

ON THE RIGOROUS DEFINITION OF SUPERFLUIDITY AND SUPERCONDUCTIVITY

Takeo Izuyama
Institute of Physics, College of General Education
University of Tokyo
Komaba, Meguro-ku, Tokyo 153, JAPAN

It is the purpose of this report to give a rigorous definition of superfluidity and to show that neither the off-diagonal long range order (ODLRO) nor the Bose-Einstein condensation can be a sufficient condition for superfluidity. The sufficient condition for superfluidity in a system possessing the ODLRO is also presented.

We start with the Hamiltonian

$$H = \sum_j \vec{p}_j^2 / 2m + V(\vec{r}_1, \dots, \vec{r}_N)$$

together with the cyclic condition

$$V(\vec{r}_1, \dots, \vec{r}_{j-1}, \vec{r}_j + \vec{L}, \vec{r}_{j+1}, \dots, \vec{r}_N) = V(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_N)$$

where $\vec{L} = (L, 0, 0)$ or $(0, L, 0)$ or $(0, 0, L)$. The impurity potential as well as the potential for interparticle forces are included in V . Suppose a uniform external field be switched on¹. It exerts the force $E(t) = E \exp(\epsilon t)$ ($\epsilon > 0$) on a particle along the positive direction of the x-axis. The field is described by the vector potential $\vec{F}(t) = (F(t), 0, 0)$ with $\partial_t F(t) = E(t)$. Then the

Hamiltonian is $\mathcal{H} = \sum_j \frac{1}{2m} (\vec{p}_j + \vec{F}(t))^2 + V$. In the infinite

past the system is supposed to be in the equilibrium state described by the canonical or the grand canonical density matrix $\rho \propto \exp\{-\beta(H - \mu N)\}$. The above situation represents the system contained in a slowly rotating torus. We follow the logic of Kubo's linear response theory². The linear response current against the external field $F(t)$ is

$$\overline{J(t)} = \left\{ \frac{N}{m} - 2 \left\langle \left\langle J \frac{H^x}{(H^x)^2 + \epsilon^2} J \right\rangle \right\rangle \right\} F(t)$$

where $J \equiv \sum_j \vec{p}_j^x / m$, $H^x \equiv [H, \dots]$, $\langle \dots \rangle = \text{Tr} \{ \dots \}$, and $\langle \langle \dots \rangle \rangle$ denotes the average over impurity distributions. The presence of impurities is crucial in a consideration on superfluidity. The response current is expressed as $j(t) \equiv N^{-1} \overline{J(t)} \equiv j_1(t) + j_2(t)$, where $j_1(t) = \Lambda F(t)$ and $j_2(t) = \sigma_\epsilon E(t)$ with

$$\Lambda \equiv \frac{1}{m} - \frac{2}{N} \left\langle \left\langle J \frac{Q}{H^x} J \right\rangle \right\rangle \quad \text{and} \quad \sigma_\epsilon \equiv \frac{2}{N} \left\langle \left\langle J \left(\frac{Q}{H^x} \frac{\epsilon}{(H^x)^2 + \epsilon^2} \right) J \right\rangle \right\rangle.$$

In the above the projection operator Q is defined by

$$(QJ)_{nm} = J_{nm} \quad \text{for } E_n \neq E_m \quad \text{and} \quad 0 \quad \text{for } E_n = E_m.$$

It is only $j_2(t)$ that corresponds to the ordinary Ohmic current.

In fact, if we take the thermodynamic limit (denoted by Lim) and then put $\epsilon \rightarrow 0$, we obtain

$$\sigma = \text{Lim} \frac{2}{N} \left\langle \left\langle J \frac{\delta(H^x)}{H^x} Q J \right\rangle \right\rangle$$

which is a generalized version of the Greenwood formula³ for the Ohmic conductivity. The other component $j_1(t)$ represents the persistent current, which is non-dissipative: If Λ is non-vanishing, then a finite current exists even for an infinitesimal $E(t)$. We have the following;

$\text{Lim } \Lambda > 0$: Superfluidity.

$\text{Lim } \Lambda = 0$: Normal fluidity.

$\text{Lim } \Lambda < 0$: The assumed (ground) state is unstable.

Note that the perfect conductor $\sigma = \infty$ and the superconductor $\text{Lim } \Lambda > 0$ are entirely different.

To see that the ODLRO does not necessarily lead to $\text{Lim } \Lambda > 0$, we consider here the ground state of ideal Bosons in a large one-dimensional ring with a single δ -function potential at the origin. The single particle Hamiltonian is $H_1 = - (1/2m) (d/dx)^2 + g \delta(x)$. The even parity solution of $H_1 \psi_k = E_k \psi_k$ is $\psi_k \propto \cos[k((L/2) - x)]$ for $0 < x < L$, where k is determined by $\tan(kL/2) = mg/k$ and $E_k = k^2/2m$. The odd parity solutions of $H_1 \phi_n = E_n \phi_n$ is $\phi_n \propto \sin[(2\pi n/L)((L/2) - x)]$ with $n = 1, 2, \dots$ and $E_n = (2\pi n/L)^2 (1/2m)$. The ground state of H_1 is described by ψ_{k_0} where k_0 is the minimum value of k . For large L , $k_0 = (\pi/L) - (2\pi/L^2 mg) + \dots$. Thus

$$\begin{aligned} \frac{2}{N} \left\langle \psi_0 \left| J \frac{1}{H^x} J \right| \psi_0 \right\rangle &= \frac{4}{m} \sum_n \frac{|\langle \phi_n | p^x | \psi_{k_0} \rangle|^2}{(2\pi n/L)^2 - k_0^2} \\ &\xrightarrow{\text{Lim}} \frac{64}{\pi^2 m} \sum_{n=1}^{\infty} \frac{4n^2}{(4n^2 - 1)^3} = \frac{1}{m}. \end{aligned}$$

The Thomas-Kuhn sum rule $\Lambda = 0$, which holds in any non-cyclic system, has been restored by a single scatterer in the cyclic system. Our system exhibits the condensation $\langle \langle \psi_0 | a_0^\dagger a_0 | \psi_0 \rangle \rangle = 8N/\pi^2$ and the ODLRO $\langle \langle \psi_0 | \psi^\dagger(x') \psi(x'') | \psi_0 \rangle \rangle = 2(N/L) \neq 0$, though there is no superfluidity.

Finally a system of interacting Bosons containing low concentration of impurities is considered. Suppose that the system possesses the ODLRO

$\lim_{|\vec{r}' - \vec{r}''| \rightarrow \infty} \lim \langle \psi(\vec{r}') \psi^\dagger(\vec{r}'') \rangle \equiv \langle \phi^2 \rangle \neq 0$. We start with the formula¹

$$\Lambda = -2N^{-1}L^2 \langle \langle J(x') (Q/H^X) J(x'') \rangle \rangle$$

where $J(x') \equiv (1/2m) \sum_j \{ p_j^x \delta(x_j - x') + \delta(x_j - x') p_j^x \}$

and $x' \neq x''$. We consider the case $|x' - x''| \rightarrow \infty$. It is proved that

$$\langle \langle J(x') \frac{Q}{H^X} J(x'') \rangle \rangle = \int dy' dz' \int dy'' dz'' \lim_{\epsilon \rightarrow +0} i \left(\int_0^\infty - \int_{-\infty}^0 \right) dt e^{-\epsilon |t|} \Gamma(\vec{r}', t | \vec{r}'', 0)$$

where

$$\Gamma(\vec{r}', t | \vec{r}'', 0) = (1/2m^2) \{ \langle \langle (\partial' \psi^\dagger(\vec{r}', t)) \psi(\vec{r}', t) \psi^\dagger(\vec{r}'', 0) (\partial'' \psi(\vec{r}'', 0)) \rangle \rangle + \langle \langle \psi^\dagger(\vec{r}', t) (\partial' \psi(\vec{r}', t)) (\partial'' \psi^\dagger(\vec{r}'', 0)) \psi(\vec{r}'', 0) \rangle \rangle \} - (1/4m^2) \partial' \partial'' \langle \langle \rho(\vec{r}', t) \rho(\vec{r}'', 0) \rangle \rangle$$

with $\partial = \partial/\partial x$ and $\rho(x)$ = the density operator. The last term in Γ does not contribute when $|x' - x''| \rightarrow \infty$. We adopt the decoupling approximation, which is believed to be valid in this limit.

$$\Gamma(\vec{r}', t | \vec{r}'', 0) = (\langle \phi^2 \rangle / 2m^2) \partial' \partial'' \{ \langle \langle \psi^\dagger(\vec{r}', t) \psi(\vec{r}'', 0) \rangle \rangle + \langle \langle \psi(\vec{r}', t) \psi^\dagger(\vec{r}'', 0) \rangle \rangle \}$$

$$\text{Then } \langle \langle J(x') \frac{Q}{H^X} J(x'') \rangle \rangle = \frac{\langle \phi^2 \rangle}{2m^2} \frac{1}{\Omega} \sum_{k \neq 0} k^2 e^{ik(x' - x'')} \int_{-\infty}^{\infty} \frac{\langle A(k, \omega) \rangle}{\omega} d\omega$$

where $k = 2\pi n/L$, Ω = volume, and

$$A(k, \omega) = \langle a_k \delta(H^X - \mu - \omega) a_k^\dagger \rangle - \langle a_k^\dagger \delta(H^X + \mu + \omega) a_k \rangle$$

with $a_k \equiv \Omega^{-1/2} \int \psi(\vec{r}) e^{-ikx} d\vec{r}$.

The quantity $\int d\omega \langle A(k, \omega) \rangle / \omega$ is obtained by a general argument.

The result is $\int_{-\infty}^{\infty} d\omega \frac{\langle A(k, \omega) \rangle}{\omega} = \frac{m^2 \langle \phi^2 \rangle}{k^2 f(k)}$, where $f(k)$ may be a

function of k in the impure system. In the case of pure systems considered by the Josephson-Baym theory^{4,5}, $f(k) = \rho_s$.

The condition for superfluidity is found to be $f(k) = \text{constant} \equiv \tilde{\rho}_s$

(for small k including the smallest one, namely, $k = 2\pi/L$).

$$\therefore \Lambda = - \frac{m \langle \phi^2 \rangle^2}{\rho \tilde{\rho}_s} \sum_{k \neq 0} \exp[ik(x' - x'')] = \frac{m \langle \phi^2 \rangle^2}{\rho \tilde{\rho}_s} > 0$$

where $\rho = mN/\Omega$. If ρ_s is defined by the London equation, then

$$\tilde{\rho}_s = \langle \phi^2 \rangle^2 / \rho_s$$

The condition $f(k) \rightarrow \tilde{\rho}_s$ ($k \rightarrow 0$) is not trivial. In the system of ideal (non-interacting) Bosons containing macroscopic number of impurities, $f(k)$ diverges as k^{-2} , which is rigorously proved. In this case $\Lambda = 0$.

References 1) T. Izuyama, Progr. Theor. Phys., 50, 841 (1973).

2) R. Kubo, Jour. Phys. Soc. Japan, 12, 570 (1957).

3) D. A. Greenwood, Proc. Phys. Soc., 71, 585 (1958).

4) B. D. Josephson, Phys. Letters, 21, 608 (1966).

5) G. Baym, in Mathematical Methods in Solid State and Superfluid Theory, edited by R. C. Clark and G. H. Derrick (Oliver & Boyd, Edinburgh 1967) p.121 ~ 156.