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Superconductivity in a quasi-two-dimensional Bose gas

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We show, within mean-field theory, that the normal state of a compressible quasi-two-dimensional Bose gas with *arbitrarily weak* attractive interactions becomes unstable with respect *to pair* condensation at a temperature T_c of order T_0, the Bose degeneracy temperature. Below T_c, the ground-state many-particle wave function is the boson analog of the Bardeen-Cooper-Schrieffer wave function and the charged gas has the principal electromagnetic properties of a conventional superconductor.

In this paper we point out that the normal ground state of a compressible quasi-two-dimensional (2D) Bose gas becomes unstable toward *pair* condensation as *arbitrarily weak* attractive interactions between its particles are switched on. This property, which does not arise for an isotropic 3D Bose gas at zero temperature[1] ($T=0$), is reminiscent of the Cooper-pair instability[2] in a Fermi gas. We show that the mean-field transition temperature, T_c, corresponding to the $T=0$ instability is of order T_0, the Bose degeneracy temperature. Below T_c, the many-particle wave function describing the ground state is the boson analog of the Bardeen-Cooper-Schrieffer (BCS)[3] wave function which was first introduced by Valatin and Butler[4] and developed by Evans and Imry[5] as a possible description of liquid ^{4}He. In consequence, the charged gas has the principal electromagnetic properties[6] of a conventional superconductor, i.e., Meissner-Ochsenfeld effect[7] and flux quantization[8] in units of $\phi_0=hc/2e$.[6] We find that the mean-field T dependences of the critical field $H_c(T)$ and pair potential $\Delta(T)$ are also similar to those of a conventional superconductor, as is roughly also that of the specific heat $C_v(T)$, although the excitation spectrum is different from that of a BCS fermion superconductor.[3] These results have possible implications for the interpretation of the superconductivity in the perovskite oxides[9] and the interpretation of the order parameter in 2D liquid ^{4}He layers.

We consider a model of an interacting 2D Bose gas of N particles of mass m whose thermodynamic potential is defined by the operator

$$K=\sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}(\varepsilon_{\mathbf{k}}-\tilde{\mu}+\rho U) - (V/2A)\sum_{\mathbf{k},\mathbf{k}'}{}' a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} a_{-\mathbf{k}'} a_{\mathbf{k}'} \,. \tag{1}$$

Here, $a_{\mathbf{k}}^{\dagger}$ and $a_{\mathbf{k}}$ are boson creation and annihilation operators, respectively, for Hartree-Fock (HF) particle states with momentum $\hbar\mathbf{k}$ and energy $\varepsilon_{\mathbf{k}}+\rho U$, where $\varepsilon_{\mathbf{k}}=\hbar^2\mathbf{k}^2/2m$ and ρU is a constant Hartree-Fock energy with $U>0$. In the absence of the second sum in (1) the latter condition ensures that the compressibility $(1/B)=2\rho^2 U$ is positive. The parameter $\tilde{\mu}$ is the chemical potential and is determined by the condition that the statistical average of $A^{-1}\sum_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}}$ be equal to $\rho=N/A$, the number of particles per unit area ($N\to\infty$, $A\to\infty$). The second term in (1) describes a weak attractive interaction V between pairs of particles of zero total momentum. This interaction is restricted to particles with $\varepsilon_{\mathbf{k}}\le\varepsilon_A$, a restriction that is denoted by the prime over the summation. V is to be considered a parametrization either of the effect of an attractive component of the direct interparticle interaction or an indirect attraction between particles mediated by the exchange of quanta with an external system to which the gas is coupled. We consider the gas to be *quasi*-2D in the sense that it exists in the 3D volume $\Omega=dA$ of a slab lying in the x-y plane with area A and thickness of the order of one or two atomic lattice spacings. The zero-point energy per particle due to localization in the z direction is considered absorbed in $\tilde{\mu}$. The model can be readily extended to include a small finite bandwidth for delocalization in the z direction.

The instability of the normal state in the presence of V may be demonstrated by calculating the amplitude $T_{\mathbf{k},\mathbf{k}'}$ for the pair scattering event $(\mathbf{k},-\mathbf{k})\to(\mathbf{k}',-\mathbf{k}')$ and looking for a possible bound state with energy $\varepsilon_B=-\omega(<0)$. At temperature T, and from Fig. 1, the t matrix is

$$T_{\mathbf{k},\mathbf{k}'}=-V\bigg/\left|1-\tfrac{1}{2}\lambda\int_{|\mu|/2k_BT}^{(\varepsilon_A+|\mu|)/2k_BT}\frac{dx\coth(x)}{x+\tilde{\omega}}\right| \,, \tag{2}$$

where $\lambda=N_0V$, $N_0=\rho/k_BT_0$ is the density of states per unit area, $T_0=2\pi\hbar^2\rho/mk_B$, $\tilde{\omega}=\omega/4k_BT$, and $\mu(T)=k_BT\ln[1-\exp(-T_0/T)]$ is the chemical potential measured relative to the constant HF term $\rho(U-\frac{1}{2}V)$. In the limit $T\to 0$, (2) yields the condition

$$\lambda^{-1}=(2k_BT_0/\omega)+\tfrac{1}{2}\ln[(2\varepsilon_A+\omega)/\omega] \tag{3}$$

for the bound state. The second term in (3) determines ε_B for the case of an isolated pair ($\rho=0$), while the first term describes the effect of the quantum statistics ($\rho\neq 0$). Clearly, Eq. (3) has solutions for *arbitrary* λ and in the

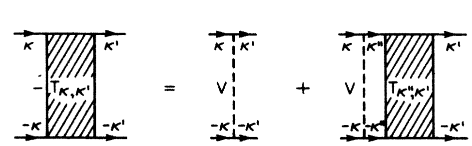

FIG. 1. Diagrams for the calculation of the t matrix $T_{\mathbf{k},\mathbf{k}'}$.

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limit $\lambda \rightarrow 0$, $\omega \sim 2\lambda k_B T_0$. This implies an instability toward a pairing phase in which pair correlations persist over radii $\xi \sim (\hbar^2/2m\lambda k_B T_0)^{1/2}$ and in which the pair potential $\Delta(0) \sim \lambda k_B T_0$ is linear in ρ. The corresponding mean-field T_c is given by $\lambda I(T_c) = 2$, where $I(T)$ is the integral in (2) with ω set equal to zero. For $\varepsilon_A \neq 0$, and $\lambda \rightarrow 0$, $T_c \sim -T_0/\ln(\lambda)$. As discussed in an elegant paper by Nozières and Saint James,[1] in 3D a pure pairing phase at $T=0$ can occur only if $V > V^*$, where $\rho V^* \sim k_B T_0 (k_B T_0/\varepsilon_A)^{1/2}$ is the minimum magnitude of V for there to be a bound state for the isolated pair problem. Since such values of V are too large to be reasonably consistent with a positive compressibility it is unlikely that a pure pairing phase could ever exist in (isotropic) 3D at $T=0$.[10] In 2D it is the *constant density of states* N_0 which is responsible for the different behavior.

To describe the mean-field state below T_c we follow Bogoliubov[7] and BCS and replace (1) by the bilinear form

$$K = \sum_{\mathbf{k}} [(\varepsilon_{\mathbf{k}} - \mu) a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + \tfrac{1}{2}\Delta_{\mathbf{k}} a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger + \tfrac{1}{2}\Delta_{\mathbf{k}}^* a_{-\mathbf{k}} a_{\mathbf{k}}] \ , \tag{4}$$

where $\Delta_{\mathbf{k}} = -V\langle a_{-\mathbf{k}} a_{\mathbf{k}} \rangle = \Delta \exp(iS)$ is the mean-field pair potential. The brackets denote a Gibbs statistical average taken over the eigenstates of (4) and both Δ and S are real. K may be brought to the diagonal form

$$K = \sum_{\mathbf{k}} E_{\mathbf{k}} \alpha_{\mathbf{k}}^\dagger \alpha_{\mathbf{k}} + \tfrac{1}{2} \sum_{\mathbf{k}} [E_{\mathbf{k}} - (\varepsilon_{\mathbf{k}} + |\mu|)] \ , \tag{5}$$

by means of the unitary Bogoliubov transformation[11]

$$a_{\mathbf{k}} = u_{\mathbf{k}} \alpha_{\mathbf{k}} - v_{\mathbf{k}}^* \alpha_{-\mathbf{k}}^\dagger, \quad a_{\mathbf{k}}^\dagger = u_{\mathbf{k}}^* \alpha_{\mathbf{k}}^\dagger - v_{\mathbf{k}} \alpha_{-\mathbf{k}} \ ,$$

where $\alpha_{\mathbf{k}}^\dagger$ and $\alpha_{\mathbf{k}}$ are new boson operators which create and destroy, respectively, quasiparticle (QP) excitations with energies

$$E_{\mathbf{k}} = [(\varepsilon_{\mathbf{k}} + |\mu|)^2 - \Delta^2]^{1/2} \tag{6}$$

relative to the ground-state value of K, which is given by the second sum in (5). The amplitudes $u_{\mathbf{k}} = |u_{\mathbf{k}}| \times \exp(iS/2)$ and $v_{\mathbf{k}} = |v_{\mathbf{k}}| \exp(-iS/2)$ satisfy $|u_{\mathbf{k}}|^2 - |v_{\mathbf{k}}|^2 = 1$ and their moduli are given by $2|u_{\mathbf{k}}|^2 = \gamma_{\mathbf{k}} + 1$, $2|v_{\mathbf{k}}|^2 = \gamma_{\mathbf{k}} - 1$, where $\gamma_{\mathbf{k}} = (\varepsilon_{\mathbf{k}} + |\mu|)/E_{\mathbf{k}}$. The many-particle wave function describing the ground state is the Valatin-Butler[2] wave function

$$\Phi_0 = \prod_{\mathbf{k}} |u_{\mathbf{k}}|^{-1} \exp[-(v_{\mathbf{k}}/u_{\mathbf{k}}) a_{\mathbf{k}}^\dagger a_{-\mathbf{k}}^\dagger] |0\rangle \tag{7}$$

and satisfies $\alpha_{\mathbf{k}} \Phi_0 = 0$ and $\Phi_0^\dagger \Phi_0 = 1$, where $|0\rangle$ denotes the vacuum. It may be interpreted as describing clusters of $n = 1, 2, \ldots, \infty$ identical time-reversed pairs. The probability that the particular cluster of n occurs is $P_{\mathbf{k},n} = |v_{\mathbf{k}}|^{2n}/|u_{\mathbf{k}}|^{2n+2}$ and satisfies $\sum_n P_{\mathbf{k},n} = 1$. The equations determining the self-consistent values of $\Delta(T)$ and $\mu(T)$ are

$$A^{-1} \sum_{\mathbf{k}}{}' E_{\mathbf{k}}^{-1} (2n_{\mathbf{k}} + 1) = (2/V) \ , \tag{8}$$

$$\rho = (2A)^{-1} \sum_{\mathbf{k}} E_{\mathbf{k}}^{-1} [(\varepsilon_{\mathbf{k}} + |\mu|)(2n_{\mathbf{k}} + 1) - E_{\mathbf{k}}] \ , \tag{9}$$

where $n_{\mathbf{k}} = [\exp(E_{\mathbf{k}}/k_B T) - 1]^{-1}$ is the number of QP's excited with momentum $\hbar\mathbf{k}$ at temperature T. Equation (7) can be evaluated exactly to give the following relationship between μ and Δ:

$$(\mu^2 - \Delta^2)^{1/2} = -2k_B T \ln\{[(x^2+4)^{1/2} - x]/2\} \ , \tag{10}$$

where $x = \exp[(|\mu| - 2k_B T_0)/2k_B T]$. Finally, the thermodynamic properties are determined from the Helmholtz free energy

$$F = \langle K + \mu N \rangle - k_B T \sum_{\mathbf{k}} [(n_{\mathbf{k}} + 1)\ln(n_{\mathbf{k}} + 1) - n_{\mathbf{k}} \ln(n_{\mathbf{k}})] \ . \tag{11}$$

We now discuss the main consequences of these results.

Equation (10) shows that the "gap" $E_g = (\mu^2 - \Delta^2)^{1/2}$ in the excitation spectrum is nonvanishing at *all* finite temperatures. For

$$\lambda = N_0 V < \lambda_0 = 1/\sinh^{-1}[(\varepsilon_A/4k_B T_0)^{1/2}] \ ,$$

however, E_g rapidly diminishes as $T \rightarrow 0$ and is precisely zero at $T=0$. For $\lambda > \lambda_0$, $E_g \neq 0$ at $T=0$. Figure 2 shows the magnitudes and temperature dependences of $\Delta(T)$ and $\mu(T)$ as calculated from (8) and (9) for cases corresponding to $\lambda < \lambda_0$ [Fig. 2(a)] and $\lambda > \lambda_0$ [Fig. 2(b)], where the parameter values employed are indicated in the figures. It is seen that $\Delta(T)$ has a BCS-like T dependence and the behavior of $\mu(T)$ is quite different from that of noninteracting gas. For $\lambda < \lambda_0$ and $T=0$, $E_{\mathbf{k}}$ is *phonon-like* for $k\xi \ll 1$, i.e., $E_{\mathbf{k}} = \hbar s k$, where $s = (|\mu|/m)^{1/2} = (\Delta/m)^{1/2}$ is the critical superfluid velocity at $T=0$. In the limit $\lambda \rightarrow 0$, with $\varepsilon_A \neq 0$, $\Delta(0) \rightarrow \rho V$. The latter result leads to a compressibility $(1/B) = 2\rho^2(U - 1.5V)$. The

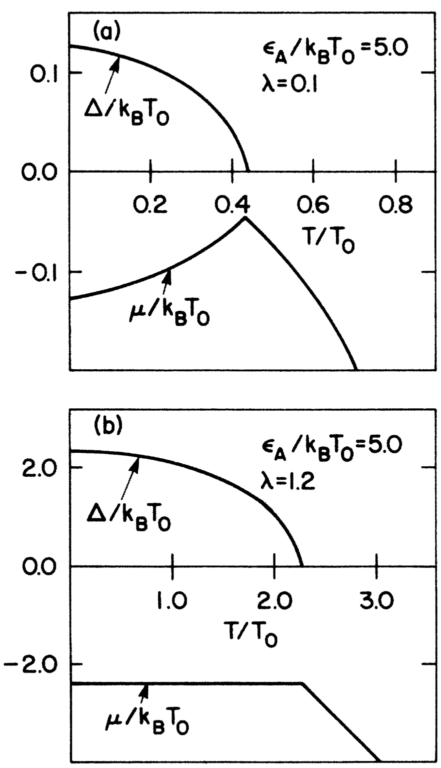

FIG. 2. $\Delta(T)/k_B T_0$ and $\mu(T)/k_B T_0$ vs T/T_0 for (a) $\lambda/\lambda_0 = 0.096$ and (b) $\lambda/\lambda_0 = 1.154$. In both cases $\lambda_0 = 1.04$.

linear spectrum gives rise to a specific heat $C_v(T)$ which varies as T^2 as $(T/T_c) \to 0$. Figure 3 shows $C_v(T)$ as calculated from (8), (9), and (10) for $\lambda = 0.6$ and $\varepsilon_A = 5k_BT_0$. In general, we find that $C_v(T)$ is linear in T immediately below T_c and the jump in C_v at T_c must be determined numerically. For $E_g \neq 0$, $C_v(T)$ falls exponentially to zero for $T \ll T_c$, as in the BCS case.

For the charged gas, the critical magnetic field $H_c(T)$ may be calculated from (11) and the relation $F_s - F_n = -(H_c^2/8\pi)$, where F_s and F_n denote the free energies of the superconducting and normal phases, respectively. Figure 3 shows $H_c(T)/H_c(0)$ vs F/T_c calculated using the same values of λ and ϵ_A that were employed for the calculation of $C_v(T)$. Within the error of our numerical calculations, the curve shown for $H_c(T)/H_c(0)$ vs T/T_c coincides with those which we have also calculated for $\lambda = 0.1$ and $\lambda = 1.2$ with the same value of ε_A; this particular functional dependence, therefore, seems to be a universal one. For the gas with infinite mean free path, the current response $\mathbf{j}_s(\mathbf{r})$ at the point $\mathbf{r}$ to a weak, slowly varying, vector potential $\mathbf{A}(\mathbf{r})$, applied in the plane (x,y) of our slab, can be calculated via linear response theory[12] to be

$$\mathbf{j}_s(\mathbf{r}) = -[n_s(T)e^2/mcd]\mathbf{A}(\mathbf{r}) ,$$

where

$$n_s(T) = \rho + A^{-1}\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \left(\frac{\partial n_{\mathbf{k}}}{\partial E_{\mathbf{k}}} \right)$$

is the number of superconducting particles per unit area. If we now consider our slab to be a disk of radius $R \to \infty$, the latter London equation implies the exclusion of weak magnetic flux, applied along the z direction, by supercurrents flowing around the disk perimeter in an annulus of thickness $\sim \eta = (mc^2d/4\pi n_s e^2)^{1/2}$. If there is a hole of radius R_1 at the center of the disk, where $R - R_1 \gg \eta$, flux passing through the hole in the z direction can be trapped in the hole only in units of $\phi_0 = (hc/2e)$. This follows from the standard argument[13] of integrating the gauge velocity

$$\mathbf{v}_s(\mathbf{r}) = (\hbar/2m)\nabla_r S(\mathbf{r}) - (e/mc)\mathbf{A}(\mathbf{r})$$

around a path in the bulk where $\mathbf{v}_s = 0$. We estimate[13] the energy E_0 is required for the flux unit ϕ_0 to actually penetrate the bulk superconducting regions of the disk to be $E_0 \simeq (\phi_0/4\pi)^2\eta^{-1}\ln(\eta/\xi)$. Finally, we note that for $\lambda < \lambda_0$, $\eta_s(T) - \rho \sim T^3$ for $T/T_c \to 0$. As in BCS, the results in this paragraph have been obtained without explicitly taking into account the long-range Coulomb interaction between the particles.

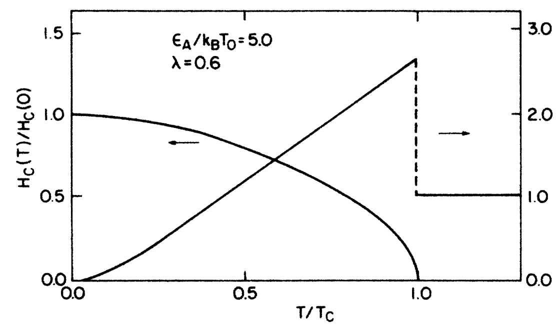

FIG. 3. $C_v(T)/Nk_B$ (right-hand scale) and $H_c(T)/H_c(0)$ (left-hand scale) vs T/T_c.

If the pertinent carriers in the oxide superconductors[9,14] are governed by Bose-Einstein rather than Fermi-Dirac statistics, as discussed by several authors in the literature,[15-17] and in particular by Kivelson, Rokhsar, and Sethna[18] in the context of the resonating-valence-bond model of Anderson,[19] our results would be able to account for the occurrence of *apparently* conventional superconductivity at high temperatures in these compounds. The origin of V could be the interaction of the carriers with phonons. With regard to liquid ^{4}He our theory could be relevant to quasi-2D liquid ^{4}He layers:[20] Our results do not affect the Kosterlitz-Thouless transition[21] but are relevant to the interpretation of the superfluid order parameter.

While it is likely that fluctuations in the local phase $S(\mathbf{r})$ will destroy long-range order in the strict 2D limit of the present problem, it is reasonable to suppose that in the actual *quasi*-2D systems of interest there will be approximate long-range order and supercurrents which will live for macroscopic times at finite temperatures sufficiently below the mean-field T_c. For the perovskite oxides weak coupling between the CuO_2 layers would imply a highly anisotropic 3D Bose gas. The considerations of Nozières and Saint James lead us to expect that such a gas will have a pairing phase for values of $V > V_1$, where V_1 is a threshold *still small* in comparison to the isotropic threshold V^*. This gas should exhibit true long-range order at finite temperature.

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theory of superconductivity, the instability in Eq. (2) can survive the presence of a stronger repulsive pair interaction $U_{\mathbf{k},\mathbf{k}'}=V_R$ provided that its range ε_R, in the pair energy space satisfies $\varepsilon_R \gg \varepsilon_A$. In this case V in Eq. (2) is to be replaced by $V_{\text{eff}}=V-\{V_R/[1+N_0V_R\ln(\varepsilon_R/\varepsilon_A)]\}$.

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