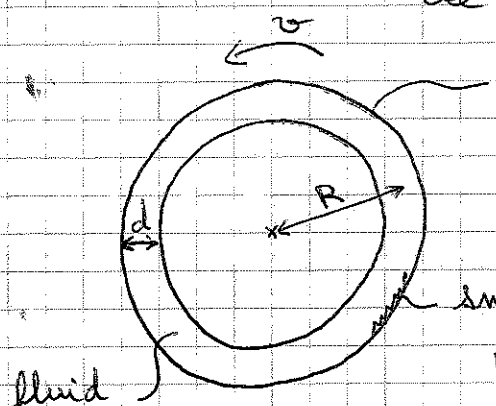
Superfluidity of the 3D Bose gas

I) Normal fraction and equilibrium in a rotating container

1) Physical motivation

Consider the following Gedankenexperiment [this is the second experiment described in G. Batrouni's Lectures. See also: Leggett, Rev. Mod. Phys. **71**, S318 (1999)]



Define $L_x = 2\pi R$

- Start at $T_{initial} > T_c$
- Start rotating the container at velocity $v \ll \frac{2\pi}{L_x} \Rightarrow$ the (normal) fluid rotates at velocity v.
- Cool to $T < T_c$

This sequences ensures that the fluid is at equilibrium with the container. What happens?

The superfluid component stops.

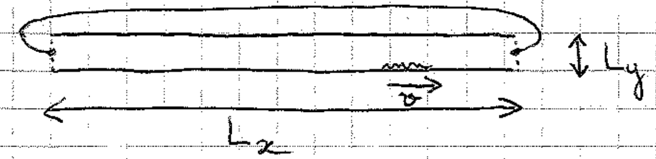
Angular momentum of the fluid: $\boxed{L = f_n(T) \cdot N \cdot R \cdot v}$ (1) — normal fraction

superfluid fraction: $f_s = 1 - f_n$.

2) Simple modelization

- For the container: a Box with $L_x \gg L_y = L_z$

Periodic boundary conditions along x (very important to mimic the toroidal geometry of the container) and along y, z (for convenience).



- For the defects : an external potential

$$U(\vec{r},t) = U_{ext}(\vec{r}-\vec{v}\,t), \text{ moving at } \vec{v} = v\cdot\vec{u}_x = \begin{pmatrix} v \\ 0 \\ 0 \end{pmatrix}$$

3) Thermodynamic equilibrium in the rotating container

The Hamiltonian of the fluid (= the gas) is

$H(t) = H_0 + H_{ext}(t)$ where H_0 is as usual

$$H_0 = \sum_{j=1}^{N} \frac{\hat{\vec{P}}_j^{\,2}}{2} + \sum_{1\leq i<j\leq N} V(\hat{\vec{r}}_i - \hat{\vec{r}}_j)$$

with $V(\vec{r}) = g\,\delta^3(\vec{r})$ [same Remark than in Part 2]

and $H_{ext}(t) = \sum_{j=1}^{N} U_{ext}(\hat{\vec{r}}_j - \vec{v}\,t)$.

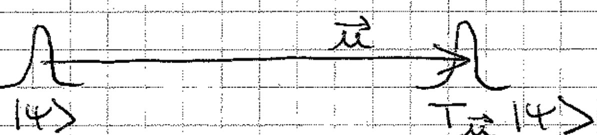
Denoting by $|\psi(t)\rangle$ the wavefunction of the fluid

[so that $\langle \vec{r}_1, \dots, \vec{r}_N | \psi(t)\rangle = \psi(\vec{r}_1,\dots,\vec{r}_N; t)$]

we have : $i\dfrac{d}{dt}|\psi(t)\rangle = H(t)|\psi(t)\rangle$.

Def (Translation operator)

$$\langle \vec{r}_1, \dots, \vec{r}_N | T_{\vec{u}} | \psi\rangle \equiv \langle \vec{r}_1 - \vec{u}, \dots, \vec{r}_N - \vec{u} | \psi\rangle$$



Idea: $T_{-\vec{v}\cdot t}|\psi(t)\rangle$ "does not move", i.e. we hope that it satisfies Schrödinger's equation with a time-independent Hamiltonian.

Ex 1 S.t. $T_{\vec{u}} = e^{-i\vec{u}\cdot\hat{\vec{P}}}$, where $\hat{\vec{P}} = \sum_{j=1}^{N} \hat{\vec{p}}_j$ is the total momentum (as in Part 2)

Solution : We have :

$$\vec{\nabla}_{\vec{u}}\langle \vec{r}_1,\dots,\vec{r}_N | T_{\vec{u}}|\psi\rangle = -\sum_{j=1}^{N} \vec{\nabla}_j \langle \vec{r}_1 - \vec{u}, \dots, \vec{r}_N - \vec{u} | \psi\rangle$$

$$= -i\sum_{j=1}^{N} \langle \vec{r}_1,\dots,\vec{r}_N | \hat{\vec{p}}_j\, T_{\vec{u}}|\psi\rangle$$

$$\Rightarrow \quad \vec{\nabla}_{\vec{u}}\left(T_{\vec{u}}|\psi\rangle\right) = -i\hat{\vec{P}}\,T_{\vec{u}}|\psi\rangle.$$

Moreover, $T_{\vec{0}}|\psi\rangle = |\psi\rangle$. Thus, $T_{\vec{u}}|\psi\rangle = e^{-i\vec{u}\cdot\hat{\vec{P}}}|\psi\rangle$. ☒

<u>Def</u> : $\boxed{|\psi'(t)\rangle = T_{-\vec{v}t}\,|\psi(t)\rangle}$.

Ex 2 | S.t. $i\dfrac{d}{dt}|\psi'(t)\rangle = \mathcal{H}\,|\psi'(t)\rangle$

where $\mathcal{H} = H_0 - \hat{\vec{P}}\cdot\vec{v} + H_{ext}(0)$

<u>Solution</u> : From the definition of $|\psi'(t)\rangle$ and Ex 1, it follows : $i\dfrac{d}{dt}|\psi'(t)\rangle = \left[-\vec{v}\cdot\hat{\vec{P}} + T_{-\vec{v}t}\,H(t)\,T_{\vec{v}t}\right]|\psi'(t)\rangle$

One then checks that :

- $T_{-\vec{v}t}\,H_0\,T_{\vec{v}t} = H_0$
- $T_{-\vec{v}t}\,H_{ext}(t)\,T_{\vec{v}t} = H_{ext}(0)$

and the result follows. ☒

Since $\mathcal{H}$ is time-independent, we can apply statistical mechanics : there exists a temperature T such that, for any few-body observable $\hat{A}$,

$$\langle\psi'(t)|\hat{A}|\psi'(t)\rangle \xrightarrow[\substack{t\to\infty \\ \text{(in some sense..)}}]{} \mathrm{tr}\left(e^{-\beta\mathcal{H}}\hat{A}\right)/\mathrm{tr}\left(e^{-\beta\mathcal{H}}\right)$$

If $[\hat{A},\hat{\vec{P}}] = \vec{0}$, $\langle\psi'(t)|A|\psi'(t)\rangle = \langle\psi(t)|A|\psi(t)\rangle$.

Finally, assuming U_{ext} is small (small defects); $\mathcal{H} \simeq \boxed{H' \equiv H_0 - \hat{\vec{P}}\cdot\vec{v}}$, and

$$\langle\psi(t)|\hat{A}|\psi(t)\rangle \xrightarrow[t\to\infty]{} \frac{\mathrm{tr}\left(e^{-\beta H'}A\right)}{\mathrm{tr}\left(e^{-\beta H'}\right)} \equiv \langle A\rangle_v$$

4 A definition of the normal fraction f_n

<u>Def</u> $\boxed{f_n(T) = \lim_{v\to 0}\dfrac{\langle\hat{P}_x\rangle_v}{N\cdot v}}$ (for $T>0$)

(in agreement with Equation (1) in 1.)

5 <u>Calculation of f_n for the 3D Bose gas</u>

As in Part 2 : $T<T_c$, $\rho a^3 \ll 1$, $a>0$. We use Bogoliubov theory.

(a) Condensate wavefunction. Since the Hamiltonian is $H' = H_0 - \hat{P}_x v$, we have to minimize the energy functional:

$$E(\psi) = N \int d\vec{r}\, \psi^*(\vec{r}) \left[-\frac{1}{2}\Delta_{\vec{r}} - \frac{1}{i}\frac{\partial}{\partial x} v \right] \psi(\vec{r}) + \frac{N^2}{2} g \int d\vec{r}\, |\psi(\vec{r})|^4 .$$

Setting $E(\psi) \equiv E_{kin}(\psi) + E_{int}(\psi)$, we have: $E_{kin}(\psi) = N \langle \psi | -\frac{1}{2}\Delta_{\vec{r}} - \frac{1}{i}\frac{\partial}{\partial x} v | \psi \rangle$

$$= N \sum_{\vec{k}} \underbrace{\left(\frac{k^2}{2} - k v \right)}_{= \frac{1}{2}[k-v]^2 - \frac{v^2}{2}} |\langle \vec{k} | \psi \rangle|^2 .$$

Defining: $\left[\begin{array}{l} |\phi\rangle \equiv |\vec{k}_0\rangle \text{ with } \vec{k}_0 = \left(\frac{2\pi}{L_x} n, 0, 0\right) \text{ and} \\ n \in \mathbb{N} \text{ such that } |\vec{k}_0 - \vec{v}| \text{ is minimal} \end{array} \right.$

one sees that $E_{kin}(\psi) > E_{kin}(\phi)$, $\forall \psi \neq \phi$.

Thus the condensate wavefunction (at equilibrium with a container moving at velocity v) is $|\phi\rangle$ (defined above).

Note: For $v = 0$ (or equivalently, without any rotating container), $n = 0$, $\vec{k}_0 = \vec{0}$ and $|\phi\rangle = |\vec{k} = \vec{0}\rangle$.

[We have used this result at the beginning of Part 2. II]

(b) f_n. Remember that in our definition of f_n (see I.4) we take the limit $v \to 0$, so that we can assume in particular: $|v| \ll \frac{2\pi}{L_x}$.

Thus we have $n = 0$ and $|\phi\rangle = |\vec{k} = \vec{0}\rangle$ (i.e. $\phi(\vec{r}) = \frac{1}{\sqrt{V}}$.)

Within Bogoliubov theory, we thus approximate H_0 by the same H_{Bog} than the one obtained in Part 2 (in the non-rotating case). Thus:

$$H' = H_0 - \hat{P}_x v \underset{\substack{\uparrow \\ \text{Bogoliubov approximation}}}{\simeq} H_{Bog} - \hat{P}_x v \underset{\substack{\uparrow \\ \text{Definition}}}{\equiv} H'_{Bog} .$$

Moreover, $\hat{P}_x = \sum_{\vec{k}\neq\vec{0}} k_x \, b^+_{\vec{k}} b_{\vec{k}}$.

Thus, $H'_{Bog} = \left[\sum_{\vec{k}\neq\vec{0}} (\varepsilon_k - k_x v) \, b^+_{\vec{k}} b_{\vec{k}}\right] + E_0$

with a corresponding density operator

$$\rho'_{Bog} \propto \exp\left[-\beta \sum_{\vec{k}\neq\vec{0}} (\varepsilon_k - k_x v) \, b^+_{\vec{k}} b_{\vec{k}}\right].$$

The effect of the rotating container is thus only to replace the quasi-particle energy ε_k by $(\varepsilon_k - k_x v)$.
Since we still have an ideal gas of quasi-particles, we have $\langle b^+_{\vec{k}} b_{\vec{k}} \rangle_v = \dfrac{1}{e^{\beta(\varepsilon_k - k_x v)} - 1}$. Thus

$$f_n \equiv \lim_{v\to 0} \frac{\langle \hat{P}_x \rangle_v}{N v}$$

$$= \lim_{v\to 0} \frac{1}{N v} \sum_{\vec{k}\neq\vec{0}} k_x \langle b^+_{\vec{k}} b_{\vec{k}} \rangle_v$$

$$= \frac{1}{N} \sum_{\vec{k}\neq\vec{0}} k_x \frac{\partial}{\partial v}\left(\frac{1}{e^{\beta(\varepsilon_k - k_x v)} - 1}\right)\Bigg|_{v=0}$$. Finally:

$$\boxed{f_n \underset{t.l.}{=} \frac{1}{3\rho T} \int \frac{d\vec{k}}{(2\pi)^3} \, k^2 \, \frac{e^{\beta\varepsilon_k}}{\left(e^{\beta\varepsilon_k} - 1\right)^2}}$$

Ex 3

S.t.:

For $T \ll \rho g$: phonons dominate (in this integral)
and: $f_n \simeq \dfrac{T^4}{720\sqrt{\pi}\,\rho^{7} a^{5}}$ (*)

For $T \gg \rho g$: free-particles dominate (in the same integral) and: $f_n \simeq f_{nc} \simeq f_{nc}^{ideal}$

Rem: • For $T \ll \rho g$ we thus have $f_n \ll f_{nc} \propto \sqrt{\rho a^3} \; (\ll 1)$

• This is qualitatively similar to liquid Helium, where at $T \to 0$, $f_n \to 0$ and it is believed that $f_{nc} \sim 0.9$

• Eq. (*), if one replaces $\sqrt{\rho g}$ by c, is the same than the one obtained for liquid Helium in e.g.: [Lifshitz and Pitaevski, "Statistical Physics, Part 2", 1980, Sections 22–23]

<u>Solution of Ex. 3</u> : $f_n = \frac{1}{\rho T \cdot 6\pi^2} \int_0^\infty dk \cdot k^4 \cdot \frac{e^{\beta \varepsilon_k}}{(e^{\beta \varepsilon_k} - 1)^2}$

. For $T \ll \rho g$: the integral is dominated by the phonon regime ($k \ll \sqrt{\rho g}$; $\varepsilon_k \simeq \sqrt{\rho g}\, k$). [This can be shown by setting $k = \sqrt{2\rho g}\, q$, as in Part 2, Exercise 8, page 2.12].

Thus: $$f_n \simeq \frac{1}{\rho T \cdot 6\pi^2} \int_0^\infty dk \cdot k^4 \cdot \frac{e^{\beta\sqrt{\rho g}\, k}}{(e^{\beta \sqrt{\rho g}\, k} - 1)^2}$$

and setting $x = \beta \sqrt{\rho g}\, k$:

$$f_n \simeq \frac{1}{6\pi^2 \rho T [\beta\sqrt{\rho g}]^5} \underbrace{\int_0^\infty dx \cdot x^4 \cdot \frac{e^x}{(e^x - 1)^2}}_{= 4!\, \zeta(4) = 4! \cdot \frac{\pi^4}{90}}$$

and the result follows.

. For $T \gg \rho g$: the integral is dominated by the free-particle regime ($k \gg \sqrt{\rho g}$, $\varepsilon_k \simeq \frac{k^2}{2}$). [This can be shown by setting $k = \sqrt{\frac{2}{\beta}}\, p$, as in Part 2, Ex. 8, page 2.13]

Thus, $$f_n \simeq \frac{1}{\rho T \cdot 6\pi^2} \int_0^\infty dk \cdot k^4 \cdot \frac{e^{\beta k^2/2}}{(e^{\beta k^2/2} - 1)^2}.$$

Integrating by parts gives:

$$f_n \simeq \frac{1}{2\pi^2 \rho} \int_0^\infty dk \cdot k^2 \cdot \frac{1}{e^{\beta k^2/2} - 1}$$

$$= \frac{1}{\rho} \int \frac{d\vec{k}}{(2\pi)^3} \frac{1}{e^{\beta k^2/2} - 1}$$

$$\underset{t.l.}{=} \frac{1}{N} \sum_{\vec{k} \neq \vec{0}} \langle n_{\vec{k}} \rangle_{ideal} = f_{nc}^{ideal,\, ANEC}$$

$$\simeq f_{nc}^{ideal} \simeq f_{nc}$$

since $T \gg \rho g$ (Part 2, Ex 8)

⑥ <u>Remark: Thermal excitation of supercurrents</u>

We briefly address the question: can the gas be thermally

excited to a state where the condensate is moving, in the sense that $|\phi\rangle = |\vec{k}\rangle$ with $\vec{k} \neq \vec{0}$?
(still assuming $v = 0$, or at least $|v| \ll \frac{2\pi}{L_x}$)
Answer (a bit handwaving but can be made rigorous, and in the t.l., see References below): No in $d = 3$, because
for $\vec{k} = \left(\frac{2\pi}{L_x}, 0, 0\right)$:
$$\Delta E \equiv E(|\phi\rangle = |\vec{k}\rangle) - E(|\phi\rangle = |\vec{0}\rangle) = N \frac{k^2}{2} = \frac{N}{2}\left(\frac{2\pi}{L_x}\right)^2 \xrightarrow[\text{t.l.}]{} +\infty .$$
But in $d = 1$ and $d = 2$, the situation is very different.
Actually, in $d = 1$, for the weakly interacting Bose gas, one finds (with the above definition of f_n) that $f_n = 1$ in the t. l.
See I. Carusotto and Y. Castin, C. R. Physique (2004), also available at cond-mat/0311601 ;
N. Prokof'ev and B. Svistunov, Phys. Rev. B 61, 11282 (2000)

II Landau's criterion for the metastability of superflow.

1 Physical motivation

Consider the same toroidal container than in I.1, but with another experimental sequence :

- Start at equilibrium at $T < T_c$ with the container at rest (and thus the fluid also at rest).
- Suddenly start rotating the container at a velocity $v \gg \frac{2\pi}{L_x}$.

What happens ?
The superfluid component stays at rest, in a metastable state, for a very long time (if $v < v_c$)
[This is analogous to the first experiment discussed in G. Batrouni's Lectures, where however it was the container

which was at rest, and the superfluid which would continue to rotate in a metastable state.]

2) Discussion

• For $v \gg \frac{2\pi}{L_x}$, the ground state has a moving condensate (according to I.5.a)

• But we can use Bogoliubov theory to (try to) describe a metastable state where the condensate is at rest! We assume an almost pure condensate, of wavefunction $\phi = \frac{1}{\sqrt{V}}$. This allows to apply the Bogoliubov approximation to the Hamiltonian:

$H' \simeq H'_{Bog}$, as in I:

$$H'_{Bog} = E_0 + \sum_{\vec{k} \neq \vec{0}} (\varepsilon_k - k_x v)\, b^+_{\vec{k}}\, b_{\vec{k}} .$$

• If $\exists\, \vec{k}_0 \,/\, \varepsilon_{\vec{k}_0} - k_{0,x} v < 0$, then there is a "thermodynamical instability": the system can decrease its energy by creating a large number of quasi-particles of wavevector $\vec{k}_0$ (these quasiparticles having negative energy) untill the condensed fraction becomes small (and the Bogoliubov approximation breaks down).
[More formally, H'_{Bog} has no ground state (in $\tilde{\mathcal{E}}_N$)]

• Thus, metastability requires: $\boxed{\underset{\vec{k}\neq\vec{0}}{\mathrm{Min}} (\varepsilon_k - k_x v) > 0.}$

("Landau's criterion")

In the t.l., this gives: $|v| < c$.

Rem: • This condition is necessary for metastability, but not always sufficient, see G. Batrouni's Lecture

• Ideal gas, $d = 3$, $T < T_c$, t.l.: $f_n = f_{nc} < 1$ (see I)
$\Rightarrow$ superfluidity in the sense of I. But Landau's criterion violated $\Rightarrow$ no metastability of superflow.

• Weakly interacting 1D Bose gas : $f_n = 1 \Rightarrow$ no superfluidity in the sense of I . (3.9)

But Landau's criterion is satisfied, and we expect metastability of superflow.

Conclusion : There are (at least) two very different aspects of superfluidity.