consequence of the excitation spectrum L.D. Landau, J. Phys. USSR 5, 71 (1941); ibid. 8, 1 (1944); ibid. 11, 91 (1947).
 - **R.P. Feynman** (1953): excitation spectrum postulated by Landau follows from quantum mechanics *R.P. Feynman, Phys. Rev. 90, 1116 (1953).*

two-fluid model allows phenomenological description of superfluid ⁴He

microscopic description is difficult \rightarrow treatment using hydrodynamics

- already in 1938: anomalous properties of superfluid ⁴He can be well described by two-fluid model:
 mixture of two non-interacting fluid components (I. Tisza, J. de Phys. et Radium 1, 164 (1938))
- formal description of superfluid ⁴He as the sum of a normal and a superfluid component

 $\rho = \rho_s + \rho_n$ $\rho_s, \rho_n =$ superfluid and normal fluid densities

$$- T = 0: \quad \rho_s = \rho \quad \text{and} \quad \rho_n = 0$$

-
$$T = T_{\lambda}$$
: $\rho_s = 0$ and $\rho_n = \rho$

> superfluid component: *no entropy:* $S_s = 0$ *zero viscosity:* $\eta_s = 0$

> normal fluid component: carries total entropy: $S_n = S$, finite viscosity: $\eta_n = \eta$

superfluid component

- description of superfluid component by macroscopic wave function

as done in superconductivity for electronic system: charged superfluid

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r})e^{i\theta(\mathbf{r})}, \qquad |\psi_0(\mathbf{r})|^2 = n_0(\mathbf{r}), \qquad N_0 = \int |\psi_0(\mathbf{r})|^2 \, \mathrm{d}^3 r \qquad n_0 = \frac{N_0}{V} = \text{particle density in condensate}$$

use quantum mechanics to derive expression for the particle current density (probability current density in 3D)

$$J_{\rho} = \frac{\hbar}{2m\iota} [\psi^*(\mathbf{r}) \nabla \psi(\mathbf{r}) - \psi(\mathbf{r}) \nabla \psi^*(\mathbf{r})]$$

$$J_{\rho} = \frac{\hbar}{2m\iota} \left[\underbrace{\sqrt{n_0} e^{-\iota\theta(\mathbf{r})}}_{\psi^*(\mathbf{r})} \underbrace{\left(e^{\iota\theta(\mathbf{r})} \nabla \sqrt{n_0} + \iota \sqrt{n_0} e^{\iota\theta(\mathbf{r})} \nabla \theta(\mathbf{r}) \right)}_{\nabla \psi(\mathbf{r})} - \underbrace{\sqrt{n_0} e^{\iota\theta(\mathbf{r})}}_{\psi(\mathbf{r})} \underbrace{\left(e^{-\iota\theta(\mathbf{r})} \nabla \sqrt{n_0} - \iota \sqrt{n_0} e^{-\iota\theta(\mathbf{r})} \nabla \theta(\mathbf{r}) \right)}_{\nabla \psi^*(\mathbf{r})} \right]$$

$$J_{\rho}(\mathbf{r}) = n_0 \underbrace{\frac{\hbar}{m} \nabla \theta(\mathbf{r})}_{v_s} = n_0 v_s(\mathbf{r})$$

current density – phase relation (as in superconductivity) $v_s =$ superfluid velocity

- what is the ratio of the normal und superfluid component? How does it depend on temperature?
 - torsional pendulum experiment: 50 Al disks, thickness: 13 μm, diameter: 3.5 cm, disk separation: 210 μm

(E.L. Andronikashvili, Zh. Eksperim. i. Teor. Fiz. 18, 424 (1948))



skin depth of viscous wave:

 $\sqrt{2\eta_n/
ho_n\omega}$

→ large compared to disk separation below T_{λ} → complete normal component is moved

> moved mass of normal component results in change of moment of inertia \rightarrow change of oscillation frequency: $\omega \propto 1/\text{mass}$



empirical relation by fitting data:



cf. normal fluid density of ideal BEC:



physical consequence of macroscopic wave function description

$$J_{\rho}(\mathbf{r}) = n_0 \frac{\hbar}{m} \nabla \theta(\mathbf{r}) = n_0 v_s(\mathbf{r}) \implies v_s(\mathbf{r}) = \frac{\hbar}{m} \nabla \theta(\mathbf{r})$$

since the curl of the gradient of a scalar function vanishes, we obtain

 $\nabla \times v_s(\mathbf{r}) = 0$

 $v_s(\mathbf{r})$ cannot take the form $\Omega \times \mathbf{r}$ corresponding to a rotating liquid

→ it is impossible to set the superfluid into rotation

note:

we will see later that this is true only for slow enough rotations of the vessel containing the superfluid. At large rotation speed, we are generating vortices in the superfluid

→ the critical rotation speed corresponds to the lower critical field in superconductors!!

I.3.2 Experimental Observations

• boiling of liquid helium

- $T > T_{\lambda}$: liquid He is boiling
 - latent heat of evaporation is removed from bath
 - temperature is decreasing
- $T \simeq T_{\lambda}$: temperature is decreasing only slowly
 - temperature does not stay constant
 - boiling suddenly stops !!!

- \rightarrow large specific heat
- \rightarrow no latent heat, 2. order phase transition



boiling of superfluid helium:

- > very high thermal conductivity
- Iow T not only at surface, but also within liquid
- no vapor bubbles in liquid
 - evaporation only from surface, no boiling
• viscosity η of superfluid ⁴He: two different measuring methods





• viscosity η of superfluid ⁴He: *experimental results*



- flow velocity v about independent of pressure
- flow velocity increases v with decreasing diameter a of capillary

expected for viscous flow through tube of length *L* and diameter *a*: $\Delta p/L \sim \eta(v/a^4)$ experimental result of Kapitza: $\Delta p \simeq 0$ independent of flow velocity $v \rightarrow \eta \simeq 0$

(laminar flow, Hagen-Poiseuille law)

- 2022)

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R. Gross

• superfluid film flow



overshooting during fill up and draining out -> oscillation of filling height

- superfluid film flow: estimate of superfluid film thickness
 - in equilibrium *chemical potentials* are identical: $\mu_{film} = \mu_{vap} = \mu_0$ (for film in saturated vapor)
 - \succ for film:

$$\mu_{\text{film}} = \mu_0 + \underbrace{mgh - \alpha / d^n}_{\uparrow = 0}$$
bulk liquid gravitation

 $(n \approx 3 \text{ for } d < 5 \text{ nm}, \alpha = \text{Hamaker constant}, \alpha \text{ is}$ determined by dielectric properties of wall and He atoms)

van der Waals potential

for vapor:

 $\mu_{\rm vap} = \mu_0 + mgh$



equilibrium condition: $\mu_{\text{film}} = \mu_0$ $d = \left(\frac{\alpha}{mgh}\right)^{1/3}$ typical values: $d (\text{nm}) \approx 30/[h (\text{cm})]^{1/3}$ $h = 5 \text{ cm} \rightarrow d = 20 \text{ nm}$

normal fluid blocked in thin film

→ superleak

• superfluid film flow: acting as a heat leak

helium pump vacuum vacuum Не bath 1.2 K

- film creeps up along the container walls and pumping line
- film creeps up to the position, where T = 2.18 K
- evaporation from film dominates, since vapor pressure at height h is much lower
- estimate of film thickness for *"unsaturated film"*

 \rightarrow d depends on gas pressure p (kinetic gas theory)

$$p(h) = p_{\text{sat}} \exp\left(-\frac{mgh}{k_{\text{B}}T}\right) \implies h = -\frac{k_{\text{B}}T}{mg} \ln\left(\frac{p(h)}{p_{\text{sat}}}\right)$$
$$d = \left(\frac{\alpha}{mgh}\right)^{1/3} \implies d = \left(\frac{-\alpha}{k_{\text{B}}T \ln(p/p_{\text{sat}})}\right)^{1/3}$$

> estimate of the flow of liquid for a critical superfluid velocity of $v_s = 30$ cm/s:

 $\dot{V}_{liq} = 2\pi R dv_s \approx 1 \text{ cm}^3/\text{h}$ for $R = 5 \text{ mm} \rightarrow \dot{V}_{gas} \approx 1 \text{ l/h}$

 \succ min. pressure achieved by vacuum pump with $\dot{V}_{
m pump} pprox 10^4$ l/h

$$p_{\min} = p \, \dot{V}_{\text{gas}} / \dot{V}_{\text{pump}} \approx 10^{-4} \, \text{bar} \qquad \Longrightarrow T_{\min} \approx 1 \, \text{K}$$

- thermomechanical effect: generate $\varDelta T$ by applying $\varDelta p$



only superfluid can flow from A to B through narrow capillary

increase/decrease of normal fluid concentration in A/B

- starting point: same filling level and temperature T of container A and B
- apply Δp → only superfluid component flows through capillary from A to B, but cannot transport heat from A to B
- temperature decreases in B and increases in A, since normal fluid fraction increases in A and decreases in B
- remove $\Delta p \rightarrow$ original state is recovered
- note: mass flow is not accompanied by heat flow since only superfluid component can flow

similar experiment:

- only superfluid flows through powder
- increase of normal fluid concentration
- increase of *T* in container



- thermomechanical effect: generate ΔT by applying Δp

G = U - TS + pV $dG = TdS - pdV + \mu dN - TdS - SdT + pdV + Vdp$ $dG = -SdT + Vdp + \mu dN$



only superfluid can flow from A to B through narrow capillary

$$\Rightarrow \text{ since } S = S_n \Delta p = \frac{S_n}{V} \Delta T = \frac{S_n}{M_n} \frac{M_n}{V} \Delta T = \sigma_n \rho_n \Delta T \Delta p = \sigma_n \rho_n \Delta T \Rightarrow \Delta p \to 0 \text{ for } \rho_n \to 0$$

the configuration can be considered as two systems A and B in equilibrium:

 $\Rightarrow \mu_A = \mu_B = \mu$ and particle number is conserved: $N = N_A + N_B$

- Gibbs-Duhem relation:

 $G(T, p, \mu_A, \mu_B) = N_A \mu_A + N_B \mu_B = N \mu$ $\Rightarrow dG = \mu dN + N d\mu$

comparison with
$$dG = -SdT + Vdp + \mu dN$$
 yields
 $-SdT + Vdp - Nd\mu = 0$
 $-S(T_B - T_A) + V(p_B - p_A) - N(\mu_B - \mu_A) = 0$
 $\downarrow 0$
 \downarrow

- since superfluid flow does not carry heat, there is no mechanism to equilibrate T_A and T_B
- ➢ nevertheless, the particle flow results in $\mu_A = \mu_B = \mu$

- thermomechanical effect: generate ΔT by applying Δp





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• inverse thermomechanical effect: generate Δp by applying ΔT



- heating generates increase of normal fluid concentration
- superfluid components flows through capillary to establish balance
- analoguous to osmotic pressure
- superfluid flows very rapidly through capillary so that a fountain pressure can be generated
 - → fountain effect

• inverse thermomechanical effect: fountain effect



- − light is absorbed by emery powder \rightarrow heating
- lower opening is closed by cotton wool \rightarrow only superfluid can enter
- a He fountain is generated by the thermomechanical effect (typical height up to 30 cm)



thermal conductivity

- thermal conductivity of superfluid ⁴He is by more than five orders of magnitude larger than that of normal liquid ⁴He
- explains disappearance of boiling below T_{λ}
- heat conduction through narrow capillaries has maximum at \approx 1.8 K
- heat current density varies as $J_Q \propto \nabla T^{1/3}$ (if we would use $J_Q \simeq -\lambda \nabla T$, then $\lambda \propto \nabla T^{-2/3}$ and would diverge for small ∇T)
- linear $J_Q \propto \nabla T$ dependence only for small heat current densities
- → no Umklapp (U) processes possible in superfluid ⁴He (no periodic lattice)
- excitations (phonons, rotons) move ballistically, only surface scattering



W.H. Keesom, B.F. Saris, L. Meyer, Physica 7, 817 (1940)

• thermal conductivity: comparison to thermal conductivity of solids

solids at low T:

- → ballistic phonons
- → N processes do not cause momentum relaxation
- ➔ only surface scattering

kinetic gas theory:



thermal conductivity κ is proportional to

ŝ

(W/K

- mean velocity of the particles
- mean free path
- density of the particles
 specific heat carried by particles



- 2022)





BAYERISCHE AKADEMIE DER WISSENSCHAFTEN Technische Universität München

Superconductivity and Low Temperature Physics II



Lecture No. 5 02 June 2022

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• two-fluid hydrodynamics

starting point for hydrodynamic description are Navier-Stokes equations:



 $\rho_s, \rho_n = \text{superfluid and normal fluid densities}$ $\mathbf{v}_s, \mathbf{v}_n = \text{superfluid and normal fluid velocities}$ $\eta_n = \text{normal fluid viscosity}$

terms have unit energy/volume

with the definition of the material derivative $D\mathbf{v}/Dt$:

$$\frac{\mathbf{D}\mathbf{v}_n}{\mathbf{D}t} = \frac{\partial \mathbf{v}_n}{\partial t} + (\nabla \cdot \mathbf{v}_n)\mathbf{v}_n \quad \text{and} \quad \nabla \cdot \mathbf{v}_n = \nabla \left(\frac{\|\mathbf{v}_n\|^2}{2}\right) + (\nabla \times \mathbf{v}_n) \times \mathbf{v}_n$$
the tensor derivative of the velocity vector curl of the velocity (called vorticity) disappears for irrotational flow (no vortices)

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two-fluid hydrodynamics

> superfluid (no viscous friction):

$$\underbrace{\rho_s \frac{D\mathbf{v}_s}{Dt}}_{\text{inertia}} = -\underbrace{\frac{\rho_s}{\rho} \nabla p}_{\text{pressure gradient}} -\underbrace{\frac{\rho_s \sigma_s \nabla T}{\rho}}_{\text{entropy}} - \underbrace{\frac{\rho_s \sigma_s \nabla T}{2\rho} \nabla (\mathbf{v_n} - \mathbf{v_s})^2}_{\text{add. term due to compressibility}} + \underbrace{\frac{\eta_s \nabla^2 \mathbf{v}_s}{\rho}}_{\eta_s = 0}$$

 $\rho_s, \rho_n = \text{superfluid and normal fluid densities}$ $\mathbf{v}_s, \mathbf{v}_n = \text{superfluid and normal fluid velocities}$ $\eta_n = \text{normal fluid viscosity}$

terms have unit energy/volume

with the definition of the material derivative Dv/Dt:

$$\frac{\mathbf{D}\mathbf{v}_{s}}{\mathbf{D}t} = \frac{\partial \mathbf{v}_{s}}{\partial t} + (\mathbf{\nabla} \cdot \mathbf{v}_{s})\mathbf{v}_{s} \quad \text{and} \quad \mathbf{\nabla} \cdot \mathbf{v}_{s} = \mathbf{\nabla}\left(\frac{\|\mathbf{v}_{s}\|^{2}}{2}\right) + (\mathbf{\nabla} \times \mathbf{v}_{s}) \times \mathbf{v}_{s}$$

$$\underset{\text{curl of the velocity (called vorticity)}}{\overset{\text{curl of the velocity (no vortices)}}}$$

- → Euler type equation for superfluid (if there are no vortices)
- → detailed treatment including vortices: Gross-Pitaevskii equation

- two-fluid hydrodynamics (1) a simplified description
 - mass flow density:

 $\mathbf{J} = \rho_n \mathbf{v}_n + \rho_s \mathbf{v}_s$ $\swarrow \qquad \uparrow$ normal superfluid component

- conservation of mass: $\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}$
 - viscosity of normal component is very small and can be neglected in most situations \rightarrow in first order approximation we treat superfluid He is ideal liquid

 \rightarrow description by *Euler equation* (motion of a compressible, inviscid fluid)

$$\frac{\partial \mathbf{J}}{\partial t} + \underbrace{\rho \mathbf{v} \cdot \nabla \mathbf{v}}_{\approx 0} = -\nabla \mathbf{p} \qquad (\mathbf{p} = \text{pressure})$$

$$\Rightarrow \text{ if } \mathbf{v} \text{ is small, quadratic terms in } \mathbf{v} \text{ can be neglected}$$

since we are neglecting dissipative effects (no viscous friction), entropy is conserved:

$$\frac{\partial S}{\partial t} = \frac{\partial(\rho\sigma)}{\partial t} = -\nabla \cdot (\rho\sigma) \mathbf{v_n} \qquad \sigma = \text{entropy per mass}$$

two-fluid hydrodynamics (2)

- exact derivation of equation of motion of normal and superfluid phase is difficult
 - \rightarrow we use approach following "Gedanken" experiment of Landau
- we are adding superfluid component at constant volume and consider change of inner energy

 \rightarrow the resulting operation only changes the mass of the superfluid component, no entropy and volume change)

$$dU = TdS - pdV + \mu dN = TdS - pdV + \underbrace{\mu_m}_{\text{potential energy}} dm$$
$$\Rightarrow -\nabla(\mu_m dm) = \mathbf{F} = dm \frac{d\mathbf{v}_s}{dt}$$

- since adding particles to the superfluid does not change the energy, we have

$$0 = TdS - pdV + \mu_m dm \qquad \Rightarrow \frac{d\mathbf{v}_s}{dt} = \frac{\Delta S}{\Delta m} \nabla T - \frac{\Delta V}{\Delta m} \nabla p = \sigma \nabla T - \frac{1}{\rho} \nabla p$$

- with $\frac{d\mathbf{v}_s}{dt} = \frac{\partial \mathbf{v}_s}{\partial t} + v_s \cdot \nabla v_s \simeq \frac{\partial \mathbf{v}_s}{\partial t}$ (neglecting quadratic terms in v_s) we obtain

 $\frac{\partial \mathbf{v}_s}{\partial t} = \sigma \, \mathbf{\nabla} T - \frac{1}{\rho} \, \mathbf{\nabla} p$

• two-fluid hydrodynamics (3)

- for the normal fluid component we obtain

$$\frac{\partial \mathbf{J}}{\partial t} = \frac{\partial (\rho_n \mathbf{v}_n + \rho_s \mathbf{v}_s)}{\partial t} = -\nabla \mathbf{p} \qquad \Rightarrow \frac{\partial \mathbf{v}_n}{\partial t} = -\frac{1}{\rho_n} \nabla \mathbf{p} - \frac{\rho_s}{\rho_n} \frac{\partial \mathbf{v}_s}{\partial t}$$

with $\frac{\partial \mathbf{v}_s}{\partial t} = \sigma \, \nabla T - \frac{1}{\rho} \, \nabla p$ we then obtain

$$\frac{\partial \mathbf{v}_n}{\partial t} = -\frac{1}{\rho_n} \nabla \mathbf{p} - \frac{\rho_s}{\rho_n} \sigma \nabla T + \frac{\rho_s}{\rho_n} \frac{1}{\rho} \nabla p = -\frac{\rho_s}{\rho_n} \sigma \nabla T + \frac{\rho_s - \rho}{\rho_n \rho} \nabla p = -\frac{\rho_s}{\rho_n} \sigma \nabla T - \frac{1}{\rho} \nabla p$$
$$\frac{\partial \mathbf{v}_n}{\partial t} = -\frac{\rho_s}{\rho_n} \sigma \nabla T - \frac{1}{\rho} \nabla p$$

equations of motion

$$\frac{\partial \mathbf{v}_s}{\partial t} = \sigma \, \mathbf{\nabla} T - \frac{1}{\rho} \, \mathbf{\nabla} p \qquad \qquad \frac{\partial \mathbf{v}_n}{\partial t} = -\frac{\rho_s}{\rho_n} \sigma \, \mathbf{\nabla} T - \frac{1}{\rho} \mathbf{\nabla} p$$

note: the equations of motion are valid only for the linear regime !

• example: explanation of thermomechanical effect:



$$\frac{\partial \mathbf{v}_s}{\partial t} = \sigma \, \boldsymbol{\nabla} T - \frac{1}{\rho} \, \boldsymbol{\nabla} p$$

- in steady state:
$$\frac{\partial \mathbf{v}_s}{\partial t} = 0$$

 $0 = \sigma \nabla T - \frac{1}{\rho} \nabla p$

$$\Delta p = \sigma \rho \; \Delta T$$

I.3.3 Two-Fluid Model

- two-fluid hydrodynamics can be used to understand sound propagation in superfluid helium
 - *first sound:* normal and superfluid component move *in-phase:*

$$v_n = v_s$$
 $v_1 = 238 \text{ m/s for } T \rightarrow 0$

- second sound: normal and superfluid component move out-of-phase: $\rho_n v_n + \rho_s v_s = 0$ $v_2 = \frac{v_1}{\sqrt{3}} \simeq 137$ m/s for $T \to 0$ (Peshkov 1944)

- third sound: waves propagating in thin He films
- fourth sound: compression wave propagating in a super leak

use two-fluid hydrodynamics to understand this behavior

(super leak: very small opening or capillary, in which normal fluid cannot move because of its finite viscosity)

- two-fluid hydrodynamics sound propagation (1)
- take time derivative of $\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{J}$ and insert into $\frac{\partial \mathbf{J}}{\partial t} + \underbrace{\rho \mathbf{v} \cdot \nabla \mathbf{v}}_{\approx 0} = -\nabla \mathbf{p}$ $\frac{\partial^2 \rho}{\partial t^2} = -\nabla \cdot \frac{\partial \mathbf{J}}{\partial t} = -\nabla \cdot (-\nabla \mathbf{p}) \Rightarrow \qquad \frac{\partial^2 \rho}{\partial t^2} = \nabla^2 p$
- elimination of terms with \mathbf{v}_n and \mathbf{v}_s in $\frac{\partial S}{\partial t} = \frac{\partial(\rho\sigma)}{\partial t} = -\nabla \cdot (\rho\sigma) \mathbf{v}_n$ and $\frac{\partial \mathbf{v}_s}{\partial t} = \sigma \nabla T \frac{1}{\rho} \nabla p$ (cannot be observed experimentally) \rightarrow after some steps and neglecting higher order terms one obtains
 - $\frac{\partial^2 \sigma}{\partial t^2} = \frac{\rho_s}{\rho_n} \sigma^2 \, \nabla^2 T$

- $\frac{\partial \mathbf{v}_s}{\partial t} = \sigma \, \nabla T \frac{1}{\rho} \, \nabla p$ $\frac{\partial \mathbf{v}_n}{\partial t} = -\frac{\rho_s}{\rho_n} \sigma \, \nabla T \frac{1}{\rho} \, \nabla p$
- in the two equations we have four variables: ρ , σ , p and $T \rightarrow$ only two of them are independent, we choose ρ and σ
 - dependence of p and T on ρ and σ can be expressed as

$$\delta p = \left(\frac{\partial p}{\partial \rho}\right)_{\sigma} \delta \rho + \left(\frac{\partial p}{\partial \sigma}\right)_{\rho} \delta \sigma \qquad \delta T = \left(\frac{\partial T}{\partial \rho}\right)_{\sigma} \delta \rho + \left(\frac{\partial T}{\partial \sigma}\right)_{\rho} \delta \sigma \qquad for all a determined on the second sec$$

we insert relations into expression for $\frac{\partial^2 \rho}{\partial t^2}$ and $\frac{\partial^2 \sigma}{\partial t^2}$

- supplementary ma

- two-fluid hydrodynamics sound propagation (2)
 - insertion yields

$$\frac{\partial^2 \rho}{\partial t^2} = \left(\frac{\partial p}{\partial \rho}\right)_{\sigma} \nabla^2 \rho + \left(\frac{\partial p}{\partial \sigma}\right)_{\rho} \nabla^2 \sigma \qquad \qquad \frac{\partial^2 \sigma}{\partial t^2} = \frac{\rho_s}{\rho_n} \sigma^2 \left[\left(\frac{\partial T}{\partial \rho}\right)_{\sigma} \nabla^2 \rho + \left(\frac{\partial T}{\partial \sigma}\right)_{\rho} \nabla^2 \sigma \right]$$

2nd oder partial differential equations

- to solve these equations we use the ansatz (1D for simplicity)

$$\rho = \rho_0 + \rho_1 \exp\left[\iota\omega\left(t - \frac{x}{v}\right)\right] \qquad \sigma = \sigma_0 + \sigma_1 \exp\left[\iota\omega\left(t - \frac{x}{v}\right)\right]$$

inserting the ansatz yields

linear system of equations

$$\left[\left(\frac{v}{v_1}\right)^2 - 1\right]\rho_1 + \left(\frac{\partial p}{\partial \sigma}\right)_\rho \left(\frac{\partial \rho}{\partial p}\right)_\sigma \sigma_1 = 0$$

$$\left(\frac{\partial T}{\partial \rho}\right)_{\sigma} \left(\frac{\partial \sigma}{\partial T}\right)_{\rho} \rho_1 + \left[\left(\frac{\nu}{\nu_2}\right)^2 - 1\right] \sigma_1 = 0$$

with abbreviations

$$v_1^2 = \left(\frac{\partial p}{\partial \rho}\right)_{\sigma}$$
$$v_2^2 = \frac{\rho_s}{\rho_n} \sigma^2 \left(\frac{\partial T}{\partial \sigma}\right)_{\rho}$$

- supplementary materia

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Chapter 1/RG 172

- two-fluid hydrodynamics sound propagation (3)
 - constraint equation for coefficients

$$\left(\frac{v}{v_1}\right)^2 - 1 \left[\left(\frac{v}{v_2}\right)^2 - 1 \right] = \left(\frac{\partial p}{\partial \sigma}\right)_{\rho} \left(\frac{\partial \rho}{\partial p}\right)_{\sigma} \left(\frac{\partial T}{\partial \rho}\right)_{\sigma} \left(\frac{\partial \sigma}{\partial T}\right)_{\rho}$$

- the r.h.s. can be rewritten by using known thermodynamic relations

$$\left[\left(\frac{v}{v_1}\right)^2 - 1\right] \cdot \left[\left(\frac{v}{v_2}\right)^2 - 1\right] = \frac{C_p - C_V}{C_p} \qquad C_p, C_V: \text{ specific heat at constant pressure/volume}$$

− for superfluid helium the difference $C_p - C_V$ is very small \rightarrow we can use the approximation

$$\left[\left(\frac{v}{v_1}\right)^2 - 1\right] \cdot \left[\left(\frac{v}{v_2}\right)^2 - 1\right] \simeq 0 \qquad \qquad v_1^2 = \left(\frac{\partial p}{\partial \rho}\right)_{\sigma} \qquad v_2^2 = \frac{\rho_s}{\rho_n} \sigma^2 \left(\frac{\partial T}{\partial \sigma}\right)_{\rho}$$

two-fluid hydrodynamics: first sound

- propagation of usual sound waves with velocity $v = v_1$ is given by

$$\left[\left(\frac{v}{v_1}\right)^2 - 1\right]\rho_1 + \left(\frac{\partial p}{\partial \sigma}\right)_\rho \left(\frac{\partial \rho}{\partial p}\right)_\sigma \sigma_1 = 0 \quad \text{if we set } \rho_1 \neq 0 \text{ and } \sigma_1 = 0$$

under these conditions we have $\nabla T = 0$ as for a usual sound waves (*first sound*)

- from
$$\frac{\partial \mathbf{J}}{\partial t} = -\nabla \mathbf{p}$$
 and $\frac{\partial \mathbf{v}_s}{\partial t} = \sigma \nabla T - \frac{1}{\rho} \nabla p$ we obtain
 $\boldsymbol{v}_n = \boldsymbol{v}_s$ (acoustic mode)

→ normal and superfluid component move in phase (first sound)

- density changes are adiabatic
- superfluid He behaves as usual liquid
- > sound velocity $v = v_1 = 238 \text{ m/s}$ for $T \to 0$
- $\succ v_1(T)$ shows anomaly at $T = T_{\lambda}$





L. Djadaojee, A. Douillet, J. Grucker, Jules, J. Low Temp. Phys. 203 (2021)

supplementary mater

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two-fluid hydrodynamics: second sound

- if we set $\rho_1 = 0$ and $\sigma_1 \neq 0$ we obtain temperature wave propagating with velocity $v = v_2$

$$\left(\frac{\partial T}{\partial \rho}\right)_{\sigma} \left(\frac{\partial \sigma}{\partial T}\right)_{\rho} \rho_{1} + \left[\left(\frac{\nu}{\nu_{2}}\right)^{2} - 1\right] \sigma_{1} = 0$$

- from
$$\frac{\partial^2 \rho}{\partial t^2} = \nabla^2 p$$
 we obtain $\nabla p = 0$

- together with Euler's equation
$$\frac{\partial \mathbf{J}}{\partial t} + \underbrace{\rho \mathbf{v} \cdot \nabla \mathbf{v}}_{\approx 0} = -\nabla \mathbf{p}$$
 we obtain: $\frac{\partial \mathbf{J}}{\partial t} = \frac{\partial (\rho_n \mathbf{v}_n + \rho_s \mathbf{v}_s)}{\partial t} = 0$

– since J cannot be constant in a closed container $\boldsymbol{\rightarrow} J=0$

 $\rho_n v_n + \rho_s v_s = 0$ (optical mode)

velocity of the temperature wave

$$v_2^2 = \frac{\rho_s}{\rho_n} \sigma^2 \left(\frac{\partial T}{\partial \sigma}\right)_{\rho} = \frac{\rho_s}{\rho_n} \sigma^2 \frac{T}{C_p}, \qquad v_2 = \frac{v_1}{\sqrt{3}} \simeq 137 \text{ m/s for } T \to 0$$

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two-fluid hydrodynamics: second sound – experiment



 \rightarrow vortex rings

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- two-fluid hydrodynamics: third sound thickness waves in thin helium films
 - we already discussed the thickness of helium films on surfaces

$$d = \left(\frac{-\alpha}{k_{\rm B}T\ln(p/p_{\rm sat})}\right)^{1/3} = \left(\frac{\alpha}{k_{\rm B}T(\ln p_{\rm sat} - \ln p)}\right)^{1/3}$$

- → film thickness depends on pressure and temperature
- → local periodic heating causes thickness variation propagating along surface



- viscous normal component is fixed at surface
- superfluid component oscillates freely parallel to surface

wave crest: surplus of superfluid \rightarrow cold wave valley: deficit of superfluid \rightarrow hot

sound velocity: $v_3 \sim$ 10 ... 100 m/s

detailed discussion complicated due to additional evaporation and condensation at surface



• two-fluid hydrodynamics: third sound – thickness waves in thin helium films



two-fluid hydrodynamics: forth sound – compression waves in superleaks

(super leak = very small opening or capillary, in which normal fluid cannot move because of its finite viscosity)

- only superfluid can move, whereas normal fluid is blocked due to its finite viscosity
- compression waves are not only density oscillations, but also oscillations of the superfluid density ρ_s/ρ_n , the pressure p, the temperature T, and the entropy σ
- sound velocity (without derivation)

$$v_4^2 \simeq \frac{\rho_s}{\rho} v_1^2 + \frac{\rho_n}{\rho} v_2^2$$



- supplementary materia

- two-fluid hydrodynamics: heat transport
 - example: mass flow \dot{V}_n through capillary of diameter d:
 - > the normal fluid component flows from hot to cold side
 - this mass flow is compensated by opposite flow of superfluid component
 - \succ due to different entropies of both components this results in a finite heat flow (limited by η_n)
 - mass flow \dot{V}_n of normal component according to classical hydrodynamics

$$\dot{V}_n = \frac{\beta}{\eta_n} \, \frac{\Delta p}{L}$$

 η_n : viscosity of normal component

L: length of capillary

 Δp : pressure difference

- the parameter β depends on the geometry of the capillary: e.g. $\beta \propto r^4$ according to Hagen-Poiseuille law
- heat flow = mass flow times heat/mass: $\dot{Q} = \rho_n \dot{V}_n \cdot \sigma_n T = \dot{V}_n S_n T$

$$\dot{Q}_{n} = \rho_{n} \underbrace{\dot{V}_{n}}_{\frac{\beta}{\eta_{n}} \frac{\Delta p}{L}} \cdot \sigma_{n}T = \rho_{n} \frac{\beta}{\eta_{n}} \frac{\Delta p}{L} \sigma_{n}T \qquad \text{with } \Delta p = \rho_{n} \sigma_{n} \Delta T \Rightarrow \qquad \dot{Q}_{n} = \frac{\beta T}{\eta_{n}L} (\rho_{n} \sigma_{n})^{2} \Delta T$$

two-fluid hydrodynamics: heat transport

$$\dot{Q}_n = \frac{\beta T}{\eta_n L} (\rho_n \sigma_n)^2 \Delta T$$

experiment: _

heat flow is found to be proportional to $\beta \propto d^3$ (for slit of width d)



Physica 22, 905-910 (1956)

WM

two-fluid hydrodynamics: momentum flow associated with heat flow



- heater generates normal fluid: phonons and rotons
- radiation to the left
- recoil to the right
- measurement of displacement of the glas plate via Newton's rings between glas plate and lens

- momentum flow (momentum / area and time): $ho ~ {f v} \cdot {f v}$
- resulting pressure on heat source:

$$p = \rho_n v_n^2 + \rho_s v_s^2$$

with heat flow per area:

 $J_h = \rho \sigma T v_n$

- and the fact that there is no mass transport, $\rho_n v_n + \rho_s v_s = 0$, we obtain pressure

$$p = \frac{\rho_n J_H^2}{\rho_s \rho T^2 \sigma^2} = \frac{J_h^2}{v_2^2 \rho C_p T}$$

two-fluid hydrodynamics: momentum flow associated with heat flow



$$p = \frac{\rho_n J_H^2}{\rho_s \rho T^2 \sigma^2} = \frac{J_h^2}{v_2^2 \rho C_p T}$$



Enns, Hunklinger,



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important question: does the formation of a condensate automatically result in superfluidity? Does and ideal Bose-Einstein condensate show superfluidity as ⁴He-II?

Answer: Structure of the excitation spectrum is crucial for observability of superfluidity (Lev Landau, 1947)

- note:

> we have used a phenomenological two-fluid model to describe superfluid current density in ⁴He-II

$$\mathbf{J}_{\rho}(\mathbf{r}) = n_0 \underbrace{\frac{\hbar}{m} \nabla \theta(\mathbf{r})}_{v_s} = n_0 \mathbf{v}_s(\mathbf{r})$$

- still unknown:

- \succ is there a maximum value for the superfluid velocity \mathbf{v}_s ?
- \succ if yes, what determines the value of \mathbf{v}_s ?
- is there a qualitative difference between a condensate of a non-interacting Bose gas and an interacting Bose gas ?

- Gedanken experiment by Lev Landau
 - what happens, if we move an object (e.g. sphere) of mass M at velocity \mathbf{v}_i through the condensate/superfluid ?
 - \rightarrow at T = 0, the deceleration of the object is possible only by the generation of excitations
 - \rightarrow at which velocity can the moving object generate an excitation of energy E_p and

momentum $\mathbf{p} = \hbar \mathbf{k}$?

- with velocity difference $v_i - v_f$ of object we obtain (energy and momentum conservation):

$$\boldsymbol{E}_{\boldsymbol{p}} = \frac{1}{2} M \left(v_i^2 - v_f^2 \right) \qquad \boldsymbol{p} = M \left(\mathbf{v}_i - \mathbf{v}_f \right)$$

- elimination of v_f yields

$$v_L = \min\left\{\frac{E_P}{|\mathbf{p}|}\right\}$$

Landau critical velocity

- \blacktriangleright there may be a minimum value of \mathbf{v}_i for which the equation can be satisfied
- \blacktriangleright mass of object can be large \rightarrow we can neglect 2nd term on rhs

Gedanken experiment by Lev Landau

$$E_p = \mathbf{p} \cdot \mathbf{v}_i - \frac{1}{2M}p^2 = \mathbf{p} \cdot \mathbf{v}_i - \mathcal{O}\left(\frac{1}{M}\right)$$

 $v_L = \min \left\{ \right.$

- for free bosons: $E_p = p^2/2m$ (*m* = mass of the boson)

$$\frac{p^2}{2m} = \mathbf{p} \cdot \mathbf{v}_i \qquad \text{equation always satisfied for cone of momentum} \\ \text{vectors } |p| = 2mv_i \cos \vartheta, \text{ where } \vartheta = \measuredangle(\mathbf{p}, \mathbf{v}_i) \end{cases}$$

→ object (e.g. a sphere) moving in superfluid can always transfer momentum to superfluid and is thereby decelerated → $v_L = 0$

ideal Bose-Einstein condensate of free (non-interacting) bosons with dispersion $E_p = p^2/2m$ does not show superfluidity !!

- motivation for Landau critical velocity
 - deceleration of moving object by generation of excitations with energy E_p only possible if $\frac{p^2}{2m} = \mathbf{p} \cdot \mathbf{v}_i$ can be satisfied

$$E_p = \mathbf{p} \cdot \mathbf{v}_i - \frac{1}{2M}p^2 \simeq \mathbf{p} \cdot \mathbf{v}_i$$

$$v_L = \min\left\{\frac{E_P}{|\mathbf{p}|}\right\}$$

how to obtain the blue dispersion curve ??
dispersion of
free particle

$$g_{H}^{0}$$

 g_{H}^{0}
 g_{H}^{0}
 g_{H}^{0}
 g_{H}^{0}
 g_{H}^{0}
 g_{L}^{0}
 p_{L}^{0}
 $p_{L}^{$

$$\Longrightarrow E_{p} = \hbar \omega = \frac{\partial E_{p}}{\partial p} \cdot \mathbf{p} = \hbar \mathbf{v}_{i} \cdot \mathbf{k} = \hbar v_{i} k \cos \vartheta \leq \hbar v_{i} k$$

$$v_{i} \geq \frac{\omega}{k} = v_{ph} \qquad v_{ph} = Phasengeschwindigkeit$$

$$v_{L} = \min(v_{ph}) \qquad v_{L} = Landau \ critical \ velocity \\ \min(v_{ph}) = 0 \ for \ free \ bosons$$

no deceleration of object, if $v_i < v_{\rm L}$

Laudau:

in order to have a superfluid, we need a dispersion relation differing significantly from that of free bosons !

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excitation spectrum of superfluid ⁴He: historical aspects (1)

dispersion relation must deviate from that of free bosons, $E_p = p^2/2m$, as in this case $v_L = 0$!!



Nikolai Bogoliubov (1947):

→ interaction effects drastically change the nature of elementary excitations collective excitations (many particles move at the same time)

 \rightarrow even for weak repulsive interaction: $E_p = c |\mathbf{p}|$ (phonon-like dispersion)



Lev Landau (1947) and Richard Feynman (1953):

- \rightarrow discussion of situation for superfluid ⁴He (stronger interaction)
- \rightarrow postulation of the following excitation spectrum (phonons and rotons):

(i) small p:



phonon-like collective excitations



(ii) higher p:
$$\lim_{|p| \to p_0} E_p = \Delta_{\text{rot}} + \frac{(|\mathbf{p}| - p_0)}{2m_{\text{rot}}}$$

roton-like collective excitations (finite energy gap Δ_{rot} for excitation)

expression **"roton"** used by Feynman due to analogy with **"smoke ring"**, since it is connected with a forward motion of a particle accompanied by a ring of back-flowing particles **→** however: detailed nature of rotons still not clarified

• excitation spectrum of superfluid ⁴He: historical aspects (2)

interacting Bose gas
 → finite stiffness
 → solid like excitations



excitation spectrum of superfluid ⁴He: historical aspects (3)

Richard P. Feynman:

(from: "The beat of a different drum" Jagdish Mehra, 1994)

"I cannot remember, how it happened. I was walking along the street... and zing! I understood it!" ...

... "But of course, that is just what liquids must do. If you measure X-ray diffraction, then because of the spatial structure of the liquid, which is almost like a solid, there will be a maximum corresponding to the first diffraction ring of the X-ray pattern! That was a terriffic moment!"



• excitation spectrum of superfluid ⁴He: plausibility considerations

physical interpretation of the phonon and roton part of the excitation spectrum





- wavelength $\lambda = 2\pi/k \gg$ atomic distance
- coupled motion of group of atoms (like for acoustic phonon in solid)

- wavelength $\lambda = 2\pi/k \simeq$ interatomic distance
- central atom moves forward while closely packed neighbors move (backward) out of the way in circular motion (like smoke ring)

in both cases we have collective excitations with dispersion $E_p(k) \rightarrow$ quasiparticles

• excitation spectrum of superfluid ⁴He: measurement by inelastic scattering experiments

ż

experimental study:

inelastic neutron scattering (coupling to density)

experimental parameter:

 $\frac{\Delta_{\rm rot}}{k_{\rm B}} = 8.61$ K, $\frac{p_0}{\hbar} = 1.92$ Å⁻¹, $m_{\rm rot} = 0.14$ $m_{\rm He}$

TABLE IV. Zero pressure roton parameters (this work) compared to previous results: Woods *et al.* [58], Stirling [14,62,64], Andersen *et al.* [68–72], Gibbs *et al.* [73,74], and Pearce *et al.* [76]. Δ_R at P = 0(shown below in italics) is taken from Refs. [62,64] in our instrument calibration procedure.

-	Δ_R (meV)	$k_R\;({\rm \AA}^{-1})$	μ_R
This work	0.7418(10)	1.918(2)	0.141(2)
Woods 1977	0.7426(10)	1.926(5)	0.126(30)
Stirling 1991	0.7418(10)	1.920(2)	0.136(5)
Andersen 1992-1994	0.743(1)	1.931(3)	0.144(3)
Gibbs 1999	0.7426(21)	1.929(2)	0.161(4)
Pearce 2001	0.7440(20)	1.926(-)	0.166(10)

H. Godfrin et al., Phys. Rev. B **103**, 104516 (2021)



R. J. Donnelly, J. A. Donnelly, R. N. Hills, J. Low Temp. Phys. **44**, 471 (1981). Inset: L. D. Landau, J. Phys. U.S.S.R. **11**, 91 (1947).

• excitation spectrum of superfluid ⁴He: measurement by inelastic scattering experiments



Liquid helium excitation spectrum S(Q, $\hbar\omega$) from inelastic neutron scattering measurements.

Main panel, excitation spectrum in 4He for 1.5 < T < 1.8 K. Data for wave vector Q ≥ 2.3 Å⁻¹ are reproduced from ref. 13, data at smaller Q are from C.L.B. and S.-H. Lee, unpublished results. Solid black line, dispersion from ref. 13; red circle with cross, spectrum termination point at Q = Q_c and $\hbar \omega = 2\Delta$. White line, Feynman–Cohen bare dispersion in absence of decays; horizontal red line at $\hbar \omega = 2\Delta$, onset of two-roton states for $\hbar \omega \geq 2\Delta$. Inset, excitations near termination point, at Q = 2.6 Å⁻¹ \approx Q_c, for several temperatures.

Quasiparticle breakdown in a quantum spin liquid Matthew B. Stone, Igor A. Zaliznyak, Tao Hong, Collin L. Broholm and Daniel H. Reich Nature **440**, 187-190 (9 March 2006)

excitation spectrum of superfluid ⁴He: qualitative understanding

periodic crystal: experimental data 16 k and k + G are equivalent linear × 12 chain liquid: (\mathbb{X}) only short distance ordering E_p/k_B \rightarrow a becomes smeared out 8 \rightarrow also $G = 2\pi/a$ is smeared out G π/a $a = 3.6 \text{ \AA} \rightarrow 2\pi/a \approx 1.8 \text{ \AA}^{-1}$ (reasonable agreement) n 0.0 0.8 1.6 2.4 3.2 $p/\hbar(A^{-1})$

excitation spectrum of superfluid ⁴He: qualitative understanding

- smearing of $G = 2\pi/a$ \rightarrow modelling by average solid + continuum
- other liquids:
 - ightarrow rotons strongly damped
- superfluid He:
 - → no damping, since there are no single particle excitations
- critical velocities:
 - $\overrightarrow{v}_L = 238 \text{ m/s for phonons}$ $\overrightarrow{v}_L \approx 60 \text{ m/s for rotons}$

measured v_L usually smaller

→ excitation of vortices



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• excitation spectrum of superfluid ⁴He: pressure dependence

- average distance *a* becomes smaller
- He becomes harder
 → sound velocity increases
- ordering increases
 - \rightarrow roton gap decreases



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• excitation spectrum of superfluid ⁴He: pressure dependence



The experimental INS phonon-roton curve for molecular para-hydrogen at T = 15.7 K. The filled symbols (inverted triangles, diamonds and crosses) depict data measured at different spectrometers and the open circles with a dot show the simulation results.

J. Dawidowski, F. J. Bermejo, M. L. Ristig, B. Fak, C. Cabrillo, et al., Phys. Rev. B 60, 15154 (1999).

• excitation spectrum of superfluid ⁴He: pressure dependence



FIG. 17. Dispersion curves $\epsilon(k)$ measured for several pressures in the 0 to 24 bar range. The individual data points are represented by small circles (best seen on-line). Accurate values for the pressures are given in Table I.

H. Godfrin, K. Beauvois, A. Sultan, E. Krotscheck, J. Dawidowski, B. Fåk, and J. Ollivier Phys. Rev. B **103**, 104516 (2021)

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BAYERISCHE AKADEMIE DER WISSENSCHAFTEN Technische Universität München

Superconductivity and Low Temperature Physics II



Lecture No. 6 09 June 2022

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- I.6 ³He / ⁴He mixtures

• specific heat of ⁴He revisited



deviations from ideal Bose gas are
 expected due to finite interactions
 → collective excitations: phonons, rotons

 $C_V(T)$ determined by freeze out of phonons and rotons at $T < T_\lambda$

2nd order phase transition is expected for interacting Bose gas

→ however, no jump of C_V at $T = T_\lambda$ is observed, as expected for 2nd order phase transition

- specific heat of ⁴He revisited: temperature dependence below T_{λ}
- T < 0.6 K:

in this temperature regime the dominant excitations are long wave length phonons

 $C_{V,ph} \propto T^3$

(corresponds to Debye model in solid state physics)

$$\frac{C_V}{M} = \frac{2}{15} \frac{\pi^2 k_B^4}{\hbar^3 v_s^3} \frac{V}{M} T^3$$
$$\frac{C_{V,ph}}{M} = \frac{2}{15} \frac{\pi^2 k_B^4}{\hbar^3 v_s^3} \frac{V}{M} T^3$$

single crystal, for single acoustic phonon branch

phononic specific heat of ⁴He-II

thermal conductivity:

$$\kappa = \frac{1}{3} C_V v \ \ell \simeq \frac{1}{3} C_V v \ f(d) \propto T^3$$

if $\ell \simeq d$ (sample dimension, Casimir regime)

absolute value of κ depends on details: e.g., $\kappa \propto d^3$ for flow through narrow slit of width d



D. S. Greywall, Phys. Rev. B **18**, 2127 (1978); see also Phys. Rev. B **21**, 1329 (1979)

Chapter 1/RG 209

• specific heat of ⁴He revisited: temperature dependence below T_{λ}

II. 0.6 K < T < 1.2 K:

in this temperature regime the dominant excitations are rotons, number N_R of rotons increases with $T \rightarrow$ thermal activation

$$C_{V,R} \propto N_R \propto \frac{1}{\sqrt{T}} \exp\left(-\frac{\Delta_{\rm rot}}{k_{\rm B}T}\right)$$

III. 1.2 K < $T < T_{\lambda}$:

- lifetime broadening of roton states comparable to Δ_{rot}
- additional excitations
- more complicated behavior

- normal fluid density
 - within two-fluid model, the normal component can be considered as formed by the excitations out of the ground state (quasiparticles)

→ normal fluid density is determined by phonon and roton density

- temperature dependence of phonon and roton density is given by

$$\rho_{n,\text{ph}} = \frac{1}{V} \int D_{\text{ph}}(E) n_{\text{ph}}(E,T) dE \qquad n_{\text{ph}}, n_{\text{rot}} = \text{occupation probability}$$

$$\rho_{n,\text{rot}} = \frac{1}{V} \int D_{\text{rot}}(E) n_{\text{rot}}(E,T) dE \qquad D_{\text{ph}}, D_{\text{rot}} = \text{density of states}$$

after some math

$$\rho_{n,\text{ph}} = \frac{2\pi^2 k_{\text{B}}^4}{45\hbar^3 v_{\text{ph}}^5} T^4 \qquad \rho_{n,\text{rot}} = \frac{2p_0^4}{3\hbar^3} \sqrt{\frac{m_{\text{rot}}}{(2\pi)^3 k_{\text{B}}T}} \exp\left(-\frac{\Delta_{\text{rot}}}{k_{\text{B}}T}\right)$$

experimental parameter:

$$\frac{\Delta_{\rm rot}}{k_{\rm B}} = 8.61 \text{ K}$$
$$\frac{p_0}{\hbar} = 1.92 \text{ Å}^{-1}$$
$$m_{\rm rot} = 0.15 m_{\rm He}$$
$$v_{\rm ph} = 238 \text{ m/s}$$

specific heat of ⁴He revisited: temperature dependence close to T_{λ}



experiment:

second order phase transition with logarithmic singularity

theory of phase transitions:

$$C_p = a^{\pm} + b^{\pm} \frac{t^{-\alpha}}{\alpha} \left(1 - c^{\pm} t^{\delta} + \cdots \right) \quad \text{with } t = \frac{T}{T_{\lambda}} - 1$$

 $\alpha \simeq -0.0127 \pm 0.0003$ (critical exponent), $\delta = 0.529$ a^{\pm} , b^{\pm} , c^{\pm} = constants (agree well with 3D XY universality class)

note that $t^{-\alpha} = \exp(-\alpha \ln t) \simeq 1 - \alpha \ln t$, since $\alpha \ln t \ll 1$

$$\Rightarrow C_p \propto b^{\pm} \frac{t^{-\alpha}}{\alpha} = \frac{b^{\pm}}{\alpha} - b^{\pm} \ln t$$

• T_{λ} depends on pressure, i.e. on the filling height of the He container

 \rightarrow results in an experimental broadening of the cusp

presicion experiment in space shuttle

• deviations also appear, if the size of the container becomes smaller than the coherence length, which diverges at T_{λ}

- specific heat and thermal conductivity of ⁴He revisited: temperature dependence close to T_{λ}



Averaged data close to the transition. Line shows the best-fit function.



Log-log plot of thermal conductivity vs reduced temperature above the lambda point. Filled circles: data, curve: theory model.

Specific heat of liquid helium in zero gravity very near the lambda point J. A. Lipa et al., Phys. Rev. B 68, 174518 (2003)

- supplementary materia

- 2022)

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Vortices





- vortices in superfluid ⁴He
 - > in the discussion of the two-fluid model, we assumed the absence of turbulence in \mathbf{J}_s : $\Rightarrow \nabla \times \mathbf{v}_s = 0$
 - > 1941: Landau proposed to check this assumption in experiments with superfluid He in rotating containers
 - > 1949: *Onsager* predicted the appearance of vortices in rotating superfluid He
 - > 1953: *Feynman* noted that circulation in superfluid ⁴He should be quantized
 - > 1961: first experimental proof of quantization by Vinen
 - → quantized vortices in superfluid ⁴He as in superconductors
 - → difference: superfluid ⁴He is not charged, neutral circulation

- vortices nomenclature and some definitions
 - ideal vortex in z-direction at position $\mathbf{r} = 0$: $\nabla \times \mathbf{v}(\mathbf{r}) = \Gamma \cdot \delta(x) \cdot \delta(y)$



• description of superfluid component by macroscopic wave function

as done in superconductivity for electronic system: charged superfluid

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r})e^{i\theta(\mathbf{r})}, \qquad |\psi_0(\mathbf{r})|^2 = n_0(\mathbf{r}), \qquad N_0 = \int |\psi_0(\mathbf{r})|^2 \,\mathrm{d}^3 r \qquad n_0 = \frac{N_0}{V} = \text{particular}$$

 $n_0 = \frac{N_0}{V}$ = particle density in condensate

- phase is related to velocity $\mathbf{v}_s(\mathbf{r})$ of superfluid:

$$\mathbf{J}_{\rho}(\mathbf{r}) = n_0 \underbrace{\frac{\hbar}{m_{\text{He}}} \nabla \theta(\mathbf{r})}_{\mathbf{v}_s(\mathbf{r})} = n_0 \mathbf{v}_s(\mathbf{r})$$

current density – phase relation (as in superconductivity) \mathbf{v}_s = superfluid velocity, n_0 = superfluid density

analogy to superconductors

$$\mathbf{J}_{s}(\mathbf{r}) = n_{s}q_{s}\left[\underbrace{\frac{\hbar}{m_{s}}\nabla\theta(\mathbf{r}) - \frac{q_{s}}{m_{s}}\mathbf{A}(\mathbf{r})}_{\mathbf{v}_{s}}\right] \qquad \mathbf{v}_{s}(\mathbf{r}) = \frac{\hbar}{m_{s}}\nabla\theta(\mathbf{r}) - \frac{q_{s}}{m_{s}}\mathbf{A}(\mathbf{r})$$
$$\mathbf{v}_{s}(\mathbf{r}) = \frac{\hbar}{m_{\mathrm{He}}}\nabla\theta(\mathbf{r})$$

superfluid He is uncharged: $q_s = 0$

circulation of superfluid component

$$\Gamma = \oint_{\mathcal{S}} \mathbf{v}_{\mathbf{s}}(\mathbf{r}) \cdot d\mathbf{r} = \frac{\hbar}{m_{\text{He}}} \oint_{\underbrace{\mathcal{S}}} \nabla \theta(\mathbf{r}) \cdot d\mathbf{r} = \frac{\hbar}{m_{\text{He}}} \cdot 2\pi \, n = \frac{h}{\underbrace{m_{\text{He}}}_{\kappa}} \cdot n$$

 \rightarrow circulation is quantized in units of $h/m_{\text{He}} = \kappa$ (vorticity)

 \rightarrow quantum number *n* corresponds to topological winding number

(counts the 2π windings along a closed contour)

- generation of vortices by rotation:

angular frequency $\Omega = \Gamma/A \iff \text{magnetic field } B = \Phi/A$ Coriolis force $\mathbf{F}_{cor} = 2m_{He}\mathbf{v}_s \times \mathbf{\Omega} \iff \text{Lorentz force } \mathbf{F}_{L} = q_s \mathbf{v}_s \times \mathbf{B}$

 $2m_{\rm He}\Omega \iff q_s B$

consequences of macroscopic quantum description of superfluid

- superfluid velocity:
$$\mathbf{v}_{s}(\mathbf{r}) = \frac{\hbar}{m_{\text{He}}} \nabla \theta(\mathbf{r}) \Rightarrow \nabla \times \mathbf{v}_{s}(\mathbf{r}) = \frac{\hbar}{m_{\text{He}}} \underbrace{\nabla \times \nabla \theta(\mathbf{r})}_{=0} = \mathbf{0}$$

- experimental observation:
 - \succ if we rotate a cylinder filled with superfluid ⁴He at angular frequency ω , the surface of the superfluid does not stay flat but shows curvature due to centrifugal force

parabolic radial height profile: $z = \frac{\omega^2}{2a} r^2$

- apparent contradiction is caused by the presence of vortices
- $\triangleright \nabla \times \mathbf{v_s}(\mathbf{r}) = 0$ is satisfied apart inside the vortex core at r = 0: macroscopic wave function $|\psi_0(0)|^2 = 0$, phase θ is not defined, superfluid density $J_s = n_0 v_s = 0$





www.wmi.badw.de

- some estimates
 - magnitude of the superfluid velocity (in circular vortex)

$$\Gamma = \frac{\hbar}{m_{\rm He}} \ n = 2\pi r \ v_{\varphi}$$



- diameter $d_{
m vc}$ of vortex core

for n = 1 and v_{φ} = critical velocity for roton formation

– energy of vortex is proportional to v_{φ}^2

$$E_{\rm v} \approx E_{\rm kin} \propto \kappa^2 \propto n^2$$

→ it is more favorable to generate two vortices with n = 1 instead of a single vortex with n = 2

- are there vortices in thermal equilibrium ?
 - excitation energy $\approx E_{kin}$ should be as small as possible:
 - \rightarrow minimum v_s $\rightarrow n = 1$ \rightarrow minimum length \rightarrow vortex rings \rightarrow smallest ring \rightarrow atomic dimension



vortex still macroscopic object

 $\rightarrow E_V \gg k_{\rm B}T$ except for $T \sim T_{\lambda}$

 \rightarrow momentum is large $\rightarrow v_L = E / p$ is small for vortex rings

- critical velocity v_L is determined by excitation of vortex rings

I.4.2 Experimental Study of Vortices



first experiments by Vinen in 1961

The detection of a single quantum of circulation in liquid helium II, W.F. Vinen, *Proc. Roy. Soc. (Lond.)* A **260**,218 (1961).



I.4.2 Experimental Study of Vortices

- what is the density of vortices inside the container ?
 - circulation at the edge of the container with radius R:

$$\Gamma = \oint_{S} \mathbf{v}(\mathbf{r}) \cdot d\mathbf{r} = 2\pi R \ v(R) = 2\pi R \ \Omega R = 2\pi R^{2} \Omega$$



- circulation must be equal to number of vortices $N_V \times$ vorticity $\kappa \times$ area πR^2

 $\Gamma = N_V \kappa \pi R^2 = 2\pi R^2 \Omega$

$$N_V = \frac{2\Omega}{\kappa} = \frac{2m_{\rm He}\Omega}{h} = \frac{m_{\rm He}\Omega}{\pi\hbar} \qquad \qquad N_V \simeq \frac{20}{\rm mm^2} \times \Omega \ [\rm Hz \]$$

I.4.2 Experimental Study of Vortices

rotating cryostats





A Compact Rotating 1K Cryostat for ⁴He Studies Takahiko Makiuchi, Satoshi Murakawa & Keiya Shirahama J. Low Temp. Phys. **187**, 633-638 (2017)


• imaging of vortices in superfluid ⁴He

- > He is covered by electrons
- electrons are trapped in vortex cores
- on applying an electric field, electrons are extracted to fluorescent screen



E.J. Yarmchuk, M.J.V. Gordon, R.E. Packard, Phys. Rev. Lett. <u>43</u>, 214 (1979) E.J. Yarmchuk, R.E. Packard, J. Low Temp. Phys. <u>46</u>, 479 (1982)

pinning of vortices at bottom of container

• imaging of vortices in a Bose-Einstein condensate of Na atoms

Formation and decay of a vortex lattice. The condensate was rotated for 400 ms and then equilibrated in the stationary magnetic trap for various hold times. (A) 25 ms, (**B**) 100 ms, (**C**) 200 ms, (**D**) 500 ms, (E) 1 s, (F) 5 s, (G) 10 s, and (H) 40 s. The decreasing size of the cloud in (E) to (H) reßects a decrease in atom number due to inelastic collisions. The field of view is about 1 mm by 1.15 mm.



Observation of Vortex Lattices in Bose-Einstein Condensates W. Ketterle et al., Science **292**, 476 (2001)



imaging of vortices



A sheet of laser light illuminates frozen hydrogen particles trapped on vortex cores, which are then captured on video.

 $\odot \odot \odot \odot$ \odot $\odot \odot \odot \odot$ (\bullet) $\odot \odot \odot \odot \odot$ \odot () \odot \odot \odot (\bullet) (\bullet) (\bullet) (\bullet) \odot \odot \odot (\bullet) (\bullet) (\bullet) \odot (\bullet) (\bullet) $\odot \odot \odot \odot$ \odot (\bullet) (\bullet) (\bullet) \odot (\bullet) \odot \odot (\bullet) (\bullet) (\bullet) \odot (\bullet) (\bullet) (\bullet) (\bullet) (\bullet) ۲ \odot

Quantized vortices arrange themselves in a triangular lattice pattern.



A still image captures the vortex lattice along the axis of rotation in a vat of superfluid helium. A perfect lattice is not observed due to waves and other boundary effects.

https://engage.aps.org/dfd/resources/virtual-pressroom/2009-pressroom/language-papers-2009/tornadoes

generation of persistent current

- rotate a normal fluid at $T > T_{\lambda}$
- cool down the rotating normal fluid to $T < T_{\lambda} \rightarrow$ the rotation is frozen in and does not decay

• generation of circulation jumps or phase slip events

- start with a non-rotating fluid at $T < T_{\lambda}$: $\kappa = 0$, n = 0
- rotate the cylindrical vessel containing the fluid:
 - ➔ normal fluid rotates at the speed of the vessel
 - ➔ superfluid stays in rest
- reduce the temperature:



- ➔ more and more particles of the normal fluid enter the superfluid
- → the lost angular momentum is transferred to the superfluid, which starts to rotate
- \rightarrow the circulations and the vorticity κ do not change continuously but in jumps of $h/m_{\rm He}$
- \rightarrow jumps are associated with additional vortex corresponding to phase change of 2π called phase slip
- \rightarrow phase slips correspond to transition between two quantum states with different quantum number n



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• basic properties of ³He

⁴ He	p⁺↑ p⁺↓	nî n↓	e⁻↑ e⁻↓	boson
³ He	p⁺↑ p⁺↓	nî	e⁻↑ e⁻↓	fermion

- ³He has spin $\frac{1}{2}$ **Fermion**
- fluid ³He: *interacting Fermi gas*
- → Fermi liquid (*ideal non-interacting Fermi gas with finite interaction*)
 → theoretical description by Landau (1956-1958)
 - L.D. Landau, Soviet. Phys. JETP <u>3</u>, 920 (1957) L.D. Landau, Soviet. Phys. JETP <u>5</u>, 101 (1957)

- solid ³He shows nuclear magnetism
 - → due to different quantum statistics:

liquid ³He has completely different properties than liquid ⁴He

- **first approximation:** description by an *ideal Fermi gas* (*non-interacting Fermions*)
 - Fermi-Dirac distribution:







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$$N = \int D(\varepsilon) f(\varepsilon) \, \mathrm{d}\varepsilon \qquad \qquad \frac{\mathrm{d}N}{\mathrm{d}\varepsilon} = D(\varepsilon) f(\varepsilon)$$

• ideal (non-interacting) Fermi gas

$$\varepsilon_{\rm F} = \frac{\hbar^2 k_{\rm F}^2}{2m} = \frac{\hbar^2}{2m} (3\pi^3 n)^{2/3}$$
Fermi energy
$$T_{\rm F} = \varepsilon_{\rm F}/k_{\rm B}$$
Fermi temperature
$$\lambda_{\rm F} = 2\pi/k_{\rm F}$$
Fermi wavelength
$$v_{\rm F} = \frac{p_{\rm F}}{m} = \frac{\hbar k_{\rm F}}{m}$$
Fermi velocity

N = particle numbern = particle density [1/m³]

 $m = m_{
m He}$ is large ightarrow expected Fermi temperature (energy) is small: $T_{
m F} \simeq 4.2$ K

comparison to electron gas in metal:

electrons in metals:

 $n \approx 10^{23} \text{ cm}^{-3} \text{ is large}, m = m_e \text{ is small}$ $\rightarrow T_F \approx 10^5 \text{ K is large}$

³He:

 $n \approx 10^{22} \text{ cm}^{-3} \text{ is smaller}, m = m_{\text{He}} \text{ is large}$ $\rightarrow T_{\text{F}} \approx \text{few K is small}$

$$T_{\rm F} = \frac{\hbar^2 k_{\rm F}^2}{2m} = \frac{\hbar^2}{2mk_{\rm B}} (3\pi^3 n)^{2/3}$$

• ideal (non-interacting) Fermi gas: specific heat



• ideal (non-interacting) Fermi gas: specific heat



- interacting Fermi gas → Fermi liquid (Landau)
- increased effective mass m^{\star}

→ smaller Fermi temperature $T_{\rm F} \propto 1/m^*$ $m^*/m_{\rm He} \simeq 2.8 \ (@\ p = 1\ bar)$ $\simeq 5.5 \ (@\ p = 30\ bar)$



- additional contribution due to spin fluctuations (paramagnons)
 - \rightarrow strong repulsive interaction at short distance \rightarrow antisymmetric orbital wavefunction
 - \rightarrow symmetric spin wavefunction \rightarrow parallel orientation of neighboring spins

• intuitive argument for increased effective mass:



interaction causes "backflow" of particles

 \rightarrow increased effective mass m^*

→ reduced Fermi temperature $T_{\rm F} \propto 1/m^{\star}$

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- magnetic susceptibility: nuclear spin $I = \frac{1}{2}$ determines magnetic properties
 - $T > T_F$: non-degenerate Fermi gas \rightarrow magnetic susceptibility follows Curie law: $\chi \propto C/T$

- $T < T_F$: degenerate Fermi gas \rightarrow temperature independent Pauli spin susceptibility (only fraction T/T_F contributes)



- transport properties
 - description by *kinetic gas theory*:

$$\rightarrow$$
 viscosity: $\eta = \frac{1}{3}\rho \nu \ell$ $(\ell = \text{mean fee path})$ \rightarrow diffusion coefficient: $D = \frac{1}{3}\nu \ell$ (self-diffusion) \rightarrow thermal conductivity: $\kappa = \frac{1}{3}C_V \nu \ell$

- classical gas: $v_{\rm th}$ = thermal velocity $v_{\rm th} = \sqrt{2k_{\rm B}T/m}$

(Maxwell-Boltzmann statistics)

– Fermi gas: $v_{\rm F}$ = Fermi velocity $v_{\rm F} = \frac{\hbar}{m} (3\pi^3 n)^{1/3}$ (Fermi statistics)

– Fermi gas, with
$$\ell = v_{
m F} au$$

$$\eta = \frac{1}{3}\rho\tau v_F^2 \propto \frac{1}{T^2} \qquad D = \frac{1}{3}\tau v_F^2 \propto \frac{1}{T^2} \qquad \kappa = \frac{1}{3}C_V \tau v_F^2 \propto \frac{1}{T}$$

 $\tau^{-1} \propto \left(\frac{T}{T_{\rm F}}\right)^2$ particle-particle scattering rate





BAYERISCHE AKADEMIE DER WISSENSCHAFTEN Technische Universität München

Superconductivity and Low Temperature Physics II



Lecture No. 7 23 June 2022

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• comparison of properties of liquid ³He with those of ideal (non-interacting) Fermi gas

	³ He	Fermi Gas	ratio	
$C_V^{\rm mol}/N_{\rm A}k_{\rm B}T$	2.78	1.0	2.78	
$v_{\rm F}$ (m/s)	56	157	2.80	
$\chi/\mu_0\mu_{ m eff}^2$ (Jm ³) ⁻¹	3.3·10 ⁵¹	3.6 ∙10 ⁵⁰	9.2	

significant deviations due to finite interactions \rightarrow Landau Fermi liquid \rightarrow effective mass

mole volume: 36.84 cm³ @ p = 0 bar, T = 0 K $\rightarrow n = 1.63 \times 10^{28}$ m⁻³ mass: $m_{3\text{He}} = 3.016$ amu = 5.006×10^{-27} kg

- comparison of phase diagrams of ³He and ⁴He
 - ⁴He mostly hcp, small region with bcc, at high *T*: fcc
 - ³He shows bcc-hcp transition at 100 bar, at high *T*: fcc
 - ³He shows minimum in melting curve at T = 0.32 K
 - → can be used for cooling of ³He Pomerantchuk effect

Isaak Jakowlewitsch Pomerantschuk (Исаак Яковлевич Померанчук; geb: 20. Mai 1913 in Warschau; gest: 14. Juli 1966 in Moskau)





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Clausius-Clapeyron equation:

$$\frac{\partial p_m}{\partial T}\Big|_{\text{melting}} = \frac{S_{\text{liq}} - S_{\text{sol}}}{V_{\text{liq}} - V_{\text{sol}}} = \frac{\Delta S_m}{\Delta V_m} = \frac{\Delta Q_m}{\Delta V_m T}$$

and $V_{\rm liq} > V_{\rm sol}$

- for T < 0.32 K: $\frac{\partial p_m}{\partial T}\Big|_{\text{melting}} < 0 \implies S_{\text{liq}} < S_{\text{sol}} \Rightarrow \text{disorder larger in solid than in liquid phase ??}$
- explanation:
 - → solid phase: atoms are ordered,
 - \rightarrow spins are disordered and determine entropy: $S_{\text{solid}} = R \ln 2$
 - at low T: antiparallel ordering of spins, S decreases towards zero
 - \rightarrow liquid phase: atoms are spatially disordered, but ordering in k-space (Fermi liquid)
 - \rightarrow entropy of Fermi liquid:



Pomerantchuk cooling



- precooling to $T < T_{\min}$
- − adiabatic compression
 → solidification and cooling
- − lowest T: ≈ 1.5 mK
 - ➔ limitation due to antiparallel spin ordering in solid ³He



Pomerantchuk cooling



Richardson, Nobel Prize Lecture (1996)

 $\frac{\Delta V}{V} \simeq 5 \%$

volume change for complete conversion of liquid to solid

Pomeranchuk's suggestion for cooling a melting mixture of ³He:

The solid phase has a higher entropy than the liquid at low temperatures. As the liquid-solid mixture is compressed, heat is removed from the liquid phase as solid crystallites form. The fractional change of volume required to completely convert liquid into solid is approximately 5%. Unlike melting water, the solid phase forms at the hottest part of the container.

• solid ³He: single crystals

110 computer-generated shape of a bcc crystal presented together with an elementary patch of a crystal habit where the facets are labeled with Miller indices.

H. Alles et al., PNAS 99, 1796-1800 (2002)



Sequence of interferograms of a growing ³He crystal at T = 0.55 mK. The dashed white lines outline the identified facets marked with Miller indices.

I.5.3 Superfluid ³He

- history of superfluid ³He
 - *initial believe*: no superfluid ³He due to Pauli's exclusion principle for fermions
 - \rightarrow no Bose-Einstein condensation of ³He
 - after development of BCS theory: pairing of ³He atoms to Cooper pairs ??
 - \rightarrow problem: liquid ³He is system of strongly interacting particles
 - → formation of Cooper pairs out of "naked" ³He atoms not possible (nature of exchange boson ??)
 - ightarrow Landau: weakly interacting quasiparticles in Fermi liquid
 - **1963**: critical pairing temperature of about 100 mK was expected
 - **1971:** discovery of superfluid ³He at T < 2.7 mK by **Osheroff**, **Richardson** and **Lee** (used Pomerantschuk cooling)

(Nobel Prize in Physics 1996 "for their discovery of superfluid ³He")

D.D. Osheroff, R.C. Richardson, D.M. Lee, Phys. Rev. Lett. **<u>28</u>**, 855 (1972), D.D. Osheroff, W.J. Gully, R.C. Richardson, D.M. Lee, Phys. Rev. Lett. <u>**29**</u>, 920 (1972)

- *initially:* two superfluid phases A and B
 later: three phases (in magnetic field additional A₁ phase)
- experimental result: pairs have spin S = 1, spin triplet pairs
 - \rightarrow pairs with S = 1 must have L = 1 (see below)
 - → occupation probability for same position is negligible (reduction of short length repulsion)



• discovery of superfluid ³He in 1971









David M. Lee, Cornell University, Ithaca, New York, USA

Robert C. Richardson, Cornell University, Ithaca, New York, USA

The Nobel Prize in Physics 1996

"for their discovery of superfluidity in helium-3"

I.5.3 Superfluid ³He

• discovery of superfluid ³He in 1971





- cool down of ³He via Pomeranchuk effect
- observation of melting curve
 - \rightarrow anomalies give hint to phase transitions

source: Nobel Prize Lecture Lee/Osheroff (1996)

I.5.3 Superfluid ³He: phase diagram for B = 0



big difference in value of T_{sf} compared to ⁴He

- normal/superfluid transition is dominated by quantum effects
- quantum statistics matters!!(bosons vs. fermions)
- nature of superfluid phase in
 ⁴He and ³He is different

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- phase diagram of ³He: note the logarithmic temperature scale. There are *two superfluid phases of ³He, A and B*.
- the line within the solid phase indicates a transition between spin-ordered and spin disordered structures (at low and high temperatures, respectively).

I.5.3 Superfluid ³He: phase diagram for B = 0

 $T_A = 2.79 \text{ mK}$ $T_B = 2.16 \text{ mK}$ paramagnetic bbc solid 40 -afm bbc solid $p = 34.4 \, bar$ pressure increases pairing interaction sf ³He-A 1. order 30 transition (bar) superfluid ³He-B 20 polycritical point (PCP) Q 21.5 bar, 2.56 mK 2. order transition 10 2. ant normal liquid ³He linear T scale !!! 0 0.8 1.2 1.6 2.0 2.4 2.8 (mK)

WM

I.5.3 Superfluid ³He: specific heat



- T_c : 2. order phase transition \rightarrow jump of C_p as for superconductor • T_{AB} : 1. order phase transition \rightarrow small change of temperature dependence
 - → small change of temperature dependence of C_p → hysteresis, latent heat
- PCP: first and second order phase transition merge

Superfluid ³He: proof of superfluidity **I.5.3**

- use of *vibrating wire*, measurement of quality factor $v / \Delta v$ $\Delta v (Hz)$ -Δν viscosity changes 10 by 5 orders of magnitude ν 10 normal fluid 10 freezes out 10
- other experiments:
 - - \rightarrow persistent flow experiments: viscosity of B phase changes at least by 12 orders of magnitude - persistent flow in A phase decays slowly (appearence of textures) - small critical velocity: 1 to 100 mm/s

0.12

0.16

0.2

0.3

0.6

7 (mK)

Persistent-Current Experiments on Superfluid He 3 - B and He 3 - A J. P. Pekola, J. T. Simola, K. K. Nummila, O. V. Lounasmaa, R. E. Packard, Phys. Rev. Lett. 53, 70 (1984)

- 2022)

I.5.3 Superfluid ³He: pairing

- ³He is strongly interacting Fermi liquid (different to electrons in metals)
 - \rightarrow exchange interaction favors parallel spin alignment
 - \rightarrow Fermi statistics favors anti-parallel spin orientation
- ³He forms Cooper pairs with spin S = 1 (*spin triplet pairs*) in contrast to electrons in metals: S = 0 (*spin singlet pairs pairs*)
- note the general requirement: *antisymmetric pair wave function* for fermions

symmetric spin wave function \rightarrow antisymmetric orbital wave function (L = 1,3,...)antisymmetric spin wave function \rightarrow symmetric orbital wave function (L = 0,2,...)

examples: (i) Cooper pairs in metallic superconductors $(L = 0, S = 0) \rightarrow s$ -wave, spin-singlet pairs (ii) Cooper pairs in high T_c superconductors $(L = 2, S = 0) \rightarrow d$ -wave, spin-singlet pairs (iii) Cooper pairs in superfluid ³He $(L = 1, S = 1) \rightarrow p$ -wave, spin-triplet pairs



p-type orbital wave function minimizes hard core repulsion

I.5.3 Superfluid ³He: in $B \neq 0$

spin triplet pairs have magnetic moment \rightarrow phase diagram depends on magnetic field



I.5.3 Superfluid ³He: in $B \neq 0$

• specific heat





W.P. Halperin et al., Phys. Rev. B**13**, 2124 (1974)

I.5.3 Superfluid ³He: in $B \neq 0$

• phase diagram of ³He





source: http://ltl.tkk.fi/research/theory/helium.html

I.5.3 Superfluid ³He: Fermi liquid description

description of liquid ³He by a Fermi liquid (interacting Fermi gas)

Landau: what happens, if we increase the interaction strength in a non-interacting systems continuously?

 \succ non-interacting system: addition/removal of one particle with momentum **k** and spin σ to ground state $|\Psi_0\rangle$

$$|\widetilde{\Psi}_{\mathbf{k}\sigma}\rangle = c_{\mathbf{k}\sigma}^{\dagger}|\widetilde{\Psi}_{0}\rangle \qquad \qquad \widetilde{\varepsilon}_{\mathbf{k}} = \frac{\hbar^{2}(k^{2} - k_{\mathrm{F}}^{2})}{2m} \qquad \qquad f_{\mathbf{k}\sigma}(T=0) = \begin{cases} 0 & \text{for } k < k_{\mathrm{F}} \\ 1 & \text{for } k > k_{\mathrm{F}} \end{cases}$$

interacting system: addition/removal of one particle changes energies of all other particles due to interaction Landau's argument of *adiabatic continuity*: quasiparticle energy has similar k-dependence: $\varepsilon_{\mathbf{k}} = \frac{\hbar^2 (k^2 - k_F^2)}{2m^*}$ $m^* = \text{effective mass}$

for k close to
$$k_{\rm F}$$
: $\varepsilon_{\bf k} = \frac{\partial \varepsilon_{\bf k}}{\partial k} \bigg|_{k=k_{\rm F}} (|{\bf k}| - k_{\rm F}) = \frac{\hbar k_{\rm F}}{m^*} (|{\bf k}| - k_{\rm F})$

 $f_{k\sigma}(T = 0)$ has shows discontinuity, but height of the discontinuity is reduced to smaller value Z < 1



- supplementary material

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I.5.3 Superfluid ³He: Fermi liquid description

description of liquid ³He by a Fermi liquid (interacting Fermi gas)

➤ total energy:
$$E = \underbrace{E_0}_{\text{ground}} + \underbrace{\sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} n_{\mathbf{k}\sigma}}_{\text{quasiparticle}} + \underbrace{\frac{1}{2} \sum_{\mathbf{k}\sigma, \mathbf{k}'\sigma'} \eta(\mathbf{k}\sigma, \mathbf{k}'\sigma') n_{\mathbf{k}\sigma} n_{\mathbf{k}'\sigma'}}_{\text{interaction energy}}$$

★ two particle energy: $\varepsilon_k + \varepsilon_{k'} + \eta(k\sigma, k'\sigma') \neq \text{ sum of single particle energies } \varepsilon_k, \varepsilon_{k'}$

describes effective interaction between two quasiparticles: is usually split in parts $\eta_1(\mathbf{k}, \mathbf{k}')$ and $\eta_2(\mathbf{k}, \mathbf{k}')$ for singlet and triplet contribution

→ at low *T*: $|\mathbf{k}|, |\mathbf{k}'| \simeq k_F$ and due to spherical symmetry $\eta(\mathbf{k}, \mathbf{k}') \propto \mathbf{k} \cdot \mathbf{k}' = k_F^2 \cos \theta$ → we can express $\eta_1(\mathbf{k}, \mathbf{k}')$ and $\eta_2(\mathbf{k}, \mathbf{k}')$ by Legendre polynoms $P_\ell(\cos \theta)$

$$g(\varepsilon_{\rm F})\eta_1(\mathbf{k},\mathbf{k}') = \sum_{\ell} F_{\ell} P_{\ell}(\cos\theta) \qquad g(\varepsilon_{\rm F})\eta_2(\mathbf{k},\mathbf{k}') = \sum_{\ell} Z_{\ell} P_{\ell}(\cos\theta)$$
$$g(\varepsilon_{\rm F}) = \text{density of states (states per energy interval)} \Rightarrow F_{\ell}, Z_{\ell} \text{ are dimensionless}$$

Theory by Leggett: \succ F_0 , F_1 are large and positive $\rightarrow m^* = m(1 + F_1/3)$ with $F_1 \simeq 5.4$ (increases with pressure)

→
$$Z_0 \simeq -3$$
 and Z_1 is small → magnetic susceptibility $\chi = \frac{m^*}{m} \frac{\chi_0}{1 + (Z_0/4)}$ with $Z_0 \simeq -2.78$
→ $\chi \simeq 9.2 \chi_0$: He is close to ferromagnetic instability


I.5.3 Superfluid ³He: pairing interaction

- interaction of ³He atoms due to van der Waals potential $V(\mathbf{r}_i - \mathbf{r}_j) = V(\mathbf{r})$

$$V(\mathbf{k}, \mathbf{k}') = \int e^{-\iota(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} V(\mathbf{r}) d^3r$$

pairing potential in *k*-space

➤ at low T: |k|, |k'| ~ k_F and due to spherical symmetry V(k, k') ~ k · k' = k_F² cos θ
→ we can express V(k, k') by Legendre polynoms P_ℓ(cos θ)

$$V(\mathbf{k}, \mathbf{k}') = \sum_{\ell} \frac{2\ell + 1}{2} V_{\ell} P_{\ell}(\cos \theta) \qquad \text{with} \quad V_{\ell} = \frac{1}{4\pi} \int V(\widehat{\mathbf{n}}(\theta, \varphi), \widehat{e}_{z}) P_{\ell}(\cos \theta) \sin \theta \, d\theta \, d\varphi$$
$$\frac{2\ell + 1}{2} = \int P_{\ell}^{2}(\cos \theta) \sin \theta \, d\theta \quad (\text{normalization})$$

- ➤ calculation of V_ℓ for van der Waals potential (e.g. by Leggett 1975): $V_0 = \text{strongly repulsive}, V_1, V_2 = \text{weakly attractive} \Rightarrow \text{cannot explain pairing in superfluid ³He}$
- attractive interaction results from exchange of virtual spin fluctuations

one ³He atom polarizes neighboring nuclear spins which then result in an effective attractive interaction for 2^{nd 3}He atom

$$V(\mathbf{k}, \mathbf{k}') \propto \frac{1}{g(\varepsilon_{\rm F})} \frac{\chi_0}{1 + (Z_0/4)} \, \hat{\mathbf{s}}_{\mathbf{k}} \cdot \hat{\mathbf{s}}_{\mathbf{k}'}$$

(Leggett 1975)

$$\hat{\mathbf{s}}_{\mathbf{k}} \cdot \hat{\mathbf{s}}_{\mathbf{k}'} = +1/4$$
 for triplet
 $\hat{\mathbf{s}}_{\mathbf{k}} \cdot \hat{\mathbf{s}}_{\mathbf{k}'} = -3/4$ for singlet

• starting point: BCS Hamiltonian

formalism of second quantization is used (>1927, Dirac, Fock, Jordan et al.)

BCS Hamiltonian for N interacting electrons



- symmetry of the pair wavefunction
 - important: pair consistst of two fermions -> total wavefunction must be antisymmetric: minus sign for particle exchange

$$\Psi(\mathbf{r}_{1}, \boldsymbol{\sigma}_{1}, \mathbf{r}_{2}, \boldsymbol{\sigma}_{2}) = \frac{1}{\sqrt{V}} e^{i \mathbf{K}_{s} \cdot \mathbf{R}_{s}} f(\mathbf{q}, \mathbf{r}) \chi(\boldsymbol{\sigma}_{1}, \boldsymbol{\sigma}_{2}) = -\Psi(\mathbf{r}_{2}, \boldsymbol{\sigma}_{2}, \mathbf{r}_{1}, \boldsymbol{\sigma}_{1}) \qquad \mathbf{R}_{s} = (\mathbf{r}_{1} + \mathbf{r}_{2})/2 \\ \mathbf{r} = (\mathbf{r}_{1} - \mathbf{r}_{2}) \\ \mathbf{r} = (\mathbf{r}_{1} - \mathbf{r}_{2}) \\ \mathbf{K}_{s} = (\mathbf{k} + \mathbf{k}')/2 \\ \mathbf{w} \text{ assume } \mathbf{K}_{s} = 0 \quad \text{part} \quad \text{part} \qquad \mathbf{q} = (\mathbf{k} - \mathbf{k}') \end{cases}$$

possible *spin wavefunctions* $\chi(\sigma_1, \sigma_2)$ for electron pairs

$$S = \begin{cases} 0 \quad m_s = 0 \qquad \chi^a = \frac{1}{\sqrt{2}} (\uparrow \downarrow - \downarrow \uparrow) \qquad \rightarrow \text{singlet pairing,} \quad \text{antisymmetric spin wavefunction} \\ symmetric orbital function: \\ L = 0, 2, \dots (s, d, \dots) \end{cases}$$

$$1 \quad m_s = \begin{cases} -1 \quad \chi^s = \downarrow \downarrow \\ 0 \quad \chi^s = \frac{1}{\sqrt{2}} (\uparrow \downarrow + \downarrow \uparrow) \\ +1 \quad \chi^s = \uparrow \uparrow \end{cases} \qquad \rightarrow \text{triplet pairing,} \quad \text{symmetric spin wavefunction} \\ antisymmetric orbital function: \\ L = 1, 3, \dots (p, f, \dots) \end{cases}$$

_

• BCS mean-field approximation

pairing amplitude:

$$\hat{c}_{-\mathbf{k}\alpha}\hat{c}_{\mathbf{k}\beta} = \underbrace{\left\langle \hat{c}_{-\mathbf{k}\alpha}\hat{c}_{\mathbf{k}\beta} \right\rangle}_{g_{\alpha\beta}(\mathbf{k})} + \underbrace{\left\{ \hat{c}_{-\mathbf{k}\alpha}\hat{c}_{\mathbf{k}\beta} - \left\langle \hat{c}_{-\mathbf{k}\alpha}\hat{c}_{\mathbf{k}\beta} \right\rangle}_{\delta g_{\alpha\beta}(\mathbf{k})} - \left\langle \hat{c}_{\mathbf{k}\alpha}^{\dagger}\hat{c}_{-\mathbf{k}\beta}^{\dagger} \right\rangle}_{\delta g_{\alpha\beta}(\mathbf{k})} + \underbrace{\left\{ \hat{c}_{\mathbf{k}\alpha}\hat{c}_{-\mathbf{k}\beta}^{\dagger} \right\}}_{g_{\alpha\beta}^{*}(\mathbf{k})} + \underbrace{\left\{ \hat{c}_{\mathbf{k}\alpha}\hat{c}_{-\mathbf{k}\beta}^{\dagger} - \left\langle \hat{c}_{\mathbf{k}\alpha}^{\dagger}\hat{c}_{-\mathbf{k}\beta}^{\dagger} \right\rangle}_{\delta g_{\alpha\beta}^{*}(\mathbf{k})} - \left\langle \hat{c}_{\mathbf{k}\alpha}\hat{c}_{-\mathbf{k}\beta}^{\dagger} \right\rangle} = \underbrace{\left\{ \hat{c}_{\mathbf{k}\alpha}\hat{c}_{\mathbf{k}\beta}^{\dagger} \right\}}_{g_{\alpha\beta}^{*}(\mathbf{k})} + \underbrace{\left\{ \hat{c}_{\mathbf{k}\alpha}\hat{c}_{-\mathbf{k}\beta}^{\dagger} \right\}}_{\delta g_{\alpha\beta}^{*}(\mathbf{k})} - \left\langle \hat{c}_{\mathbf{k}\alpha}\hat{c}_{-\mathbf{k}\beta}^{\dagger} \right\rangle}_{g_{\alpha\beta}^{*}(\mathbf{k})} = \underbrace{\left\{ \hat{c}_{\mathbf{k}\alpha}\hat{c}_{-\mathbf{k}\beta}^{\dagger} \right\}}_{g_{\alpha\beta}^{*}(\mathbf{k})} =$$

- make use of pairing potential
$$\Delta_{\alpha\beta}(\mathbf{k}) \equiv -\sum_{\mathbf{k}',\gamma,\delta} V_{\alpha\beta\gamma\delta}(\mathbf{k},\mathbf{k}') g_{\alpha\beta}(\mathbf{k}')$$
four component function due to two values α,β of spin spin structure orbital structure

$$\mathcal{H}_{BCS} - \mathcal{N}\mu = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu) c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - \sum_{\mathbf{k},\alpha,\beta} \left[\Delta_{\alpha\beta}(\mathbf{k}) \hat{c}^{\dagger}_{\mathbf{k}\alpha} \hat{c}^{\dagger}_{-\mathbf{k}\beta} + \Delta^{*}_{\alpha\beta}(\mathbf{k}) \hat{c}_{\mathbf{k}\alpha} \hat{c}_{-\mathbf{k}\beta} \right]$$

- with $\alpha, \beta = \uparrow, \downarrow$: two fermions with $\mathbf{s} = \frac{1}{2}$ and $\alpha, \beta = m_s = \uparrow, \downarrow$

$$g(\mathbf{k}) \equiv \begin{pmatrix} \langle \hat{c}_{-\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}\uparrow} \rangle & \langle \hat{c}_{-\mathbf{k}\uparrow} \hat{c}_{\mathbf{k}\downarrow} \rangle \\ \langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \rangle & \langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\downarrow} \rangle \end{pmatrix} \qquad g^*(\mathbf{k}) \equiv \begin{pmatrix} \langle \hat{c}_{-\mathbf{k}\uparrow}^{\dagger} \hat{c}_{\mathbf{k}\uparrow}^{\dagger} \rangle & \langle \hat{c}_{-\mathbf{k}\uparrow}^{\dagger} \hat{c}_{\mathbf{k}\downarrow}^{\dagger} \rangle \\ \langle \hat{c}_{-\mathbf{k}\downarrow}^{\dagger} \hat{c}_{\mathbf{k}\uparrow}^{\dagger} \rangle & \langle \hat{c}_{-\mathbf{k}\downarrow}^{\dagger} \hat{c}_{\mathbf{k}\downarrow}^{\dagger} \rangle \end{pmatrix} \qquad \Delta(\mathbf{k}) = \begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} \qquad \Delta^*(\mathbf{k}) = \begin{pmatrix} \Delta_{\uparrow\uparrow}^*(\mathbf{k}) & \Delta_{\uparrow\downarrow}^*(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}^*(\mathbf{k}) & \Delta_{\downarrow\downarrow}^*(\mathbf{k}) \end{pmatrix}$$

4 components covering all spin orientations before and after interaction

Superfluid ³He: superfluid phases **I.5.3**

diagonalization of mean-field Hamiltonian by Bogoliubov transformation

(Nambu, 1962)



- 4 x 4 matrix equation instead of 2 x 2 matrix equation for spin singlet superconductor
- diagonalization by suitable Bogoliubov transformation
- \blacktriangleright two positive eigenvalues $E_{\mathbf{k}n}$ (n = 1,2) and two negative eigenvalues $-E_{\mathbf{k}n}$
- general gap equation allows for both spin singlet and spin triplet pairing
- symmetry properties of pairing amplitude and pairing potential (follows from anti-commutation relation of fermionic operators)

$$g_{\alpha\beta}(\mathbf{k}) = \langle \hat{\mathbf{c}}_{-\mathbf{k}\alpha} \, \hat{\mathbf{c}}_{\mathbf{k}\beta} \rangle = -\langle \hat{\mathbf{c}}_{\mathbf{k}\beta} \, \hat{\mathbf{c}}_{-\mathbf{k}\alpha} \rangle = -g_{\beta\alpha}(-\mathbf{k})$$
$$\Delta_{\alpha\beta}(\mathbf{k}) = -\Delta_{\beta\alpha}(-\mathbf{k})$$

- supplementary mat

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- representation of the energy gap matrix $\Delta_{\alpha\beta}(k)$ by a scalar gap function $\Delta(k)$ and a vector d(k)

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \iota \left[\Delta(\mathbf{k}) \mathbf{I} + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma} \right] \sigma_{y}$$
Pauli spin matrix $\sigma_{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Scalar gap function
$$\mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \mathbf{d}\text{-vector}$$

$$\sigma = \begin{pmatrix} \sigma_{x}, \sigma_{y}, \sigma_{z} \end{pmatrix} = \text{vector of Pauli matrices}$$

$$\sigma_{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_{x}(\mathbf{k}) + \iota d_{y}(\mathbf{k}) & \Delta(\mathbf{k}) + d_{z}(\mathbf{k}) \\ -\Delta(\mathbf{k}) + d_{z}(\mathbf{k}) & d_{x}(\mathbf{k}) + \iota d_{y}(\mathbf{k}) \end{pmatrix}$$



- > amplitude |d| (d is vector with complex components): pair density $|d|^2 = d_x^2 + d_y^2 + d_z^2 = n_s$
- direction $\hat{\mathbf{d}} = \mathbf{d}/|\mathbf{d}|$:
 spatial orientation of spin wave function: $\hat{\mathbf{d}} \cdot \mathbf{S} = 0$

Superfluid ³He: superfluid phases **I.5.3**

- parity consideration
 - with $g_{\alpha\beta}(\mathbf{k}) = -g_{\beta\alpha}(-\mathbf{k})$ and $\Delta_{\alpha\beta}(\mathbf{k}) = -\Delta_{\beta\alpha}(-\mathbf{k})$ we obtain

$$\Delta(\mathbf{k}) = \Delta(-\mathbf{k})$$
scalar component is **even** with
respect to inversion $\mathbf{k} \to -\mathbf{k}$
vector component is **odd** with
respect to inversion $\mathbf{k} \to -\mathbf{k}$

-k

anti-symmetry of pair wave function requires

• spin singlet
$$(S = 0)$$
:
• spin triplet $(S = 1)$:

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} 0 & \Delta(\mathbf{k}) \\ -\Delta(\mathbf{k}) & 0 \end{pmatrix}$$
• spin triplet $(S = 1)$:

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_{\chi}(\mathbf{k}) + \iota d_{\chi}(\mathbf{k}) & +d_{Z}(\mathbf{k}) \\ +d_{Z}(\mathbf{k}) & d_{\chi}(\mathbf{k}) + \iota d_{\chi}(\mathbf{k}) \end{pmatrix}$$

 $L = 1,3,5, \dots$



 $\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_{\chi}(\mathbf{k}) + \iota d_{\chi}(\mathbf{k}) & \Delta(\mathbf{k}) + d_{z}(\mathbf{k}) \\ -\Delta(\mathbf{k}) + d_{z}(\mathbf{k}) & d_{\chi}(\mathbf{k}) + \iota d_{\chi}(\mathbf{k}) \end{pmatrix}$

- representation of the scalar function $\Delta(\mathbf{k})$ and vector $\mathbf{d}(\mathbf{k})$
 - we can restrict ourselves to wave vectors near the Fermi level
 - \rightarrow due to spherical symmetry, we can use spherical harmonics Y_{lm} to represent

$$d_i(\mathbf{k}) = \sum h_{ilm} Y_{lm}(\theta_{\mathbf{k}}, \varphi_{\mathbf{k}}) \qquad i = x, y, z$$

> spin singlet: *l* = 0,2,4, ...
 > spin triplet: *l* = 1,3,5, ...

in general, one has to sum up over all angular momentum quantum numbers l

- practically, one can restrict oneself to a particular quantum number (dominating pairing channel, all other channels have much smaller T_c)
- > for superfluid ³He, the dominating pairing channel is the l = 1 channel mediated by spin fluctuations

$$p_{x}(\theta_{k},\varphi_{k}) = \sqrt{3/4\pi} \cos \varphi_{k} \sin \theta_{k}$$

$$p_{y}(\theta_{k},\varphi_{k}) = \sqrt{3/4\pi} \sin \varphi_{k} \cos \theta_{k}$$

$$p_{y}(\theta_{k},\varphi_{k}) = \sqrt{3/4\pi} \cos \theta_{k}$$

$$p_{z}(\theta_{k},\varphi_{k}) = \sqrt{3/4\pi} \cos \theta_{k}$$

complex matrix elements have to be determined by solving BCS gap equation



• superfluid phases of ³He

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_x(\mathbf{k}) + \iota d_y(\mathbf{k}) & +d_z(\mathbf{k}) \\ +d_z(\mathbf{k}) & d_x(\mathbf{k}) + \iota d_y(\mathbf{k}) \end{pmatrix} \qquad d_i(\mathbf{k}) = \sum h_{im} p_j(\theta_{\mathbf{k}}, \varphi_{\mathbf{k}}) \qquad h_{im} = \begin{pmatrix} h_{xx} & h_{xy} & h_{xz} \\ h_{yx} & h_{yy} & h_{yz} \\ h_{zx} & h_{zy} & h_{zz} \end{pmatrix}$$

- Anderson-Brinkman-Morrel (ABM or A) phase

$$h_{im} = \begin{pmatrix} 1 & \iota & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \Rightarrow d_x(\mathbf{k}) = p_x + \iota p_y \qquad |\psi\rangle_{ABM} = (p_x + \iota p_y) |\downarrow\downarrow\rangle - (p_x - \iota p_y) |\uparrow\uparrow\rangle$$

linear combination of $S_z = \pm 1$ (i) $B = 0: |h_{xx}| = |h_{xy}|$ $\rightarrow \langle S_z \rangle = 0$ (ii) $B \neq 0: |h_{xx}| \neq |h_{xy}|$ $\rightarrow \langle S_z \rangle \neq 0$ (anisotropic, paramagnetic)

- Anderson-Brinkman-Morrel (ABM or A) phase

$$|\psi\rangle_{ABM} = (p_x + \iota p_y) |\downarrow\downarrow\rangle - (p_x - \iota p_y) |\uparrow\uparrow\rangle$$

- both spins are always parallel
- \succ all paired atoms are moving in plane perpendicular to L



➤ unpaired atoms moving in L direction do not perturb → no energy gap in L-direction





- supplementary material

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• superfluid phases of ³He

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_{\chi}(\mathbf{k}) + \iota d_{y}(\mathbf{k}) & +d_{z}(\mathbf{k}) \\ +d_{z}(\mathbf{k}) & d_{\chi}(\mathbf{k}) + \iota d_{y}(\mathbf{k}) \end{pmatrix} \qquad d_{i}(\mathbf{k}) = \sum h_{im} p_{j}(\theta_{\mathbf{k}}, \varphi_{\mathbf{k}}) \qquad h_{im} = \begin{pmatrix} h_{xx} & h_{xy} & h_{xz} \\ h_{yx} & h_{yy} & h_{yz} \\ h_{zx} & h_{zy} & h_{zz} \end{pmatrix}$$

- Balian-Werthamer (BW or B) phase

$$h_{im} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Rightarrow d_x(\mathbf{k}) = p_x, \ d_y(\mathbf{k}) = p_y, \ d_z(\mathbf{k}) = p_z,$$
$$|\psi\rangle_{BW} = (p_x + \iota p_y) |\downarrow\downarrow\rangle - (p_x - \iota p_y) |\uparrow\uparrow\rangle + p_z(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$$

linear combination of $S_z = -1,0, +1$ (all spin states are represented equally)

 $|h_{xx}| = |h_{yy}| = |h_{zz}| \neq 0 \quad \Rightarrow \quad \langle S_z \rangle = 0$ (isotropic, non-magnetic)

 $B \neq 0$: $S_z = 0$ component is non-magnetic $\rightarrow \chi_{BW} = \frac{2}{3}\chi_{ABM}$

BW phase energetically less favorable tan ABM phase in applied magnetic field !!

Balian-Werthamer (BW or B) phase

 $|\psi\rangle_{\rm BW} = (p_x + \iota p_y) |\downarrow\downarrow\rangle - (p_x - \iota p_y) |\uparrow\uparrow\rangle + p_z(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)$





• superfluid phases of ³He

$$\begin{pmatrix} \Delta_{\uparrow\uparrow}(\mathbf{k}) & \Delta_{\uparrow\downarrow}(\mathbf{k}) \\ \Delta_{\downarrow\uparrow}(\mathbf{k}) & \Delta_{\downarrow\downarrow}(\mathbf{k}) \end{pmatrix} = \begin{pmatrix} -d_x(\mathbf{k}) + \iota d_y(\mathbf{k}) & +d_z(\mathbf{k}) \\ +d_z(\mathbf{k}) & d_x(\mathbf{k}) + \iota d_y(\mathbf{k}) \end{pmatrix} \qquad d_i(\mathbf{k}) = \sum h_{im} p_j(\theta_{\mathbf{k}}, \varphi_{\mathbf{k}}) \qquad h_{im} = \begin{pmatrix} h_{xx} & h_{xy} & h_{xz} \\ h_{yx} & h_{yy} & h_{yz} \\ h_{zx} & h_{zy} & h_{zz} \end{pmatrix}$$

- A_1 phase (only for B > 0)

$$h_{im} = \begin{pmatrix} 1 & \iota & 0 \\ \iota & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \xrightarrow{\bullet} d_x(\mathbf{k}) = p_x + \iota p_y$$
$$\Rightarrow d_y(\mathbf{k}) = \iota p_x + p_y \qquad |\psi\rangle_{\mathbf{A}_1} = 2(p_x + \iota p_y) |\uparrow\uparrow\rangle$$

only state $|\uparrow\uparrow\rangle$ contributes: $\langle S_z \rangle = 1$ ("ferro" magnetic)

➔ long-range ordered magnetic liquid

I.5.3 Superfluid ³He: broken symmetries

disordered state

(isotropic with respect to orientation of both degrees of freedom)





broken gauge symmetry "superfluid"



broken gauge and rotational symmetry in spin space "ferromagnetic superfluid"





broken gauge and rotational symmetry in orbital space "ferroorbital superfluid"



only symmetry related to relative orientation is broken







rotational symmetry is broken separately in spin and orbital space

³He

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BAYERISCHE AKADEMIE DER WISSENSCHAFTEN Technische Universität München

Superconductivity and Low Temperature Physics II



Lecture No. 8 30 June 2022

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> I.6 ³He / ⁴He mixtures



- why interesting:
 - → model system for testing Fermi liquid theories (³He is fermion, can be diluted in passive ⁴He background → change of interaction strength)
 - → technical application in cooling machines
 - H.E. Hall, P.J. Ford and K. Thomson, Cryogenic 6 (1966) 80B.S. Neganov, N.S. Borisov and M.Yu. Liburg, Zh. Exp. Teor. Fiz. 50 (1966) 1445.
- experimental observations:
 - → specific heat vs. T curve of ⁴He is shifted to lower T on adding ³He, but does not change its shape
 - \rightarrow phase separation of ⁴He and ³He at low T



I.6 ³He/⁴He mixtures: phase diagram

• high T:

³He reduces $T_{\lambda} \propto n_4$ (⁴He concentration)

- tricritical point $T_{\text{tri}} = 0.87 \text{ K}$
- $T < T_{tri} = 0.87$ K: • phase separation

³He rich phase: lighter ³He poor phase: heavier

- $T \rightarrow 0$:
 - → incomplete phase separation

6.5% of ³He still dissolved in ⁴He

- concentrations: $x_3 = \frac{n_3}{n_3 + n_4}; \quad x_4 = 1 x_3 = \frac{n_4}{n_3 + n_4}$
- limiting concentrations:

$$x_4 = aT^{3/2}e^{-b/T}$$
 ($a = 0.85 \text{ K}^{-3/2}$, $b = 0.56 \text{ K}^{-1}$)

$$x_3 = 0.0648 (1 + cT^2 + dT^3)$$
 ($c = 8.4 \text{ K}^{-2}, d = 9.4 \text{ K}^{-3}$)



- at $T_{\text{phase sep}} < T < T_{\lambda}(x_4)$:
 - → ⁴He forms superfluid with negligible amounts of excitations (phonons, rotons)
 - \rightarrow viscosity, entropy and specific heat go to zero:
 - → ⁴He = inert superfluid background

- ³He obeys Fermi statistics
 - \rightarrow Fermi temperature is about 1 K for pure ³He
 - \rightarrow dissolving ³He in ⁴He reduces the Fermi temperature

$$T_{\rm F} = \frac{\hbar^2}{2m_{3\rm He}^*} (3\pi^3 n_{3\rm He})^{2/3} \propto x_3^{2/3}$$

 m_{3He}^* : effective mass of ³He dissolved in ⁴He $n_{3He} = \frac{N_{3He}}{V} = \frac{x_3N}{V}$: density of ³He atoms 100

³He



I.6 ³He/⁴He mixture as diluted Fermi liquid WM

specific heat



- Fermi gas ($T \ll T_{\rm F}$) ٠
- classical gas $(T > T_F)$ ٠

$$C_{\rm mol} = \frac{\pi^2}{2} R \frac{T}{T_{\rm F}}$$

$$C_{\rm mol} = \frac{3}{2} N_{\rm A} k_{\rm B} = \frac{3}{2} R$$

 $T_{\rm F}$ increases with x_3 ۲





I.6 ³He/⁴He mixtures: miscibility gap in binary systems

• bonding:



- $V_{AB} > \frac{1}{2}(V_{AA} + V_{BB})$ complete miscibility (e.g. water and alcohol)
- $\frac{1}{2}(V_{AA} + V_{BB}) > V_{AB}$ phase separation (e.g. water and petrol)
- → optimization of binding total energy U complete phase separation @ T = 0



increasing mixing with increasing T:

 $F = U - TS \rightarrow min$ bindina thermal energy motion

→ minimization of free energy

I.6 ³He/⁴He mixtures: finite solubility of ³He in ⁴He

binding energy of ³He in ³He (V_{33}) and ⁴He (V_{34}):

 $L_3 = U_{\text{vap}} - U_{\text{liq}} + p\Delta V$ $p\Delta V =$ work done against ambient pressure

i. single ³He atom in liquid ³He: average binding energy is given by the latent heat of evaporation L_3 :

binding energy for single ³He atom: $\epsilon_{3,c} = -\frac{L_3}{N_A} = \mu_{3,c}$ $\mu_{3,c} = chemical potential of pure (concentrated) liquid$

ii. single ³He atom in liquid ⁴He:

binding energy for single ³He atom: $\epsilon_{3,d}$

 $\epsilon_{3,d}(x_3 \to 0) = \mu_{3,d}(x_3 \to 0)$ $\mu_{3,d} = chemical potential of dilute phase$

- $|\epsilon_{3,d}(0)| > |\epsilon_{3,c}|$ or vice versa ?

³He has smaller mass \rightarrow larger zero point fluctuations \rightarrow occupies larger volume

 \rightarrow binding of ³He is larger in ⁴He than in ³He due to larger density of ⁴He

 $\rightarrow |\epsilon_{3,d}(0)| > |\epsilon_{3,c}|$ (it is energetically more favorable to add a ³He atom to the ⁴He superfluid than to pure ³He)

→ corresponds to case $V_{AB} > \frac{1}{2}(V_{AA} + V_{BB})$ → complete miscibility expected,

why miscibility only up to 6.5% ??

- questions
 - why can't we dissolve more than 6.5% of ³He in ⁴He at T = 0?

we have to take into account two effects:

- ³He forms degenerate Fermi liquid
 - \rightarrow $T_{\rm F}$ increases with x_3

 \rightarrow for $x_3 > 6.5\%$, the increase of Fermi energy exceeds the gain in binding energy

ii. effective attraction between two ³He atoms (*magnetic and volume effect*)

 $\rightarrow |\epsilon_{3,d}(x_3)| > |\epsilon_{3,d}(x_3=0)|$

- why don't we have a complete phase separation into pure ³He and pure ⁴He at T = 0?
 - \rightarrow incomplete phase separation results in finite disorder, violation of 3rd law of thermodynamic ?
 - → no: we have degenerate Fermi gas, ordering in k-space



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I.6 ³He/⁴He mixtures: finite solubility of ³He in ⁴He



for $x_3 > 6.5\%$: $\left| E_{\text{pot}}(x_3) + k_{\text{B}}T_{\text{F}}(x_3) \right| < \left| \epsilon_{3,c} \right| = \left| E_{\text{pot}}(x_3 = 1) + k_{\text{B}}T_{\text{F}}(x_3 = 1) \right|$

→ separation of pure ³He

I.6 ³He/⁴He mixtures: cooling effect

• ³He/⁴He dilution refrigeration

- operation principle:
 - ightarrow remove ³He atoms from the dilute phase below $T_{
 m tri}~=~0.87~
 m K$
 - \rightarrow transport of ³He atoms across phase boundary to maintain equilibrium concentration
 - \rightarrow corresponds to evaporation of ³He from concentrated phase
 - \rightarrow cooling effect as the latent heat of evaporation is removed
- for Fermi liquid:
 - $\rightarrow C_{V,\text{concentrated}} < C_{V,\text{diluted}} (x_3 = 0.065) \qquad (C_V \propto T/T_F, \ T_F \propto n_{3\text{He}}^{2/3})$

- with
$$U = Q = \int_0^T C_V(T') dT' = \frac{\gamma}{2} T^2$$
 we therefore obtain ($C_V = \gamma T, \gamma =$ Sommerfeld coefficient)

 $\boldsymbol{U}_{\text{concentrated}}(\boldsymbol{T}) < \boldsymbol{U}_{\text{diluted}}(\boldsymbol{T})$

on transition across phase boundary:

$$dG = 0 = dU - TdS \Rightarrow dU = TdS = dQ$$

- → removal of heat $\Delta Q = T\Delta S = T [S_{dil}(T) S_{con}(T)]$ → cooling effect
- \rightarrow ³He/⁴He dilution refrigerator



concentrated

(lighter)

³He

diluted,6.5%

(heavier)

³Не

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I.6 ³He/⁴He mixtures: cooling effect

- ³He/⁴He dilution refrigeration: cooling power
 - assumption: one mole of ³He crosses boundary between diluted and concentrated phase —
 - removed heat: $\Delta Q = T \Delta S = T \left[S_{\text{dil}}(T) - S_{\text{con}}(T) \right]$

- cooling power:
$$\Delta \dot{Q} = \left(\frac{\Delta Q}{n_{3He}}\right) \cdot \dot{n}_{3He} \Rightarrow \Delta \dot{Q} = \dot{n}_{3He} T \left[s_{dil}(T) - s_{con}(T)\right] \qquad S_{dil} = \frac{s_{dil}}{n_{3He}}, S_{con} = \frac{s_{con}}{n_{3He}}$$

since there is no volume change:

$$dQ = dU = TdS = C_V dT, \qquad U(T) = \int_0^T C_V dT', \qquad S(T) = \int_0^T \frac{C_V}{T'} dT'$$

$$\Rightarrow \text{ with } C_{\text{mol}} = \frac{\pi^2 N_A k_B^2 T}{2\varepsilon_F} \text{ and } \varepsilon_F = \frac{\hbar^2}{2m_{3\text{He}}^*} \left(\frac{3\pi^2 N_{3\text{He}}}{V}\right)^{2/3} = \frac{\hbar^2}{2m_{3\text{He}}^*} \left(\frac{3\pi^2 N_A}{V_{\text{mol}}}\right)^{2/3} \text{ (standard expressions for Fermi liquid)}$$

we obtain the entropy
$$S_{\rm mol} = \frac{\pi^2 N_A k_B^2 m_{3\rm He}^*}{\hbar^2} \left(\frac{V}{3\pi^2 N_{3\rm He}}\right)^{2/3} T \propto \frac{T}{n_{3\rm He}}$$

 $S_{\rm con} < S_{\rm dil}$ (as $n_{3,\rm con} > n_{3,\rm dil}$) $Q(\dot{T}) = 84 \dot{n}_{3He} T^2$ [W] (cooling power $\propto {}^{3}$ He throughput \dot{n}_{3} [mol/s])

Т

WM

I.6 ³He/⁴He mixtures: cooling effect

• ³He/⁴He dilution refrigeration: plausibility consideration



entropy increases going from concentrated to diluted phase

removed heat: dQ = TdS