

Condensate superfluidity and infrared structure of the single-particle Green's function: The Josephson relation

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(Received 28 March 2007; revised manuscript received 2 July 2007; published 21 September 2007)

We derive the Josephson relation in a superfluid between the condensate density, the superfluid mass density, and the infrared structure of the single-particle Green's function by means of diagrammatic perturbation theory. The derivation is valid for finite systems and two dimensions.

DOI: [10.1103/PhysRevB.76.092502](https://doi.org/10.1103/PhysRevB.76.092502)

PACS number(s): 05.30.Jp, 03.75.Hh

Although the phenomena of superfluidity and Bose condensation¹ are intimately related, the connection between the condensate density n_0 and the superfluid mass density ρ_s is only indirect. In the limit of dilute gases, the superfluid mass density simply equals the condensate density times the particle mass m . More generally, the two quantities are related via the infrared structure of the single-particle Green's function G . The detailed relation was given by Josephson,^{2,3}

$$\rho_s = -\lim_{k \rightarrow 0} \frac{n_0 m^2}{k^2 G_{11}(k, 0)}, \quad (1)$$

where $G_{11}(k, 0)$ is the single-particle Green's function at momentum k and zero Matsubara frequency.

This relation, applied in the critical region of Bose condensation in a three dimensional system, determines the scaling structure of the superfluid density.⁴ Furthermore, it implies that in a two dimensional interacting Bose gas, superfluidity can exist below the Kosterlitz-Thouless-Berezinskii transition temperature, even in the absence of condensation in the thermodynamic limit.^{5,6} The Josephson relation was derived originally by heuristic arguments. In this note, we derive the Josephson relation at finite temperature within the framework of diagrammatic perturbation theory, for infinite as well as large but finite size systems. The present derivation, which follows a different path from that of Josephson, extends to finite temperatures the discussion of Gavoret and Nozières⁷ of the microscopic connection between superfluidity and condensation at zero temperature (see also Talbot and Griffin⁸). Our derivation, in yielding the correct Josephson relation for finite systems, is of immediate experimental importance for ultracold trapped atomic gases.

A superfluid effectively has an extra dynamical degree of freedom, the velocity of the superfluid, v_s , with respect to the wall velocity.⁹ In the presence of superflow, the free energy density F of the system is

$$F(v_s, T, \mu) = F(0, T, \mu) + \frac{1}{2} \rho_s v_s^2, \quad (2)$$

where T is the temperature and μ the chemical potential. Thus, thermodynamically,

$$\rho_s = \frac{\partial^2}{\partial v_s^2} F(v_s, T, \mu) \Big|_{v_s=0}, \quad (3)$$

and the normal density ρ_n is given by $\rho_n = \rho - \rho_s$, where ρ is the mass density of the system.

The Hamiltonian $H(v_s)$ in the rest frame of the superfluid, written in terms of the variables of the "lab" frame, in which the walls are at rest and the superfluid flows in the z direction, is

$$H(v_s) = H - P_z v_s + \frac{1}{2} M v_s^2, \quad (4)$$

where \mathbf{P} is the total momentum operator. We work in a system of large volume V and assume periodic boundary conditions in the z direction.¹⁰ We consider the free energy density of a system with a nonzero superfluid velocity with respect to the walls, in the frame moving with the superfluid. Differentiating the partition function with respect to v_s , we obtain

$$\partial F / \partial v_s = -\langle P_z - M v_s \rangle / V, \quad (5)$$

and then, noting that the total momentum operator in the z direction commutes with H , we have

$$\partial^2 F / \partial v_s^2 = \rho - \beta \langle P_z^2 \rangle / V, \quad (6)$$

at $v_s=0$ and $\beta=1/k_B T$. Thus, the normal mass density is given by

$$\rho_n = \beta \langle P_z^2 \rangle / V. \quad (7)$$

In a normal system, the total momentum \mathbf{P} has a classical Boltzmann distribution with probability $\propto \exp(-\beta P^2 / 2M)$, where M is the total mass, which implies $\beta \langle P_z^2 \rangle / V = M / V = \rho$, and thus $\rho_n = \rho$. Only deviations of the distribution of states with total momentum P from the classical distribution can give rise to superfluidity; in the superfluid phase, the distribution of total momentum is no longer classical as a consequence of entanglement of the total momentum and superfluid velocity.

Microscopically, the superfluid and normal mass densities are defined in terms of the transverse current-current correlation function.^{3,11} In fact, the microscopic definition is, as we shall see, equivalent to Eq. (7). We consider a superfluid contained in an infinitely long cylindrical vessel oriented along the z axis. If the walls of the container move with a

small velocity \mathbf{v}_z in the z direction, the normal mass density moves with the walls, while the superfluid remains at rest in the laboratory frame. The response of the fluid flow to the motion of the walls is specified by the current-current correlation function

$$Y_{ij}(\mathbf{r}, \mathbf{r}', \omega) = \int dt e^{i\omega(t-t')} \langle [j_i(\mathbf{r}, t), j_j(\mathbf{r}', t')] \rangle, \quad (8)$$

where the current density \mathbf{j} is given by

$$\mathbf{j}(\mathbf{r}) = \frac{1}{2im} [\psi^\dagger(\mathbf{r}) \nabla \psi(\mathbf{r}) - \nabla \psi^\dagger(\mathbf{r}) \psi(\mathbf{r})], \quad (9)$$

with $\psi(\mathbf{r})$ as the particle annihilation operator. The Fourier transform to momentum \mathbf{k} and real frequency ω can be decomposed into longitudinal (L) and transverse (T) parts as

$$Y_{ij}(\mathbf{k}, \omega) = \frac{k_i k_j}{k^2} Y_L(k, \omega) + \left(\delta_{ij} - \frac{k_i k_j}{k^2} \right) Y_T(k, \omega). \quad (10)$$

The longitudinal and transverse components of the time-ordered current-current correlation function in the imaginary time have Fourier transforms to Matsubara frequency z_ν ,

$$\Xi_{L,T}(k, z_\nu) = \int \frac{d\omega}{2\pi} \frac{Y_{L,T}(k, \omega)}{z_\nu - \omega}. \quad (11)$$

The long-wavelength static longitudinal response function—describing the response of the system in a tube with closed ends moved along the z direction^{3,10}—obeys

$$\Xi_L(k \rightarrow 0, 0) = \lim_{k_z \rightarrow 0} \lim_{k_\perp \rightarrow 0} \Xi_{zz}(\mathbf{k}, z_\nu = 0) = -\rho/m^2, \quad (12)$$

where \perp denotes the directions perpendicular to z . Then

$$\rho = \lim_{k \rightarrow 0} m^2 \int \frac{d\omega}{2\pi} \frac{Y_L(k, \omega)}{\omega}, \quad (13)$$

where ρ is the total mass density. This relation follows from the f -sum rule together with the continuity equation. On the other hand, the long-wavelength limit of the transverse response, which describes the response of the system in an open ended moving container (or with periodic boundary conditions), reduces to the normal mass density, $\rho_n = \rho - \rho_s$,

$$\Xi_T(k \rightarrow 0, 0) = \lim_{k_\perp \rightarrow 0} \lim_{k_z \rightarrow 0} \Xi_{zz}(\mathbf{k}, z_\nu = 0) = -\rho_n/m^2, \quad (14)$$

or

$$\rho_n = \lim_{k \rightarrow 0} m^2 \int \frac{d\omega}{2\pi} \frac{Y_T(k, \omega)}{\omega}. \quad (15)$$

While the order of limits in Eq. (12) describes a system closed in the z direction, the order in Eq. (14) describes a system open in the z direction.³

A superfluid is characterized by $\rho_n < \rho$. As long as the two-particle Green's function is regular, the $k_x, k_y, k_z \rightarrow 0$ limits in Eqs. (12) and (14) cannot depend on the order of limits, and thus $\rho_n = \rho$. Superfluidity implies that the two-particle Green's function behaves singularly in the infrared limit.

Furthermore, since $\int d\mathbf{r} \mathbf{j}(\mathbf{r}) = \mathbf{P}(t)/m$, we have

$$\lim_{k_\perp \rightarrow 0} \lim_{k_z \rightarrow 0} \Xi_{zz}(\mathbf{k}, 0) = -\frac{i}{m^2 V} \int_0^{-i\beta} dt \langle P_z(t) P_z(0) \rangle, \quad (16)$$

where V is the system volume. Since for an infinite system, P_z is independent of t , we rederive Eq. (7).

Having established the equivalence of the two definitions of ρ_s , we turn to deriving Josephson's relation in a Bose system, using definition (3). We take the free energy density to be a functional of the order parameter, $\langle \psi(\mathbf{r}) \rangle$, of the system and the single-particle matrix Green's function,

$$\mathcal{G}(\mathbf{r}t, \mathbf{r}'t') = -i \langle \langle T[\Psi(\mathbf{r}t)\Psi^\dagger(\mathbf{r}'t')] \rangle \rangle - \langle \Psi^\dagger(\mathbf{r}'t') \rangle \langle \Psi(\mathbf{r}t) \rangle. \quad (17)$$

Here, the two-component field operator is $\Psi(\mathbf{r}t) = [\psi(\mathbf{r}t), \psi^\dagger(\mathbf{r}t)]$. In equilibrium, the first order variation of F with respect to the order parameter vanishes, $\delta F / \delta \langle \Psi \rangle = \delta F / \delta \langle \Psi \rangle^* = 0$. Static variations of F with respect to the order parameter are then given in terms of the inverse of the single-particle matrix Green's function,

$$V \delta F = -\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \delta \langle \Psi(\mathbf{r}) \rangle^* \mathcal{G}^{-1}(\mathbf{r}, \mathbf{r}') \delta \langle \Psi(\mathbf{r}') \rangle, \quad (18)$$

where $\langle \Psi \rangle = (\langle \psi \rangle, \langle \psi \rangle^*)$ is the two-component order parameter.

The dependence of F on the superfluid velocity enters through the phase of the order parameter,

$$\langle \psi(\mathbf{r}) \rangle_{v_s} = \sqrt{n_0} e^{imv_s z} + \mathcal{O}(v_s^2), \quad (19)$$

where n_0 is the condensate density evaluated at $v_s = 0$. To second order in v_s , the dependence of the free energy density on the superfluid velocity arises solely from the momentum $m\mathbf{v}_s$ of the condensate wave function. To lowest order in v_s , $\delta \langle \psi(\mathbf{r}) \rangle = im\mathbf{v}_s \cdot \mathbf{r} \sqrt{n_0}$, so that the second order change in F is

$$\begin{aligned} \delta F &= \frac{n_0 m^2}{V} \int d\mathbf{r} d\mathbf{r}' (\mathbf{v}_s \cdot \mathbf{r}) (\mathbf{v}_s \cdot \mathbf{r}') [(\mathcal{G}^{-1})_{11} - (\mathcal{G}^{-1})_{12}](\mathbf{r}, \mathbf{r}') \\ &= -\frac{n_0 m^2}{2} \lim_{k \rightarrow 0} (\mathbf{v}_s \cdot \nabla_k)^2 [(\mathcal{G}^{-1})_{11}(k, 0) - (\mathcal{G}^{-1})_{12}(k, 0)]. \end{aligned} \quad (20)$$

Since the inverse of the static Green's function has the form

$$\mathcal{G}^{-1}(k, 0) = \begin{pmatrix} \mu - \varepsilon_k - \Sigma_{11} & -\Sigma_{12} \\ -\Sigma_{21} & \mu - \varepsilon_k - \Sigma_{22} \end{pmatrix}, \quad (21)$$

where $\varepsilon_k = k^2/2m$ and the $\Sigma_{ij}(k, 0)$ are the self-energies; the variation of the free energy density [Eq. (20)] is given in terms of the Σ 's by

$$\delta F = \frac{1}{2} n_0 m^2 v_s^2 \frac{\partial^2}{\partial k_z^2} [\varepsilon_k + \Sigma_{11}(k, 0) - \Sigma_{12}(k, 0)]_{k=0}. \quad (22)$$

After a brief algebra, we obtain

$$\begin{aligned} (\mathcal{G}_{11})^{-1}(k, 0) &= -2[\varepsilon_k - \mu + \Sigma_{11}(k, 0) - \Sigma_{12}(k, 0)] \\ &\quad - \frac{[\mu - \varepsilon_k - \Sigma_{11}(k, 0) + \Sigma_{12}(k, 0)]^2}{\mu - \varepsilon_k - \Sigma_{11}(k, 0)}. \end{aligned} \quad (23)$$

We assume that below the critical temperature T_c , the

single-particle excitation spectrum is gapless. Then, Eq. (22) reduces to Eq. (1). In this case, the chemical potential μ , which depends on n_0 , is determined by the Hugenholtz-Pines relation¹³

$$\mu = \Sigma_{11}(0,0) - \Sigma_{12}(0,0). \quad (24)$$

Thus, the final term in Eq. (23) is of order k^4 and can be neglected as $k \rightarrow 0$. Rewriting Eq. (22) in terms of $G_{11}^{-1}(k,0)$, we find

$$\rho_s = -\frac{1}{2}n_0m^2 \lim_{k \rightarrow 0} \frac{\partial^2}{\partial k_z^2} (G_{11})^{-1}(k,0), \quad (25)$$

which in the gapless phase implies the Josephson relation [Eq. (1)]. Further, since we have explicitly used a finite system with periodic boundary conditions, we note that the thermodynamic limit has to be taken after the $k \rightarrow 0$ limit in Eqs. (1) and (25) has been performed.

Equivalently, we can derive ρ_n by carrying out a gauge transformation on the G_{ij} in which

$$\begin{aligned} G_{11}(\mathbf{r},\mathbf{r}',0) &\rightarrow e^{imv_n(\mathbf{r}-\mathbf{r}')}G_{11}(\mathbf{r},\mathbf{r}',0), \\ G_{12}(\mathbf{r},\mathbf{r}',0) &\rightarrow e^{imv_n(\mathbf{r}+\mathbf{r}')}G_{12}(\mathbf{r},\mathbf{r}',0), \\ G_{21}(\mathbf{r},\mathbf{r}',0) &\rightarrow e^{-imv_n(\mathbf{r}+\mathbf{r}')}G_{21}(\mathbf{r},\mathbf{r}',0), \\ G_{22}(\mathbf{r},\mathbf{r}',0) &\rightarrow e^{-imv_n(\mathbf{r}-\mathbf{r}')}G_{22}(\mathbf{r},\mathbf{r}',0). \end{aligned} \quad (26)$$

Under this transformation, the free energy density changes by

$$\delta F = \frac{1}{2}\rho_n v_n^2. \quad (27)$$

Now, the first order variation of the free energy density with δG gives a purely kinetic contribution,

$$\delta F_{kin} = -\frac{1}{2V}\text{Tr}(G_0^{-1}\delta G) \quad (28)$$

$$= \frac{1}{2}(\rho - mn_0)v_n^2, \quad (29)$$

since $(G_0^{-1})_{11}(\mathbf{r},\mathbf{r}') = (\mu + \nabla_{\mathbf{r}}^2/2m)\delta(\mathbf{r}-\mathbf{r}')$, $(G_0^{-1})_{11}(\mathbf{r},\mathbf{r}') = (G_0^{-1})_{22}(\mathbf{r},\mathbf{r}')$, and $(G_0^{-1})_{12}(\mathbf{r},\mathbf{r}') = (G_0^{-1})_{21}(\mathbf{r},\mathbf{r}') = 0$. The second order variation is given by¹²

$$\delta F_{int} = -\frac{1}{2V}\text{Tr}_1\text{Tr}_2\delta G(1)\mathcal{L}^{-1}(1,2)\delta G(2). \quad (30)$$

The connected two-particle correlation function, $\mathcal{L}(1,2) = \mathcal{G}_2(1,2) - \mathcal{G}(1)\mathcal{G}(2)$, is the two-particle Green's function, \mathcal{G}_2 , with the uncorrelated one-particle Green's function contribution subtracted. To evaluate Eq. (30) with Eq. (26), we note that under the gauge transformation coupled with the transformation $\langle \psi(\mathbf{r}) \rangle \rightarrow \langle \psi(\mathbf{r}) \rangle e^{imv_n \mathbf{r}}$, the diagrams involving the interaction are invariant. Thus, from Eq. (22), we see that Eq. (30) contributes

$$\delta F_{int} = -n_0m^2v_n^2 \frac{\partial}{\partial k_z^2} [\Sigma_{11}(k,0) - \Sigma_{12}(k,0)]_{k=0}. \quad (31)$$

Assembling the pieces and using Eq. (25), we find that under the transformation [Eq. (26)]

$$\delta F = \frac{1}{2} \left[\rho + n_0m^2 \lim_{k \rightarrow 0} \frac{\partial}{\partial k_z^2} G_{11}^{-1}(k,0) \right] v_n^2 = \frac{1}{2}(\rho - \rho_s)v_n^2, \quad (32)$$

as expected.

We note that our derivation of the Josephson relation is, in fact, valid in a finite size system. There, the Green's functions are defined only on a discrete set of points in k space, the limit $k \rightarrow 0$ in Eq. (1) is replaced by the limit $k \rightarrow k_0$, with $k_0 = 2\pi/L$, and the Josephson relation becomes discretized. In addition, the relation remains valid in two dimensions in the gapless phase⁵ since we do not need to explicitly specify the number of dimensions in the derivation.

This research was supported in part by NSF Grants No. PHY03-55014 and No. PHY05-00914 and facilitated by the Projet de Collaboration CNRS/UIUC. LPTMC is a Unité Associée au CNRS, UMR 7600. We are grateful to the Aspen Center for Physics where much of this work was carried out.

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