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†National Science Foundation Cooperative Fellow.

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BOSE-EINSTEIN PHASE TRANSITION IN AN INTERACTING SYSTEM*

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It is shown that for both the Hartree-Fock and Bogoliubov models of interacting bosons associated with the disappearance of the Bose-Einstein condensation at a temperature T_c, the specific heat C_V has a square root singularity, $C_V \sim A(T_c-T)^{-1/2}$, and the superfluid density ρ_S is discontinuous, with $\rho_S(T)-\rho_S(T_c-0) \sim B(T_c-T)^{1/2}$ for temperatures $T \to T_c - 0$. Except near $T_c = T_\lambda$ the theoretical and experimental results for ρ_S are in good agreement.

It is well known that in an ideal (Bose-Einstein) gas of He^4 atoms, the specific heat C_V is continuous but $\partial C_V/\partial T$ is discontinuous at $T_I = 3.13°K$.[1] By contrast, the measured specific heat of liquid He^4 is logarithmically singular at $T_\lambda = 2.18°K$.[2] Because of calculational difficulties inherent in studies of phase transitions, little progress has been made in showing that the introduction of interactions between atoms leads to agreement between the predicted and observed values of C_V.[3-5] We report here that for both the Hartree-Fock and Bogoliubov models of a system of bosons interacting via repulsive two-body potentials, C_V has a square-root singularity, $C_V \sim A(T_c - T)^{-1/2}$, as T is raised to a transition temperature T_c. Further, for the Hartree-Fock model, we have calculated the superfluid mass density, ρ_S, as a function of temperature, and it is in good agreement with the experimental results, when $T_c = T_\lambda$, except for temperatures in the immediate vicinity of T_λ.

Consider a system of N bosons in a cubic container of volume V, where the particle density is $n(\mathrm{He}^4) = (3.58\ \mathrm{Å})^{-3}$ and each particle has mass $m(\mathrm{He}^4) = 6.64 \times 10^{-24}$ g. We assume that the particles interact via a central, repulsive, two-body potential possessing a Fourier transform $v(\vec{p})$. In the following,[6] it suffices to specify the form of $v(\vec{p})$ for small p:

$$v(\vec{p}) \approx v_0[1-(p^2/p_c{}^2)], \quad v_0 > 0. \tag{1}$$

In the Hartree-Fock approximation the Hamiltonian of the system is (we choose units so that $\hbar = 1$)

$$\mathcal{H}_{\mathrm{H-F}} = \sum_{\vec{p}} \left(\frac{p^2}{2m} - \mu\right) N_{\vec{p}} + (2V)^{-1} \sum_{\vec{p}, \vec{p}'(\neq \vec{p})} [v_0 + v(\vec{p}-\vec{p}')] N_{\vec{p}} N_{\vec{p}'} + (2V)^{-1} v_0 \sum_{\vec{p}} N_{\vec{p}}{}^2, \tag{2}$$

where μ is the chemical potential, and $N_{\vec{p}} = a_{\vec{p}}{}^\dagger a_{\vec{p}}$ is the number operator for the single-particle state $V^{-1/2}\exp(i\vec{p}\cdot\vec{r})$ satisfying periodic boundary conditions with respect to V. As shown elsewhere,[7] for temperatures below some critical value T_c it is possible to choose μ so that in the volume limit $[N, V \to \infty,\ N/V = n(\mathrm{He}^4)]$, the excitation energy of the $\vec{p} = 0$ single-particle state vanishes, and thus the thermal equilibrium occupation number, $\langle a_0{}^\dagger a_0 \rangle \equiv n_0 V$, of this state is $O(N)$ (Bose-Einstein condensation). With this choice for μ, and $v(\vec{p})$ as given in (1), the excitation energy for a state $\vec{p}(\neq 0)$ is

$$\epsilon_{\vec{p}} = (p^2/2m^*) + n_0 v_0, \tag{3}$$

where

$$m^* = m(1 - 2mnv_0/p_c{}^2)^{-1} > m. \tag{4}$$

The equilibrium occupation number of this state is

$$\langle N_{\vec{p}} \rangle = [\exp(\beta\epsilon_{\vec{p}}) - 1]^{-1}, \tag{5}$$

where $1/\beta = k_B T$.

The condition that the total number of particles is N yields an implicit equation for n_0,

$$n_0 = n - \lambda^{-3} F_{3/2}(\beta n_0 v_0),$$
$$F_\sigma(z) = \frac{1}{\Gamma(\sigma)} \int_0^\infty dx \frac{x^{\sigma-1}}{\exp(x+z)-1},$$
$$\lambda = \left(\frac{2\pi}{m^* k_B T}\right)^{1/2}. \tag{6}$$

We have solved Eq. (6) analytically for those cases where $\alpha = m^* n v_0 (m k_S T)^{-1} \ll 1$,[8] and $\alpha \geqslant 10$, as well as numerically for intermediate values. In all cases studied, the curve of n_0/n vs T displays the same general behavior as is shown in Fig. 1. As the temperature is raised form $T = 0$, the quantity n_0/n slowly decreases from unity; and at a temperature T_c, which depends upon m^*/m and $nv_0/(k_B T_I)$, n_0/n drops discontinuously to zero. Furthermore, $n_0(T) - n_0(T_c - 0) \propto D(T_c - T)^{1/2}$ for $0 < T_c - T \ll T_c$. To obtain the curve in Fig. 1 we have chosen $v_0 = 4\pi a/m$, the Fermi pseudopotential for a hard sphere of diameter $a = 2.2$ Å,[9] and p_c so that $T_c = T_\lambda$ $(m^*/m = 5.52)$. Also shown in Fig. 1 are graphs of the superfluid fraction ρ_S/ρ, where ρ_S is the superfluid mass density and $\rho = mn$, as obtained experimentally[10] and by the formula[11]

$$\rho_S(T)/\rho = mn_0(T)[m^*n - (m^*-m)n_0(T)]^{-1}. \tag{7}$$

The theoretical curve has a discontinuity at T_λ and, as for $n_0(T)$, $\rho_S(T) - \rho_S(T_\lambda - 0) \propto B(T_\lambda - T)^{1/2}$ just below T_λ. This power-law behavior for ρ_S may be compared with the recent finding of Clow and Reppy[12] whereby $\rho_S(T) \sim C(T_\lambda - T)^\gamma$, $\gamma = 0.67 \pm 0.03$. Except near T_λ the two curves are in moderately good agreement.

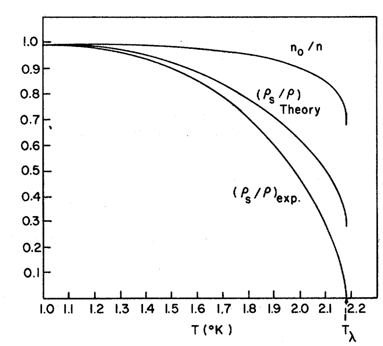

FIG. 1. Experimental results for the superfluid fraction ρ_S/ρ, and ρ_S/ρ and Bose-Einstein condensation fraction n_0/n versus temperature for the Hartree-Fock model when $m^*/m = 5.52$ and $nv_0(k_B T_\lambda)^{-1} = 3.5$.

The internal energy of the system can be obtained by replacing the operator N_p in the expression for $\mathcal{H}_{\text{H-F}}$ by its thermal average, $\langle N_{\vec{p}}\rangle$ of (5), and by omitting the terms $\mu\sum_{\vec{p}}\langle N_{\vec{p}}\rangle$. Using Eq. (1) for $v(\vec{p})$, the internal energy per unit volume is

$$U/V=\tfrac{3}{2}(\beta\lambda^3)^{-1}F_{5/2}(\beta n_0 v_0)+(n^2-\tfrac{1}{2}n_0^{\,2})v_0. \quad (8)$$

Because of the appearance of the terms containing n_0, the dominant behavior of $C_V=(\partial U/\partial T)_{V,N}$ for $0<T_c-T\ll T_c$ is given by

$$C_V\sim-\tfrac{1}{2}Vv_0(3n-n_0)(\partial n_0/\partial T)_{V,N}\propto(T_c-T)^{-1/2}. \quad (9)$$

In Figs. 2(a) and 2(b) we have plotted the results of the numerical evaluation of the complete expression for C_V as a function of T for the same choice of parameters v_0 and $p_c^{\,2}$ as were used to obtain ρ_S/ρ of Fig. 1.

We have extended the above calculations to a generalized version of the Bogoliubov model[13] described by

$$\mathcal{H}_{\text{B}}=\mathcal{H}_{\text{H-F}}+\tfrac{1}{2}n_0\sum_{\vec{p}(\neq 0)}v(\vec{p})(a_{\vec{p}}^{\dagger}a_{-\vec{p}}^{\dagger}+a_{-\vec{p}}a_{\vec{p}}), \quad (10)$$

where $n_0=\langle a_0^{\dagger}a_0\rangle/V$, the ensemble average being taken with respect to $\mathcal{H}_{\text{B}}$. For this model when $nv_0\ll k_{\text{B}}T_I$, we find that $T_c/T_I\approx 1+0.15nv_0\times(k_{\text{B}}T_I)^{-1}$ and

$$n_0(T_c-0)/n=0.23nv_0/(k_{\text{B}}T_I),$$

$$n_0(T)-n_0(T_c-0)\sim 1.17n(nv_0/k_{\text{B}}T_I)^{1/2}[(T_c-T)/T_I]^{1/2}, \quad (11)$$

for temperatures $0<T_c-T\ll T_c$.[14] To obtain this result we have used the relation[5]

$$\langle a_{\vec{p}}^{\dagger}a_{\vec{p}}\rangle=\tfrac{1}{2}[(f_{\vec{p}}/\epsilon_{\vec{p}})\coth(\tfrac{1}{2}\beta\epsilon_{\vec{p}})-1],$$

$$f_{\vec{p}}=\frac{p^2}{2m}+n_0v_0,\quad \epsilon_{\vec{p}}=\left[\frac{p^2}{2m}\left(\frac{p^2}{2m}+n_0v_0\right)\right]^{1/2}, \quad (12)$$

and, for simplicity, we have assumed $v(\vec{p})=v_0$, so that $m^*=m$. The similar temperature behavior of n_0/n for both the Hartree-Fock and Bogoliubov models also applies to C_V just below T_c. In particular, for the Bogoliubov model $C_V\propto T^3$ and $(T_c-T)^{-1/2}$ for $T\ll T_c$ and $0<T_c-T\ll T_c$, respectively.

The present results for C_V and ρ_S, although obtained for two simplified models of a system of interacting bosons, give new impetus to London's idea[1] that the condensation of a macroscopic number of particles into a single quantum state plays a primary role in effecting the unusual properties of He II.

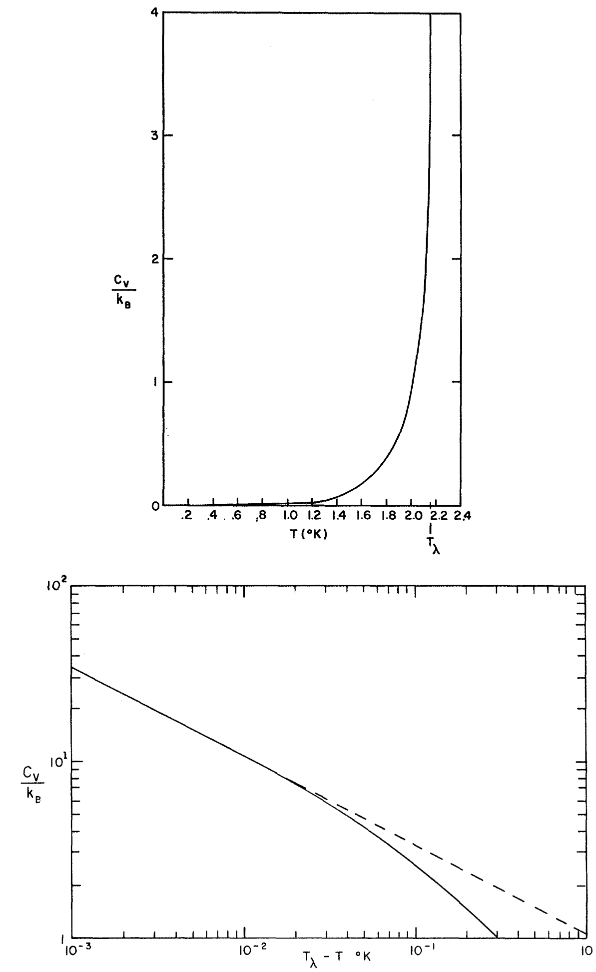

FIG. 2. (a) Specific heat C_V as a function of temperature for the Hartree-Fock model with the same parameters as used in Fig. 1. (b) Log(C_V) vs log($T_\lambda-T$) for $0<T_\lambda-T\ll T_\lambda$ showing that $C_V\propto(T_\lambda-T)^{-1/2}$ in this region. The dashed straight line has slope $-\frac{1}{2}$.

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[6]A careful analysis shows that the replacement of $v(\vec{p})$ by the right-hand side of Eq. (1) leads to negligible errors when $m^* n v_0 (m k_B T_I)^{-1}$ is large compared with unity, or, when small, if $p_c^2 (2m^* k_B T_I)^{-1} \gtrsim 3$. In any event our conclusions concerning the behavior of C_v and ρ_S near the phase transition are in no way affected.

[7]The discussion in W. D. Grobman and M. Luban, Phys. Rev. 147, 166 (1966), Sec. VI, Appendix C, is relevant to this matter.

[8]This work made use of computer facilities at Princeton University which are supported in part by National Science Foundation Grant No. NSF-GP 579.

[9]The quantity $a = 2.2$ Å is the closest distance of approach of two He atoms [see D. G. Henshaw, Phys. Rev. 119, 14 (1960)].

[10]J. G. Dash and R. D. Taylor, Phys. Rev. 105, 7 (1957).

[11]The quantity $\rho_S(T)$ is derived by using the relation $\vec{P} = \rho_S \vec{v}_S$, where $\vec{P}$ is the net momentum per unit volume when a single state of low momentum $\vec{k}(\neq 0)$ is macroscopically occupied and $\vec{v}_S = \vec{k}/m$. Macroscopic occupation of the state $\vec{k}$ is achieved by choosing μ so that $\epsilon(\vec{k}) = 0$. In this case, for small values of $\vec{q} = \vec{p} - \vec{k}$, Eq. (3) is modified to read

$$\epsilon_{\vec{p}} = \frac{q^2}{2m^*} + n_0 v_0 + \frac{\vec{q}\cdot\vec{k}}{m^*} + \frac{2\vec{q}\cdot\vec{p}v_0}{p_c^2}.$$

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