Macroscopic effects in Bose fluids: Bose-Einstein condensation and superfluidity

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(Dated: October 11, 2023)

I. BOSE-EINSTEIN CONDENSATION (BEC) – OFF-DIAGONAL LONG RANGE ORDER

The complete absence of any interparticle interactions enables explicit analytical calculations for an ideal gas, but may also introduce artifacts when compared to real situations (even on a very elementary level, all particles with non vanishing mass interact with each other, photonic systems must be discussed separately). Let us therefore first start with characterizing the phenonema of Bose-Einstein condensation in a general context, not relying on any model system, giving a precise meaning to what is commonly refered to as a "macroscopic (occupation of a) quantum state".

Reduced single particle density matrix. Probably the most general and conceptually clear definition of a Bose condensed state was proposed by Penrose and Onsager [1] in terms of the reduced single particle density matrix

$$\begin{aligned}
\rho^{(1)}(\mathbf{r}',\mathbf{r};\beta) &\equiv \langle \psi^\dagger(\mathbf{r}')\psi(\mathbf{r})\rangle && (1)\\
&= \frac{N}{Z}\int d\mathbf{r}_2 d\mathbf{r}_3\cdots d\mathbf{r}_N \langle \mathbf{r}',\mathbf{r}_2,\mathbf{r}_3,\ldots,\mathbf{r}_N|e^{-\beta H}|\mathbf{r},\mathbf{r}_2,\ldots,\mathbf{r}_N\rangle && (2)\\
&= \frac{N}{Z}\sum_n e^{-\beta E_n}\int d\mathbf{r}_2 d\mathbf{r}_3\ldots d\mathbf{r}_N \Psi_n^*(\mathbf{r}_1',\mathbf{r}_2,\ldots,\mathbf{r}_N)\Psi_n(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) && (3)
\end{aligned}$$

where in the first line we have used the (second quantized) field operators creating or annihilating a particle at position $\mathbf{r}$), $\psi^\dagger(\mathbf{r})$ and $\psi(\mathbf{r})$, respectively, whereas the second line represents its relation with the full N-particle density matrix, Z is the partition function. In the last lime, we have explicitly expressed the density operator in terms of exact (properly normalized) energy eigenstates, $H\Psi_n = E_n\Psi_n$, of the full N-boson system. For any non-interacting system, these eigenstates can be expressed in terms of single particle states, such that the integrations can be done explicitly. However, second quantized forms are in general simpler (or faster) to manipulate in this case, see below for the ideal gas.

Regarded as a matrix with respect to $\mathbf{r}$ and $\mathbf{r}'$ (discrete indices can be obtained projection on a basis set of function covering the (single-particle) Hilbert space), we can diagonalize $\rho^{(1)}$ and write

$$\rho^{(1)}(\mathbf{r}',\mathbf{r};\beta) = \sum_n N_n \varphi_n^*(\mathbf{r}')\varphi_n(\mathbf{r}) \qquad (4)$$

where N_n ($n = 0, 1, \ldots$) are the (real) eigenvalues (for convenience decreasing $N_0 \geq N_1 \geq N_2 \ldots$) and $\varphi_n(\mathbf{r})$ are the corresponding eigenfunctions, both will in general depend on temperature (β). Note that the eigenfunctions are normalized, $\int d\mathbf{r}|\varphi_n(\mathbf{r})|^2 = 1$. Bose-Einstein condensation is then characterized by having a macroscopic occupation of one of the modes

$$\text{BEC} \quad \Longleftrightarrow N_0 \sim N \qquad (5)$$

Some properties/ advantage of the Penrose-Onsager definition

- Penrose-Onsager's criterium of BEC is an operational definition, it can be used in microscopic calculations as well as for measurements (of course this does not mean that it is easy, but can/has been done within some reasonable assumptions, e.g. using neutron/light scattering)
- BEC is characterized without any reference to a single particle approximation, neither relying on perturbation theory. The criterium can be applied to any Hamiltonian of interacting particles in the presence of absence of an external potential.
- Although the system is described by a single (many-body) wave function at zero temperature, $T = 0$, there might be no BEC, e.g. BEC is not "a macroscopic occupation of the ground state".
- The concept and definition of BEC, $N_0 \sim N$, remains meaningful for finite systems, independent of the (spatial) dimensionality. In order to quantify uniquely phase boundaries, one usually takes the thermodynamic limit, $N \to \infty$, $V \to \infty$ keeping the density $n = N/V$ or some similar extensions in the case of inhomogeneous or quasi 1D/2D systems.

- Symmetry considerations can be used to (partially) determine the mode structure of reduced single particle density matrix. For a translational invariant system, the eigenmodes are plane waves, Bose condensation will in general occur in the $\mathbf{k} = 0$ uniform state. In a rotational invariant geometry, one can characterize the eigenmodes by angular momentum eigenstates.

- Let us verify the ideal gas limit. Using the field decomposition $\psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{r}} a_{\mathbf{k}}$ where $a_{\mathbf{k}}$ is the annihilation operator of a particle of momentum $\hbar\mathbf{k}$, we get

$$\rho^{(1)}(\mathbf{r}', \mathbf{r}; \beta) = \frac{1}{V} \sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}'\cdot\mathbf{r}' - \mathbf{k}\cdot\mathbf{r})} \langle a^\dagger_{\mathbf{k}'} a_{\mathbf{k}} \rangle = \frac{1}{V} \sum_{\mathbf{k}} e^{-i\mathbf{k}(\mathbf{r}-\mathbf{r}')} \langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}} \rangle = \frac{N_0}{V} + \frac{1}{V} \sum_{\mathbf{k}\neq 0} \frac{e^{i\mathbf{k}(\mathbf{r}'-\mathbf{r})}}{e^{\beta(\hbar^2 k^2/2m - \mu)} - 1} \tag{6}$$

from where we can read off the eigenvalues $N_{\mathbf{k}} = \langle a_{\mathbf{k}} a_{\mathbf{k}} \rangle$ and the corresponding (normalized) eigenfunctions $\varphi_{\mathbf{k}} = e^{-i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$. The macroscopic occupation of the $k = 0$ mode of the ideal gas in the Bose condensed phase corresponds, as expected, to a macroscopic eigenvalue of the reduced single particle density matrix, all other eigenvalues, $N_{\mathbf{k}\neq 0}$, given by the Bose-Einstein distribution, remain of order 1.

Off-diagonal long range order (OLRO). The macroscopic occupation of a single eigenfunction of $\rho^{(1)}$ directly leads to the concept of off-diagonal long range order [2]

$$\rho^{(1)}(\mathbf{r}', \mathbf{r}; \beta) = N_0 \varphi_0^*(\mathbf{r}') \varphi(\mathbf{r}) + \widetilde{\rho}^{(1)}(\mathbf{r}', \mathbf{r}; \beta) \tag{7}$$

where $\widetilde{\rho}^{(1)}$ is a positive operator independent of the boundary conditions, e.g.

$$\widetilde{\rho}^{(1)}(\mathbf{r}', \mathbf{r}; \beta) \to 0 \quad \text{for} \quad |\mathbf{r} - \mathbf{r}'| \to \infty \tag{8}$$

in the limit of a macroscopic system, and $\varphi_0(\mathbf{r})$ is commonly refered to as condensate wave function.

It is important to note that perturbation theory usually simplifies in the thermodynamic limit (e.g. link cluster expansions, Wick's theorem, etc.). Bose condensation with an extensive occupation of a single mode, as well as the sensitivity of the condensate wave function on the boundaries, in general invalidate usual pertubation theory as well as diagrammatic expansions constructed in the normal phase. They need to be adapted to treat Bose condensation by explicitly separating condensate contributions. Technically, it is most convenient to split the condensate contribution to the field operator

$$\psi(\mathbf{r}) = \langle \psi(\mathbf{r}) \rangle + \widetilde{\psi}(\mathbf{r}) \tag{9}$$

such that

$$\langle \psi(\mathbf{r}) \rangle \equiv \varphi_0(\mathbf{r}), \quad \widetilde{\rho}^{(1)}(\mathbf{r}', \mathbf{r}; \beta) = \langle \widetilde{\psi}^\dagger(\mathbf{r}') \widetilde{\psi}(\mathbf{r}) \rangle \tag{10}$$

This is commonly refered to $U(1)$ symmetry breaking. For (stable) particles of non-vanishing mass, in particular bosonic atoms as mainly considered here, $U(1)$ symmetry breaking is strickly speaking not possible, directly violating experimental facts of atomic number/mass conservation. However, it can be simply regarded as a practical tool which correctly reproduces all expectation values up to corrections $\sim N_0^{-1/2}$ (see e.g. [3, 4]). The well known Bogoliubov approximation [5] is one practical demonstration of the simplifications of symmetry breaking; a detailed discussion of number conservation may be found in [6].

The concepts of BEC and OLRO introduced here, do not rely on the assumption of thermal equilibrium and generalize with out complications to out-of-equilibrium and time-dependent situations as the description in terms of the reduced density matrix is completely general.

Dilute Bose gas. In dilute gases where the mean interparticle distance $n^{-1/3}$ greatly exceeds the typical distance r_0 characterizing the effective inter atomic/molecular, collisional properties are quantitatively described by the phase shifts in the asymptotic behavior of the wave function. At low temperatures, two particle scattering is in general dominated by zero energy s-wave scattering, fully characterized by a single parameter, the scattering length a, which in case of a hard sphere model system corresponds to the diameter of the spheres. How is the ideal gas BEC modified by interaction? Let us first focus on the dilute limit $na^3 \to 0$, which applies well to many ultacold atom experiments.

- The critical temperature of Bose condensation assuming a homogeneous system is slightly increased $T_c/T_c^{ideal} = 1 + c\, a n^{-1/3}$, linearly in the scattering length, by an universal constant c [7]. The universality class of the phase transition in a dilute gas is different from the ideal gas.

- At low temperatures the gas is, to leading order, well described by the Bogoliubov approximation. At $T = 0$, the energy per particle is given by

$$E_0/N = \frac{2\pi a n}{m}\left[1 + \frac{128}{15}\sqrt{na^3/\pi}\right] \tag{11}$$

  Please note that the subleading term increases the energy. The leading order term is frequently derived by assuming a Hartree wave function, a simple product state of single particle wave functions.

  The Bogoliubov result demonstrate that the leading order term is not an upper bound on the energy for any $a > 0$. Contrary to many derivations in the literature, the Hartree ansatz is not a valid variational wave function. Why? The Hartree ansatz actually gives an upper bound of the energy $v_0 n/2m$ involving $v_0 = \int d\mathbf{r} v(r)$ of the bare interaction potential instead of the scattering length a. In Ref. [8], explicit calculations for a simple exponential interaction potential, shows that this approximation describes rather badly the dilute gas limit $nv_0^3 \to 0$ and fails to obtain already the leading order term of the energy per particle, $2\pi a n/m$, where a is the scattering length for this potential. It rather corresponds to the extremely dense fluid, $nv_0^3 \to \infty$, which is of limited experimental interest, at least so far. One can also convince oneself, that this simple Hartree approximation becomes completely useless in the hardcore/pseudopotential limit describing ultracold atomic gases where $v_0 \to +\infty$ approaching a zero-range potential, $r_0 \to 0$, such that the scattering length a remains constant.

- At $T = 0$, the condensate fraction is given by

$$\frac{n_0}{n} = \frac{N_0}{N} = 1 - \frac{8}{3}\sqrt{na^3/\pi} \tag{12}$$

  within the Bogoliubov approach. In general, the condensate gets depleted by interaction, $N_0/N < 1$ even at zero temperature, at variance with the superfluid fraction which will be one (see below).

- At low energies, the system can still be described in terms of stable eigen-modes, with phonon (sound) dispersions $\varepsilon(k) \sim \sqrt{k^2/2m(k^2/2m + 4\pi n/m)} \sim c|k|$. Following the discussion of finite size effects of the ground state energy of an ideal phonon gas, we also expect that the ground state energy extrapolates as $1/L^{d+1}$ to the thermodynamic limit.

Local density approximation (LDA). Let us consider the effect of an external potential $U_{\rm ext}$. In the grand canonical ensemble, the partition function writes

$$Z = \mathrm{Tr} e^{-\beta(H+U-\mu N)} \tag{13}$$

where H is the Hamitonian of the homogeneous system. Writing

$$U - \mu N = \int d\mathbf{r}\left[u_{\rm ext}(\mathbf{r}) - \mu\right] n(\mathbf{r}) \tag{14}$$

we can either regard the chemical potential as a constant shift of the external potential, or gather both terms introducing $\mu(\mathbf{r}) \equiv \mu - u_{\rm ext}(\mathbf{r})$. The later expression suggest that the effect of a slowly varying external potential can be described by using the homogeneous result of some observable at the local chemical potential $\mu(\mathbf{r})$.

Thomas-Fermi approximation. Let us start by determining the chemical potential of the homogeneous system at zero temperature to leading order in a

$$\mu = \frac{dE_0}{dN} = \frac{4\pi a n}{m} \tag{15}$$

or, inverting $\mu(n)$ to obtain $n(\mu)$, we get

$$n_0 = \frac{m}{4\pi a}\mu \tag{16}$$

were we have replaced n by the condensate density n_0 within the same order. The condensate density of the inhomogenous system then writes

$$n_0(\mathbf{r}) = \frac{m}{4\pi a}\left[\mu - u_{\rm ext}(\mathbf{r})\right]\theta\left[\mu - u_{\rm ext}(\mathbf{r})\right] \tag{17}$$

where $\theta(x)$ is the step function, needed since a non-vanishing condensate density can only arise for a locally positive chemical potential $\mu - uu_{\rm ext}(\mathbf{r})$. The total number of condensed particles can be calculated by $N_0 = \int d\mathbf{r} n_0(\mathbf{r})$

The local density approximation may fail to describe variations of the density profile at scale comparable or smaller than the healing length ξ where kinetic energy effects are comparable to the chemical potential $1/2m\xi^2 = 4\pi an/m$. Thus, spatial variations of the density profile on the scale of ξ must be small within the LDA.

In the dilute limit, one can show that the condensate wave function is described by a non-linear Schrödinger equation called Gross-Pitaevskii equation in this context

$$i\frac{\partial \Psi_0(\mathbf{r},t)}{\partial t} = \left[-\frac{\nabla^2}{2m} + u_{\rm ext}(\mathbf{r},t) + \frac{4\pi a N_0}{m} |\Psi_0(\mathbf{r},t)|^2 \right] \Psi_0(\mathbf{r},t) \tag{18}$$

which describes the spatial and time dependence of the condensate. At thermal equilibrium $\Psi_0(\mathbf{r},t) = e^{-i\mu t}\Psi_0(\mathbf{r})$. The local density approximation is obtained, neglecting the kinetic energy of the laplacian, the so-called Thomas-Fermi approximation.

Experiments. Experiments on ultracold atoms in magneto-optical traps [9] have been the most convincing experimental realisations of BEC in dilute gases, $na^3 \sim 10^{-6}$. BEC was probed by time-of-flight measurements: After thermalization, the external trapping potential are suddenly switched off, and the gas expands, such that the long time density distribution basically reflects the initial momentum distribution. A strong peak around zero momentum suddenly rises when crossing the critical temperature where the local phase space density in the center of the trap exceeds the critical value ≈ 2.61. Detailed analysis showed that a mean-field description based on the Gross-Pitaevskii equation quantitatively describes these early experiments to a very high accuracy, and the condensate fraction rapidely saturates very close to 100% within the experimental accuracy. This must be compared with the condensate fraction of $\approx 7\%$ in liquid ^4He at zero temperature [10], clearly demonstrating that for helium fluids the ideal/dilute gas description does not apply quantitatively.

II. SUPERFLUIDITY

The macroscopic occupation can lead to very strong violation of classical behavior in quantum liquids and gases. One of the consequences of Bose condensation is the occurence of superfluidity, observed in liquid ^4He below the lambda transition. However, several quite different in- and out-of-equilibrium observations are in general associated with superfluidity, and it is important to properly characterize (and possibly distinguish) them.

Here, I will only discuss the thermodynamic characterization of superfluidity by the occurence of a "non-classical moment of inertia" or the "Hess-Fairbank " effect, the analog of the Meissner effect in superconductors [6].

Moving frames. Superfluidity can be defined as a thermodynamic effect via a response to a slow rotation (or translation for a fully translational invariant system) [11, 12]. For this we will briefly review statistical description of moving systems (we are only interested in the non-relativistic limit). Let us consider two different frames, one denoted by a prime moving with a velocity $\mathbf{u}$ compared to the unprimed frame.

Let $\mathbf{r}$ denote the position of some particle at time t in the labframe, moving to $\mathbf{r} + d\mathbf{r}$ at $t + dt$. We then have

$$\begin{array}{rcl} d\mathbf{r}' &=& d\mathbf{r} - \mathbf{u}dt, \\ dt' &=& dt, \end{array} \qquad \mathbf{u} = \begin{cases} \mathbf{v} = \text{const} & \text{(translation)} \\ \vec{\omega} \times \mathbf{r} = \vec{\omega} \times \mathbf{r}' & \text{(rotation)} \end{cases} \tag{19}$$

or

$$\dot{\mathbf{r}}' = \dot{\mathbf{r}} - \mathbf{u} \tag{20}$$

since $t = t'$ up to an irrevalant constant.

Quantum mechanics is usally adressed via the Hamiltonian. In order to determine the correct Hamiltonian of both frames, we need the respective canonical momentum.

Since the action $\int dt \mathcal{L}(\dot{r}_i, r_i, t)$ is a scalar quantity, the classical equations of motion can be derived from extremizing it independent of the coordinate system used for its description.

Using the Lagragian $\mathcal{L} = \sum_i m\dot{r}_i^2 - V(r_i)$ of our Lab system (the unprimed one), we can simply express the action in terms of our primed coordinates and determine the (classical) equation of motion in our new frame. From the respective canonical momenta, we can then obtain the Hamiltonian of our quantized system in both frames, and relate them.

Let us concentrate on the kinetic energy of a single particle first, and argue later how to generalize these results

$$S = \int dt \frac{m}{2}\dot{r}^2 = \int dt' \frac{m}{2}\left(\dot{r}' + \mathbf{u}\right)^2 = \int dt' \begin{cases} \frac{m}{2}\left(\dot{r}'\right)^2 & + \frac{d}{dt'}\left[m\mathbf{v}\cdot(\mathbf{r}' + \mathbf{v}t'/2)\right] \\ \frac{m}{2}\left(\dot{r}' + \mathbf{u}\right)^2 & \end{cases} \tag{21}$$

The total derivative occuring for the translational motion can be dropped as it does not affect the equation of motions (this is not the case for rotational motion since $\mathbf{u}$ depends on $\mathbf{r}$) and we can directly read of the kinetic part of the Lagrangian in the moving frames

$$\mathcal{L}'(\dot{r}') = \begin{cases} \frac{m}{2}\left(\dot{r}'\right)^2 \\ \frac{m}{2}\left(\dot{r}' + \mathbf{u}\right)^2 \end{cases} \tag{22}$$

from where get the canonical momentum and their relation between both frames

$$\mathbf{p} \;=\; \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}} = m\dot{\mathbf{r}} \tag{23}$$

$$\mathbf{p}' \;=\; \frac{\partial \mathcal{L}'}{\partial \dot{\mathbf{r}}'} = \begin{cases} m\dot{\mathbf{r}}' = m(\dot{\mathbf{r}} - \mathbf{v}) = \mathbf{p} - m\mathbf{v} \\ m(\dot{\mathbf{r}}' + \mathbf{u}) = m\dot{\mathbf{r}} = \mathbf{p} \end{cases} \tag{24}$$

The Hamiltonian then follows from

$$H \;=\; -\mathcal{L} + \mathbf{p}\cdot\dot{\mathbf{r}} = \frac{\mathbf{p}^2}{2m} \tag{25}$$

$$H' \;=\; -\mathcal{L}' + \mathbf{p}'\cdot\dot{\mathbf{r}}' = \begin{cases} \frac{(\mathbf{p}')^2}{2m} = \frac{(\mathbf{p}-m\mathbf{v})^2}{2m} = H - \mathbf{v}\cdot\mathbf{p} + \frac{m\mathbf{v}^2}{2} \\ \frac{(\mathbf{p}')^2}{2m} - \mathbf{p}'\cdot\mathbf{u} = \frac{\mathbf{p}^2}{2m} - \mathbf{p}\cdot(\omega\times\mathbf{r}) = H - \omega\cdot\mathbf{l} \end{cases} \tag{26}$$

where $\mathbf{l} = \mathbf{r}\times\mathbf{p}$ is the angular momentum.

Let us now consider the generic Hamiltonian in our laboratory frame

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} v(|\mathbf{r}_i - \mathbf{r}_j|) + \sum_i u_{\text{ext}}(\mathbf{r}_i, t) \tag{27}$$

where $u_{\text{ext}}(\mathbf{r}, t)$ is an external potential, e.g. modelling the walls of the container.

Let us first consider the container at rest in the laboratory frame. Then the external potential $u_{\text{ext}}(\mathbf{r})$ is time-independent, and, thermodynamic equilibrium in the laboratory frame will be eventually established, such that the probability for a state of energy E to occur is $\sim e^{-\beta E}$.

Now consider that the container is put into rotation or translation (Note that translation is conceptually more difficult, and should be regarded as the limiting case of rotating a nearly cylindrically symmetric annular container with very large diameter.). In the laboratory frame, the interaction with the walls becomes time-dependent, $u_{\text{ext}}(\mathbf{r}, t) \equiv u_{\text{ext}}(\mathbf{r} - \mathbf{u}t) \equiv u_{\text{ext}}(\mathbf{r}')$, whereas the walls are at rest in the coordinate system of the co-moving/rotating frame ($u_{\text{ext}}(\mathbf{r}')$ is time independent). Statistical equilibrium will then be reached in the comoving frame, and statistical properties can be obtained by the density operator in the comoving frame,

$$\rho' \;=\; e^{-\beta H'} \tag{28}$$

$$H' \;=\; \sum_i \frac{\mathbf{p}_i'^2}{2m} + \sum_{i<j} v([\mathbf{r}_i' - \mathbf{r}_j'|) + \sum_i u_{\text{ext}}(\mathbf{r}_i') \tag{29}$$

Then the Hamiltonian H' can be expressed in terms of the lab frame coordinates and momenta, $\mathbf{r}$ and $\mathbf{p}$, respectively,

$$H'(\mathbf{r}', \mathbf{p}', t') \;=\; \begin{cases} H(\mathbf{r}, \mathbf{p}, t) - \mathbf{v}\cdot\mathbf{P} + \frac{Nm}{2}v^2 \\ H(\mathbf{r}, \mathbf{p}, t) - \omega\cdot\mathbf{L} \end{cases} \tag{30}$$

where $\mathbf{P} = \sum_i \mathbf{p}_i$ is the center of mass momentum and $\mathbf{L} = \sum_i \mathbf{l}_i$ the total angular momentum of the system, as can be seen rather straightforward extending our previous derivation of the canonical momentum. Now, since in the co-moving frame the Hamiltonian is time independent, let us choose to look at the system at periodic times $t_n' = \Delta t + 2n\pi/\omega$, $n = 1, 2 \ldots$ with Δt fixed , such that the conditions at times t_n' in the lab frame are equal and $u_{\text{ext}}(\mathbf{r}, t_n)$ is independent of n (again we need to consider translational moves as rotation with large diameter). At these times, all properties of the system do not depend on n in the lab system and are described by the effective Hamiltonian $H - \omega\cdot\mathbf{L}$ with $u_{\text{ext}}(\mathbf{r}, t_n)$, without any symmetry requirements on u_{ext}.

Quantum statistical mechanics. Turning back to a quantum description, once we have identified the canonical momenta, we can upgrade them to operators imposing the usual commutation relations. However, this is not enough: we also have to specify the states the operators act on. In particular,we need to specify the boundary conditions of the corresponding wave functions, which, at least in the case of ideal bosons, become important even on a macroscopic scale below temperatures of Bose-Einstein condensation, as they determine the condensate wave function. When discussing BEC of the ideal gas above, we have as usual assumed periodic boundary conditions of the underlying single particle wave functions, $\varphi(x+L)=\varphi(x)$, to mimic the bulk of a macroscopic system. However, this explicitly involves to chose a reference frame. Does this choice influences thermodynamics, and, if so, which one is correct?

Let us start considering a rotating container. Due to the walls of the container the density of our fluid will eventually vanish at large enough radial distances (remember that $|\mathbf{r}'|=|\mathbf{r}|$). Independent of the reference frame, that of the laboratory or the co-moving/rotating one, we can therefore assume vanishing wave functions at infinity. However, using radial coordinates, we also have to impose single valueness of all underlying wave functions, $\phi(r,\varphi+2\pi)=\phi(r,\varphi)$, which leeds to the quantization of angular momentum. Physically, the laboratory and the rotating frame are not equivalent, e.g. a person in the rotating frame can measure and determine that he is actually rotating, whereas the laboratory frame is to sufficiently high precision an inertial system (e.g. with respect to the fixed stars). Therefore, we need to impose the single valueness of the wave function in the laboratory frame, and not in the co-moving one.

Since the translational motion must be regarded as the limiting description of a rotational motion of an annulus of large diameter, the laboratory frame is also the correct choice of reference frame to impose periodic boundary conditions, $\varphi(x+L)=\varphi(x)$, in this case.

Normal/superfluid mass density: translational invariant system. Let us now focus on the translational invariant system, moving with constant velocity $\mathbf{v}$ compared to our laboratory frame. The system thus thermalizes in the comoving (primed) frame, such that thermodynamics is given by the corresponding parition function

$$Z_{\mathbf{v}}=\mathrm{Tr}e^{-\beta H'} \tag{31}$$

Let us now measure the total momentum in the lab frame

$$\langle\mathbf{P}\rangle_{\mathbf{v}}\equiv\frac{1}{Z_v}\mathrm{Tr}\left[\mathbf{P}e^{-\beta H'}\right] \tag{32}$$

and consider a very small motion such that we can expand to leading order in $v\to 0$,

$$\langle\mathbf{P}\rangle_{\mathbf{v}}=\beta\langle\mathbf{P}[\mathbf{P}\cdot\mathbf{v}]\rangle_{v=0}+\mathcal{O}(v^2) \tag{33}$$

For a classical system, momenta are always Boltzmann distributed, and the center-of-mass momentum is therefore $\propto\exp[-\beta\mathbf{P}^2/2M]$, as we have seen above, and we have $\langle\mathbf{P}\rangle_v=M\mathbf{v}$. This simply tells us that the center of mass momentum of a system which moves with velocity $\mathbf{v}$ is given by $M\mathbf{v}$ as we expect from daily live. In general, quantum systems will give rise to deviations from the classical behavior. However, the center of mass motion, being a macroscopic object, is expected to behave classical at any non vanishing temperatures.

The normal fraction of the fluid ρ_N/ρ is defined as the part of the center of mass motion which behaves classical and moves with the system, thus having a non-vanishing momentum in the lab frame

$$\langle\mathbf{P}\rangle_{\mathbf{v}}=\frac{\rho_N}{\rho}M\mathbf{v} \tag{34}$$

whereas the superfluid density, $\rho_s=\rho-\rho_N$, remains fix in the lab frame.

We can relate the total momentum to the free energy difference $\Delta F_v\equiv -T\log Z_v/Z$ using

$$\langle\mathbf{P}\rangle_{\mathbf{v}}=-\frac{dF_{\mathbf{v}}}{d\mathbf{v}}+M\mathbf{v} \tag{35}$$

or

$$\frac{\rho_s}{\rho}=\frac{dF_{\mathbf{v}}}{d(M\mathbf{v})}=\frac{dF_v}{d\left(\frac{1}{2}Mv^2\right)} \tag{36}$$

where we have used that the free energy difference can only depend on v^2 for an isotropic system.

For liquid helium, below the lambda transition, some fraction of the liquid will stay at rest in the laboratory frame. Only the normal part of the fluid will behave classical and move as expected. The occurence of a superfluid fraction is a thermodynamic effect, since the fraction can be modified reversely by changing temperature.

Superfluidity: ideal gas Let us first discuss the response of the homogeneous d-dimensional Bose gas to a moving system with small velocities. From the discussion above, we need to calculate the total momentum squared, e.g. in the x-direction

$$\begin{aligned}\langle P_x^2\rangle=\left\langle\left[\sum_{\mathbf{k}}k_xN_{\mathbf{k}}\right]^2\right\rangle=\sum_{\mathbf{k}}\sum_{\mathbf{p}}k_xp_x\langle N_{\mathbf{k}}N_{\mathbf{p}}\rangle&=\sum_{\mathbf{k}}k_x^2\left[\langle N_{\mathbf{k}}^2\rangle-\langle N_{\mathbf{k}}\rangle^2\right]+\sum_{\mathbf{k}}\sum_{\mathbf{p}}k_xp_x\langle N_{\mathbf{k}}\rangle\langle N_{\mathbf{p}}\rangle\\&=\frac{1}{d}\sum_{\mathbf{k}}k^2\frac{\partial}{\partial(-\beta\varepsilon_k)}\langle N_{\mathbf{k}}\rangle\Big|_{\beta\mu}+\sum_{\mathbf{k}}\sum_{\mathbf{p}}k_xp_x\langle N_{\mathbf{k}}\rangle\langle N_{\mathbf{p}}\rangle\end{aligned} \tag{37}$$

Whereas the last term on the rhs vanishes identically by symmetry, we now use that $\varepsilon_k = k^2/2m$, and integrate by part

$$\langle P_x^2 \rangle = -\frac{2mT}{d}\alpha_d V \int dk k^{d-1} k^2 \frac{\partial}{2k\partial k}\langle n_k \rangle = mTV\alpha_d \int dk k^{d-1}\langle n_k\rangle = (N-N_0)mT = (M-N_0 m)T \tag{38}$$

where α_d is a geometrical surface factor depending on the spatial dimension d. We see that for $N \leq N_c$ the system behaves "normal", however, for $N > N_c$ the particles in the condensate have zero momenta and will not contribute to the fluctuations of the total momenta and we have

$$\langle \mathbf{P} \rangle_{\mathbf{v}} = (N - N_0)m\mathbf{v} \tag{39}$$

and the normal mass is smaller than the total mass leading to a the superfluid mass density $N_0 m/V$ in the non-interacting system [17]

Landau's criterium of superfluidity. Let us consider a translational invariant system close to zero temperature, such that the lowest energy eigenstates of the system at rest in the lab frame can be described in terms of quasiparticle occupation number $\mathcal{N}_{\mathbf{p}}$ with

$$E = E_0 + \sum_{\mathbf{p}} \mathcal{N}_{\mathbf{p}}\varepsilon_{\mathbf{p}} \tag{40}$$

$$\mathbf{P} = \mathbf{P}_0 + \sum_{\mathbf{p}} \mathcal{N}_{\mathbf{p}}\mathbf{p} \tag{41}$$

and we could have also assumed $\mathbf{P}_0 = 0$, and $\mathcal{N}_{\mathbf{p}} = 0$ at $T = 0$.

When we move the system with a small uniform velocity $\mathbf{v}$ compared to the lab frame, we expect the system to thermalize in the co-moving frame where energies and momenta are given by

$$E' = = E - \mathbf{P}\mathbf{v} + \frac{1}{2}mv^2 \tag{42}$$

$$= E_0 + \sum_{\mathbf{p}} \mathcal{N}_{\mathbf{p}}\left(\varepsilon_{\mathbf{p}} - \mathbf{p}\cdot\mathbf{v}\right) + \frac{1}{2}mv^2 \tag{43}$$

whereas

$$\mathbf{P}' = \mathbf{P} - Nm\mathbf{v} = \mathbf{P}_0 - Nm\mathbf{v} + \sum_{\mathbf{p}} \mathcal{N}_{\mathbf{p}}\mathbf{p} \tag{44}$$

Focusing on zero temperature, the partition function in the comoving frame simplifies to the contribution of only one state which minimizes the total energy, E', with respect to the occupation numbers $\mathcal{N}_p \geq 0$. The minimal energy of the co-moving frame will not have any non-vanishing quasiparticle occupation unless $\varepsilon_{\mathbf{p}} - \mathbf{p}\cdot\mathbf{v} < 0$.

Assuming a linear phonon-like dispersion relation for the quasi-particle excitation energies, $\varepsilon_{\mathbf{p}} = c|\mathbf{p}|$ where c is the speed of sound, we have

$$\varepsilon_{\mathbf{p}} - \mathbf{p}\cdot\mathbf{v} = p\left(c - \cos\theta v\right) \geq p(c - v) \tag{45}$$

and for small velocities, $v < c$, the state remains in the ground state of the lab frame. In particular, since $\mathbf{P} = \mathbf{P}_0$, the normal fraction is expected to vanish approaching zero temperature, or, equivalently, $\rho_s = \rho$. Once the velocity exceeds the speed of sound, superfluidity will disappear. However, this criterium should not be taken too literal, as the true ground state of the system will change already much before, however, in practice, the system will remain still metastable, but one needs to go beyond a pure thermodynamic description.

Please note that in dilute systems described by the Bogoliubov approximation at low temperatures, the dispersion relation is indeed linear. Therefore, althouth the condensate fraction is depleted by interaction even at zero temperature, the superfluid density equals the total density in this limit.

For an ideal Bose gas, the excitation spectrum is quadratic, so from Landau's criterium, one would expect a vanishing critical velocity in the thermodynamic limit.

Let us stress that we have used a macroscopic observable, here the center of mass momentum, to define superfluidity as the deviation of its mean value compared to the classical expectation. In addition, in our idealized situation, this observable commutes with the Hamiltonian, so that the energy values could be (at least in principle) characterized by quantum numbers of the center of mass momentum. The dependence of the energy on this quantum numbers gave rise to superfluidity, even in the case of an ideal gas where this dependence occurs purely due to statistical reasons. In practice, not $\mathbf{P}$, but the total moment of intertia is used for experimental definition of superfluidity.

Winding numbers. The sensitivity of superfluidity to the boundary conditions ("topology") can be read off from the so-called winding number estimator used in Path-Integral Monte Carlo calculations [13] considering again the response of a translational invariant system described by periodic boundary condition in a slowly moving frame. Here, the center of mass momentum commutes with the Hamiltonian, $[H, P] = 0$, and we can always separate the center of mass motion

$$H = \frac{\mathbf{P}^2}{2M} + \widetilde{H} \tag{46}$$

where $M = Nm$ is the total mass, and $\widetilde{H}$ is independent of the center of mass coordinate $\mathbf{R} = \sum_i \mathbf{r}_i/N$, $[\widetilde{H}, P] = 0$. The Hamiltonian of the co-moving frame only affects the center of mass motion

$$H' = \frac{(\mathbf{P} - M\mathbf{v})^2}{2M} + \widetilde{H} \tag{47}$$

Let us thus consider the density matrix of the center-of-mass separately inserting a complete set of momentum eigenstates $P|\mathbf{K}\rangle = \mathbf{K}|\mathbf{K}\rangle$

$$\langle \mathbf{R}'|e^{-\beta\frac{(\mathbf{P}-M\mathbf{v})^2}{2M}}|\mathbf{R}\rangle = \int d\mathbf{K}\langle \mathbf{R}'|\mathbf{K}\rangle e^{-\beta\frac{(\mathbf{K}-M\mathbf{v})^2}{2M}}\langle \mathbf{K}|\mathbf{R}\rangle = \int d\mathbf{K} e^{i\mathbf{K}\cdot(\mathbf{R}'-\mathbf{R})-\beta\frac{(\mathbf{K}-M\mathbf{v})^2}{2M}} \sim e^{i(\mathbf{R}'-\mathbf{R})\cdot M\mathbf{v}-\frac{M(\mathbf{R}'-\mathbf{R})^2}{2\beta}} \tag{48}$$

or

$$\frac{\langle \mathbf{R}'|e^{-\beta\frac{(\mathbf{P}-M\mathbf{v})^2}{2M}}|\mathbf{R}\rangle}{\langle \mathbf{R}'|e^{-\beta\frac{\mathbf{P}^2}{2M}}|\mathbf{R}\rangle} = e^{i\sum_i(\mathbf{r}'_i-\mathbf{r}_i)\cdot m\mathbf{v}} \tag{49}$$

Since the center of mass momentum commutes with the Hamiltonian, we can relate the density matrix of the co-moving frame to that of the laboratory frame, but some care is needed. Let us first consider the density matrix of distinguishable (Boltzmann) particles in the position representation

$$\rho_B(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \mathbf{r}'_2, \ldots \mathbf{r}'_N; \beta) \equiv \langle \mathbf{r}'_1| \otimes \langle \mathbf{r}'_2| \otimes \cdots \otimes \langle \mathbf{r}'_N|e^{-\beta H}|\mathbf{r}\rangle \times \cdots \otimes |\mathbf{r}_N\rangle \tag{50}$$

where we can directly relate both frames by

$$\rho'_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots \mathbf{r}'_N; \beta) = \rho_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots \mathbf{r}'_N; \beta) e^{i\sum_i(\mathbf{r}'_i-\mathbf{r}_i)\cdot m\mathbf{v}} \tag{51}$$

Indeed, it is straighforward to show that ρ'_B satisfies the Bloch equation $-\partial_\beta \rho'_B = H'\rho'_B$ from Eq. (51) if we have $-\partial_\beta \rho_B = H\rho_B$, since

$$\begin{aligned}
\partial_\beta \rho'_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots \mathbf{r}'_N; \beta) &= e^{i\sum_i(\mathbf{r}'_i-\mathbf{r}_i)\cdot m\mathbf{v}} \partial_\beta \rho_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots \mathbf{r}'_N; \beta) && (52)\\
H'\rho'_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots \mathbf{r}'_N; \beta) &= \left[-\frac{\hbar}{2m}\sum_i (\partial_{\mathbf{r}_i} + im\mathbf{v})^2 + \sum_{i<j} V(r_i - r_j)\right] \rho'_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots \mathbf{r}'_N; \beta)\\
&= e^{i\sum_i(\mathbf{r}'_i-\mathbf{r}_i)\cdot m\mathbf{v}} \left[-\frac{\hbar}{2m}\sum_i \partial^2_{\mathbf{r}_i} + \sum_{i<j} V(r_i - r_j)\right] \rho_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots \mathbf{r}'_N : \beta)\\
&= e^{i\sum_i(\mathbf{r}'_i-\mathbf{r}_i)\cdot m\mathbf{v}} H\rho_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}'_1, \ldots \mathbf{r}'_N; \beta) && (53)
\end{aligned}$$

(It equally holds if the Hamiltonian would act on the primed coordinates of ρ'_B or ρ_B, respectively, with the corresponding change of sign in front of the $i\mathbf{v}$ term, since $\mathbf{p} = i\hbar\nabla$.)

The partition function of Bosons with periodic boundary is given by symmetrizing with respect to permutations considering all closed paths modulus periodic images in space. We then get

$$Z = \frac{1}{N!}\sum_P \sum_M \int d\mathbf{r}_1 \ldots d\mathbf{r}_N \rho_B(\mathbf{r}_1, \ldots, \mathbf{r}_N; \mathbf{r}_{P(1)} + m_1 L, \ldots, \mathbf{r}_{P(N)} + m_N L) \tag{54}$$

and we from the path integral expression of ρ_B we can relate the partition function of the co-moving frame with that of the lab frame

$$e^{-\beta\Delta F_v} \equiv \frac{Z_{\mathbf{v}}}{Z} = \langle e^{i\sum_i(\mathbf{r}'_{P(i)}-\mathbf{r}_i)\cdot m\mathbf{v}}\rangle \tag{55}$$

where the expectation value is taken with the expressions of the lab frame $v = 0$ and we have denoted by $\mathbf{r}'_{P(i)}$ the unwided coordinate given by $\mathbf{r}'_{P(i)} = \mathbf{r}_{P(i)} + m_1 L$.

From the free energy difference, we then obtain the so-called winding number estimator for the superfluid fraction

$$\frac{\rho_s}{\rho} = \frac{mL^2}{3\beta N}\langle W^2\rangle \tag{56}$$

where the winding number is defined as

$$\sum_i (\mathbf{r}'_{P(i)} - \mathbf{r}_i) = \mathbf{W}L \tag{57}$$

Since the paths have to close modulus periodic images, the winding number is an integer and cannot change continuously between different configuration. It thus represents a topological number characterizing configurations of paths.

The topological character of $\mathbf{W}$ becomes clear when switching to a system without translational invariance. Although our derivation above was based on total momentum conservation, the final formula remains unchanged when used in path-integral calculations, in general, not relying on translational symmetry, only on periodic boundary conditions, as the integer winding numbers are not affected. Explicitly one can use for small imaginary times, $\tau = \beta/M$, that

$$e^{\tau H'} = e^{-\tau H} e^{+\tau \mathbf{P}^2/2M} e^{-\tau(\mathbf{P}-Mv)^2/2M} \tag{58}$$

to leading order τ and directly copy the above results into the path-integral expression. However, since $\mathbf{R}' - \mathbf{R} = \int d\tau \dot{\mathbf{R}}(\tau)$ must be an integer fraction of the system size, the final formulas remains unaffected. A different derivation can be found in Ref.[13].

The extrapolation to zero temperature might need some care, e.g. in a translational invariant time-reversal system, since we expect that the ground state is an eigenstate of zero total momentum.Classicaly, of course, none of the particles is moving, the ground state should be a crystal minimizing the potential energy. The response to a small rotation/translation will be quite different.

Let us use Eq. (36), replacing the free energy by the ground state energy, to discuss the superfluid fraction at zero temperature

$$\frac{\rho_s}{\rho} = \frac{dE_v}{d(Mv^2/2)} \tag{59}$$

where E_v is the ground state expectation value of H'. For a homogenous system, we can use the total momentum $\mathbf{P}$ to label energy eigenstates of H such that we have

$$E_v = \min_{\mathbf{P}} \left[E_0(\mathbf{P}) - \mathbf{P}v + \frac{1}{2}Mv^2 \right] \tag{60}$$

and $E_0(\mathbf{P})$ is the ground state energy of H with $\mathbf{P}$.

Bogoliubov's approximation and Landau's theory assumes $E_0(\mathbf{P}) \sim |\mathbf{P}|$, such that the system is fully superfluid at zero temperature. Gavoret and Nozières [14] have performed a diagrammatic analysis which shows that this is true to all orders in perturbation theory, provided perturbation theory converges.

Feynman's argumentation is based on the nodeless ground state of a Bose liquid, constructing low energy excitations (phonon) basically by small changes in the phase [15]. Walter Kohn [16] further discusses the relation of the response to a small gauge field (ou $\mathbf{v}$) based on localization properties of the ground state wave function.

III. SOME REMARKS

- role of spatial dimensions: for $D = 2$, Kosterlitz-Thouless transition, below T_{KT} superfluid phase, but no BEC at finite T (Mermin-Wagner theorem)
- Fermions: BCS transition (pairing!), BCS-BEC cross-over
- excitons: bound e-h pairs, composite bosonic quasi-particles with life-time
- exciton-polarons: BEC but out-of-equilibrium

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[1] * O. Penrose and L. Onsager, Phys. Rev. 104, **576** (1956).
[2] * C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962).
[3] * P. C. Hohenberg and P. C. Martin, Annals of Physics **34**, 291 (1965).
[4] S. T. Beliaev, Soviet Physics JETP **7**, 289 (1958).
[5] N. Bogolubov, J. Phys. U.S.S.R. **11**, 23 (1947).
[6] A. J. Leggett, *Quantum Liquids*, Oxford University Press (2006).
[7] G. Baym, J.-P. Blaizot, M. Holzmann, F. Lalo, and D. Vautherin, Phys. Rev. Lett. **83**, 1703 (1999).
[8] E. A. Carlen, M. Holzmann, I. Jauslin, and E. H. Lieb, Phys. Rev. A **103**, 053309 (2021).
[9] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell, Science **269**, 198 (1995).
[10] H. R. Glyde, R. T. Azuah, and W. G. Stirling Phys. Rev. B **62**, 14337 (2000).
[11] * G. Baym, in *Mathematical Methods in Solid State and Superfluid Theory*, edited by R. C. Clark and G. H. Derrick (Oliver and Boyd, Edinburgh, 1969), p. 121.
[12] A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
[13] * E. L. Pollock and D. M. Ceperley, Phys. Rev. B **36**, 8343 (1987).
[14] J. Gavoret and P. Nozières, Ann. Phys. **28**, 349 (1964).
[15] R.P. Feynman, *Statistical Mechanics*, (Benjamin/ Cummings, Reading, MA, 1972).
[16] * W. Kohn, Phys. Rev. **133**, A171 (1964).
[17] Note that we have actually assumed that v is arbitrary small. That it remains actually valid for finite v must be adressed separately and is connected with the metastability of a superflow. The ideal gas is pathological, as our thermodynamic considerations predicts superfluidity, but there is actually no superflow at finite v in the thermodynamic limit.