

Microscopic theory of two-dimensional liquid helium*

A. Isihara and Chung-In Um

*Statistical Physics Laboratory, Department of Physics and Astronomy,
State University of New York at Buffalo, Buffalo, New York 14260*

(Received 28 March 1978)

Starting with real boson particles interacting with a soft potential, it is shown that the excitation spectrum and thermodynamical properties of the system in two dimensions are characterized by the Landau-type quasiparticles. The structure factor, specific heat, and the pair distribution function are explicitly evaluated. The pair-distribution function decreases as r^{-3} at large distances. This decrease corresponds to the existence of a phonon spectrum for small momenta. The normal-fluid density divided by the product of the mass density and absolute temperature cubed is constant near absolute zero, reaches to a minimum, and increases at around 0.4 °K. The roton energy gap is given by the position of the minimum energy and the structure factor at this point. Our value is what we might expect by extrapolating the data by Washburn, Rutledge, and Mochel. It also agrees with the recent result by Rutledge, McMillan, and Mochel. The ground-state energy is also evaluated analytically.

I. INTRODUCTION

Recently, there has been a surge of interest in the properties of two-dimensional liquid helium on Grafoil, Vycor glass, and other substrates.¹ The helium films show amazingly complex properties, some of which depend on the film thickness, others on substrates. Extensive studies of the density, specific heat, and other quantities have revealed two-dimensional (2-D) peculiarities as well as bulk properties.

Although the films have complex properties, it has been considered that at high densities they are in a condensed state. Indeed, the specific heat of the films on some substrates showed a quadratic temperature-dependence characteristic of a Debye solid in two dimensions. However, more recently Cray and Vilches found that the specific heat on argon-plated Grafoil showed an exponent of 3.3, indicating nontrivial effects from the substrates.¹ Therefore, real helium films are more complicated than considered hitherto. On the other hand, at low densities, it has been reported that the films are gas-like. In between the two regions of density, a transition takes place. This transition is not in first order and depends on the thickness and substrates. It is probable that the low-temperature side of the specific-heat peak of ⁴He on grafoil represents a two-phase region.

Since the real films are very complicated, we intend to investigate the properties of an idealized 2-D system from the microscopic point of view. We remark that it has been shown that there is no long-range order in a 2-D Bose system.² Therefore, we shall not consider particles of zero momentum in a special

way. We shall try to find the excitation spectrum and thermodynamical properties of an interacting Bose gas in comparison with the bulk case.

Miller and Woo made a variational approach to a similar Bose system, with Jastrow-type trial functions.³ Another approach was made by Padmore.³ Hipólito and Lobo³ used a self-consistent method in which the structure factor, given by the susceptibility sum rule, determines in turn a self-consistent potential for the susceptibility.

Stimulated by these works, we shall present in what follows yet another statistical-mechanical approach. Instead of the approach in which the excitation spectrum is evaluated for absolute zero, we shall make a finite-temperature approach. Anticipating a Landau-type spectrum, we shall treat collective couplings between boson particles interacting with each other with a soft potential. For the bulk case, Samulski and Isihara⁵ showed recently that a grand-ensemble method can be employed effectively to show how phonon or roton quasiparticles can be obtained by starting with real boson particles, giving a new molecular basis to Landau's phenomenological approach. Therefore, we shall extend their theory to two dimensions, neglecting the effects of the substrate.

In Sec. II, we shall present our basic results and formulas for the pair-distribution function and energy. In Sec. III, the excitation energy will be evaluated explicitly for a soft potential with a Lennard-Jones attractive tail. Section IV will discuss the phonon and roton energies, their specific heats and other thermodynamical functions. The ground-state energy is also given in Sec. IV. Section V gives an explicit asymptotic formula for the pair-distribution function. Fi-

nally, in Sec. VI we compare our results with recent works and present our theoretical results in terms of graphs and tables.

In this paper, we shall use units in which we have $\hbar=1$ and $2m=1$, where m is the particle mass, except for the cases in which \hbar or m should appear explicitly.

II. BASIC FORMULA

In this section, we shall present several important formulas which will be used in Secs. III, IV, and V. for the derivation of the energy spectrum and other quantities. For our purpose of treating a helium film, we shall employ an approach based on the pair distribution function rather than a partition-function approach. One of the reasons is that the pair distribution function is directly related to the structure factor which plays an important role in the theory of liquid helium.

For the evaluation of the pair distribution function, we shall adopt the chain-diagram approximation. The pair distribution function evaluated in this approximation is known to represent collective couplings between the particles and to yield the energy in the ring diagram approximation.¹ We shall assume that the interaction between the helium particles is characterized by a repulsive peak which appears at zero momentum followed by a weak attractive tail. Therefore, a small momentum approximation can be introduced.

We shall start with real bosons with pairwise in-

teractions. Starting with these real particles with mass, we shall show first that the thermodynamic properties of the system can be described by quasiparticles obeying Bose statistics. The numbers of these quasiparticles are not conserved. This transition from real particles to quasiparticles will be made possible based on a finite-temperature approach. In this respect, our approach is different from that of Bogolieubov and Zubarev, or Feynman and Cohen for the 3-D case.⁵

In the chain-diagram approximation, the pair distribution function of a Bose fluid is given by⁶

$$\rho_2(r) = n^2 + I(r) - \frac{1}{\beta(2\pi)^{1/2}} \times \sum_{j=-\infty}^{\infty} \int d\bar{q} \frac{u(q)\lambda_j^2(q)}{1+u(q)\lambda_j(q)} e^{i\bar{q}\cdot\bar{r}}, \quad (2.1)$$

where $I(r)$ is the ideal-gas contribution, we have $\beta=1/kT$, n is the density, $u(q)$ is the Fourier transform of the interaction potential, and the λ_j 's are the eigenvalues of the effective boson propagator representing the unit process in the chain configuration of the particles. In the first approximation, we can show that the eigenvalues are given by⁶

$$\lambda_j(q) = 2nq^2 / \left[q^4 + \left(\frac{2\pi j}{\beta} \right)^2 \right] \quad (2.2)$$

The same form appears for the 3-D case. However, different from the 3-D case, the number density of a 2-D Bose system does not include a condensate.

Introducing Eq. (2.2) into Eq. (2.1) we find

$$\begin{aligned} \rho_2(r) &= n^2 + I(r) - \frac{n}{2\pi} \frac{1}{\beta} \sum_{j=-\infty}^{\infty} \int_0^{\infty} dy y^3 J_0(ry) \left(\frac{1}{y^2+x^2} - \frac{1}{y^4+2nu(y)y^2+x^2} \right) \\ &= n^2 + I(r) - \frac{n}{2\pi} \int_0^{\infty} dy y J_0(ry) \left(1 - \frac{1}{[y^2+2nu(y)]^{1/2}} \right), \end{aligned} \quad (2.3)$$

where $I(r)$ is the ideal-gas contribution and x and y represent

$$x = 2\pi j/\beta, \quad y = q.$$

The summation over j in Eq. (2.1) has been converted into integration for the lowest temperature. For finite temperatures, we must use the summation.

In terms of the pair distribution function, the internal energy is given by

$$U(T) = U_0(T) + \frac{1}{2}n^2S \int d\bar{r} \phi(r) - \frac{1}{2}nS \int \frac{d\bar{q}}{(2\pi)^2} u(q) + \frac{1}{2}S \frac{\partial}{\partial\beta} \left(\sum_{j=-\infty}^{\infty} \int_0^1 d\xi \int \frac{d\bar{q}}{(2\pi)^2} \frac{u(q)\lambda_j(q)}{1+\xi u(q)\lambda_j(q)} \right), \quad (2.4)$$

where $U_0(T)$ is the ideal-gas energy, S is the total area of the system, and $\phi(r)$ is the interaction potential.

Using Eq. (2.2) and performing the summation, we arrive at

$$\begin{aligned}
U(T) &= \frac{1}{2} n^2 S \int d\bar{r} \phi(r) \\
&+ \frac{1}{2} S \int \frac{d\bar{q}}{(2\pi)^2} [\epsilon(q) - q^2 - nu(q)] \\
&+ S \int \frac{d\bar{q}}{(2\pi)^2} \epsilon(q) f(\epsilon(q)) , \quad (2.5)
\end{aligned}$$

where $f(\epsilon)$ is the Bose distribution function for quasiparticles,

$$f(\epsilon) = 1/(e^{\beta\epsilon} - 1) , \quad (2.6)$$

and

$$\epsilon(q) = q[q^2 + 2nu(q)]^{1/2} \quad (2.7)$$

is their energy. Equation (2.7) agrees with what Bogoliubov and Zubarev gave.⁷

The internal energy given by Eq. (2.5) consists of the ground-state energy (first term) and the quasiparticle excitation energy (second term). Therefore, we have in effect shown that a Landau type quasiparticle description is possible for the 2-D Bose system.

In Sec. III, we shall further analyze the quasiparticle energy. Before concluding the present section, we remark that if the quasiparticles move with an average drift velocity \bar{v} with respect to the rest system, we expect the total momentum to be

$$\bar{P} = \frac{\hbar^2 S}{4\pi^2} \bar{v} \int dq q^3 \left[-\frac{\partial f(\epsilon(q))}{\partial \epsilon(q)} \right] . \quad (2.8)$$

If this momentum is associated with the "normal fluid", then its density is given by

We find then

$$\begin{aligned}
u(q) &= 2\pi a^2 V_0 \frac{J_1(qa)}{qa} + 2\pi a^2 \mathcal{E} \left[-\frac{(qa)^9}{10!!^2} + \frac{4}{10!!} (qa)^7 - \frac{64}{10!!} (qa)^5 + \left(\frac{6}{10 \times 10!!} - \frac{1}{4!!^2} \right) (qa)^3 \right. \\
&\quad \left. + \left(\frac{4}{4!!^2} - \frac{4 \times 48}{5 \times 10!!} \right) (qa) \right] J_1(qa) \\
&+ 2\pi a^2 \mathcal{E} \left[\frac{2}{10!!} (qa)^8 - \frac{2559}{10!! \cdot 10 \times 8} (qa)^6 + \frac{1}{10!! \times 10} (qa)^4 + \frac{3}{10^2} (qa)^2 - \frac{3}{20} \right] J_0(qa) \\
&- 2\pi a^2 \mathcal{E} \left[\frac{(qa)^4}{4!!^2} + \frac{(qa)^{10}}{10!!} \right] \left[-2\text{Ci}(qa) + \gamma + \ln qa - \sum_{k=1}^{\infty} \frac{(-)^k (\frac{1}{2} qa)^{2k}}{2k(k!)^2} \right] . \quad (3.4)
\end{aligned}$$

For small q , we can further expand the right-hand side as follows:

$$\begin{aligned}
2nu(q) &= A^2(0) + A_1^2 q^2 + A_2^2 q^4 - A_3 q^4 \ln qa - A_4 q^6 + \dots , \quad A^2(0) = 2\pi n a^2 (V_0 - \frac{3}{10} \mathcal{E}) , \\
A_1^2 &= \pi \frac{n a^4}{2^2} (\frac{3}{2} \mathcal{E} - V_0) , \quad A_2^2 = 4\pi n a^6 \left[\frac{V_0}{2^6 \times 3!} - \frac{\mathcal{E}}{10 \times 10!!} (1016 + 48 \times 10^2 \gamma) \right] , \quad \gamma = .5771 . \quad (3.5)
\end{aligned}$$

For the potential, we find the energy spectrum in the following form:

$$\epsilon(q) = A(0)q + Bq^3 + Cq^5 + \dots , \quad (3.6)$$

$$\rho_N(T) = \frac{1}{4\pi} \int_0^\infty q^3 dq \left[-\frac{\partial f(\epsilon(q))}{\partial \epsilon(q)} \right] . \quad (2.9)$$

III. EXCITATION ENERGY

The energy given by Eq. (2.7) is the type Bogoliubov and Zubarev gave for three dimensions. For small momentum, the spectrum is phonon-like with the sound velocity given by

$$c = \left[\frac{nu(0)}{m^*} \right]^{1/2} = [2nu(0)]^{1/2} , \quad (3.1)$$

where $u(0)$ is the value of $u(q)$ at zero momentum and is assumed to be positive.

For higher momentum, the energy can be expanded as follows:

$$\epsilon(q) = q^2 + nu(q) - \frac{1}{2} \{ [nu(q)]^2 / q^2 \} + \dots . \quad (3.2)$$

The right-hand side depends on $u(q)$. Note that in general the energy is particle-like whenever $u(q)$ vanishes.

To have a more explicit form for the energy, let us assume a soft potential with a Lennard-Jones tail,

$$\phi(r) = \begin{cases} V_0 , & r \leq a \\ \mathcal{E} \left[\left(\frac{a}{r} \right)^{12} - \left(\frac{a}{r} \right)^6 \right] , & r \geq a \end{cases} . \quad (3.3)$$

where

$$B = [1/2A(0)](1 + A_1^2) ,$$

$$C = [1/2A(0)] \{A_2^2 - [1/4A^3(0)](1 + A_1^2)^2\} . \quad (3.7)$$

On the other hand, for large q , the first term in $u(q)$ is dominant so that we could use

$$\epsilon(q) = q [q^2 + (4\pi na^2/qa) V_0 J_1(qa)]^{1/2} . \quad (3.8)$$

The Bessel function is oscillatory, therefore, there can be a minimum in the energy curve plotted against q . Around this minimum, we can have

$$\epsilon(q) = \Delta + (\hbar^2/2m^*)(q - q_0)^2 , \quad (3.9)$$

where the effective mass and the energy gap are given by

$$\frac{m}{m^*} = \frac{1}{S(q)} - \frac{q_0^2 S''(q_0)}{2S(q_0)^2} , \quad (3.10)$$

$$\Delta = \frac{\hbar^2 q_0^2}{2mS(q_0)} , \quad S(q) = \frac{q}{[q^2 + 2nu(q)]^{1/2}} .$$

$S(q)$ is the structure factor. The position of the minimum energy is determined from

$$2[q_0^2 + 2nu(q_0)] = nq_0[-u'(q_0)] . \quad (3.11)$$

IV. THERMODYNAMIC FUNCTIONS

In view of the energy spectrum we follow Landau's theory to obtain the phonon and roton energies. Using the small- q expansion of the energy

$$\epsilon(q) = A(0)q + Bq^3 + Cq^5 + \dots , \quad (4.1)$$

we obtain

$$\epsilon_{\text{ph}} = \frac{1}{2\pi} \left[\frac{2\zeta(3)}{A^2(0)} (kT)^3 + \frac{4 \times 4! B \zeta(5)}{A^5(0)} (kT)^5 + \frac{6! C \zeta(7)}{A^7(0)} (kT)^7 + \dots \right] . \quad (4.2)$$

For the roton part, we make use of Eq. (3.10) to obtain

$$\epsilon_{\text{rot}} = (m^*/2\pi\hbar^2)^{1/2} q_0 \left[\frac{1}{2} (kT)^{3/2} + \Delta (kT)^{1/2} \right] e^{-\Delta/kT} . \quad (4.3)$$

The corresponding specific heats are given by

$$C_{\text{vph}} = \frac{k}{2\pi} \left[\frac{3! \zeta(3)}{A^2(0)} (kT)^2 + \frac{4 \times 5! \zeta(5) B}{A^5(0)} (kT)^4 + \frac{7! \zeta(7) C}{A^7(0)} (kT)^6 + \dots \right] , \quad (4.4)$$

$$C_{\text{vrot}} = \left(\frac{m^* k T}{2\pi \hbar^2} \right)^{1/2} k q_0 \left[\frac{3}{4} + \frac{\Delta}{kT} + \left(\frac{\Delta}{kT} \right)^2 \right] e^{-\Delta/kT} . \quad (4.5)$$

Note that the phonon part of the specific heat is an even function of temperature with the first quadratic term which is characteristic of two dimensions. The roton part is characterized by the energy gap Δ and the roton momentum q_0 . Because of the exponential factor, it is small for low temperatures.

Our theoretical expressions for the free energy, entropy, and pressure are

$$F_{\text{ph}}(T) = -\frac{1}{2\pi} \left[\frac{\zeta(3)}{A^2(0)} (kT)^3 + \frac{4! \zeta(5) B}{A^5(0)} (kT)^5 + \dots \right] , \quad (4.6)$$

$$F_{\text{rot}}(T) = -q_0 \left(\frac{m^*}{2\pi \hbar^2} \right)^{1/2} (kT)^{3/2} e^{-\Delta/kT} , \quad (4.7)$$

$$S_{\text{ph}}(T) = \frac{k}{2\pi} \left[\frac{3\zeta(3)}{A^2(0)} (kT)^2 + \frac{5! \zeta(5) B}{A^5(0)} (kT)^4 + \dots \right] , \quad (4.8)$$

$$S_{\text{rot}}(T) = \left(\frac{m^* k T}{2\pi \hbar^2} \right)^{1/2} k q_0 \left[\frac{3}{2} + \frac{\Delta}{kT} \right] e^{-\Delta/kT} , \quad (4.9)$$

$$p_{\text{ph}} = \frac{1}{\pi} \left[\frac{\zeta(3)}{A^2(0)} (kT)^3 + \frac{2 \times 4! B_1 \zeta(5)}{A^5(0)} (kT)^5 + \dots \right] , \quad (4.10)$$

$$p_{\text{rot}} = \left(\frac{m^*}{2\pi \hbar^2} \right)^{1/2} q_0 (kT)^{3/2} e^{-\Delta/kT} , \quad (4.11)$$

where

$$B_1 = \frac{1}{2A(0)} (1 + \frac{3}{4} A_1^2) .$$

We consider that the normal fluid consists of the phonon and roton parts. Using Eq. (2.9), we obtain

$$\rho_{N\text{ph}}(T) = \frac{3! \zeta(3) \hbar}{4\pi A(0)} \left[\frac{kT}{\hbar A(0)} \right]^3 - \frac{6! \zeta(6) B \hbar}{8\pi m A^3(0)} \left[\frac{kT}{\hbar A(0)} \right]^5 + \dots , \quad (4.12)$$

$$\rho_{N\text{rot}}(T) = \frac{1}{2} \left(\frac{m^* \hbar^2}{2\pi k T} \right)^{1/2} q_0^3 e^{-\Delta/kT} . \quad (4.13)$$

The ground-state energy is obtained from Eq. (2.5) as follows:

$$E_g = \frac{1}{2} n^2 S \int \phi(r) d\bar{r} + \frac{1}{2} S \int \frac{d\bar{q}}{(2\pi)^2} [\epsilon(q) - q^2 - nu(q)] \quad (4.14)$$

$$= I_1 + I_2 + I_3 . \quad (4.15)$$

For the soft potential which has been adopted we find

$$I_1 = \frac{1}{2} \pi n a^2 S V^* \quad (4.16)$$

where

$$V^* = (V_0 - \frac{3}{10} \epsilon) \quad (4.17)$$

For the second integral, we use $u(q)$ expanded to order q^2 . We then obtain

$$I_2 = \frac{1}{6} \frac{N}{n a^2} \left(\frac{n V^*}{2\pi} \right)^{1/2} \left[1 - \frac{3}{4} n a^2 \left(\frac{2\pi V^*}{n} \right)^{1/2} \right] \quad (4.18)$$

For the third integral I_3 we expand the square root in the integrand and use

$$I_3 = -\frac{(2\pi n a^2 V_0)^2}{8\pi} S \int_{\alpha_0}^{\infty} \frac{J_1(x)}{x^3} dx, \quad \alpha_0 = q_0 a \quad (4.19)$$

We then make use of the Bessel-function formulas,

$$\int_{\alpha_0}^{\infty} \frac{J_1^2(x)}{x^3} dx = \frac{1}{4} \frac{J_1^2(\alpha_0)}{\alpha_0^2} + \frac{1}{2} \int_{\alpha_0}^{\infty} \frac{J_0(x) J_1(x)}{x^2} dx,$$

$$\int_{\alpha_0}^{\infty} \frac{J_0(x) J_1(x)}{x^2} dx = \frac{1}{2} \frac{J_0(\alpha_0) J_1(\alpha_0)}{\alpha_0} + \frac{1}{2} \int_{\alpha_0}^{\infty} \frac{J_0^2(x)}{x} dx - \frac{1}{2} \int_{\alpha_0}^{\infty} \frac{J_1^2(x)}{x} dx,$$

$$\int \frac{J_{\nu+1}^2(x)}{x^{2\nu+1}} dx = -\left(\frac{1}{(4\nu+2)x^{2\nu}} \right) [J_{\nu}^2(x) + J_{\nu+1}^2(x)],$$

to arrive at

$$I_3 = -\frac{(2\pi n a^2 V_0)}{8\pi} S \left\{ J_1^2(1) - 2J_0(1)J_1(1) - J_0^2(1) + 4\text{Ci}(1) + 2\gamma - \sum_{k=1}^{\infty} \frac{(-)^k}{2^{2k} k (k!)^2} \right. \\ \left. + 2 \sum_{n=1}^{\infty} \frac{1}{n} J_1(1) J_{2n}(1) - \sum_{n=1}^{\infty} \frac{1}{n^2} [J_{2n+1}(1) J_0(1) - J_{2n}(1) J_1(1)] \right\} \quad (4.20)$$

Therefore, assembling these results, we finally obtain

$$\epsilon_0 = \frac{E_g}{N} = \frac{1}{2} \pi n a^2 V^* \left\{ 1 - \frac{1}{4\pi} \frac{1}{n a^2} \left[1 - \frac{4}{3} \frac{1}{n a^2} \left(\frac{n}{2\pi V^*} \right)^{1/2} \right] + \frac{(a V_0)^2}{V^*} \delta \right\}, \quad (4.21)$$

where

$$\delta = \left\{ J_1^2(1) - 2J_0(1)J_1(1) - J_0^2(1) - 4\text{Ci}(1) + 2\gamma - \sum_{k=1}^{\infty} \frac{(-)^k}{2^{2k} k (k!)^2} + 2 \sum_{n=1}^{\infty} \frac{1}{n} J_1(1) J_n(1) \right. \\ \left. - \sum_{n=1}^{\infty} \frac{1}{n^2} [J_{2n+1}(1) J_0(1) - J_{2n}(1) J_1(1)] \right\} \quad (4.22)$$

Here, the parameter δ appears from I_3 of Eq. (4.20).

The above results for a soft potential can be used for the case of an approximate pseudopotential for a hard-sphere repulsion. Although most of the results can be derived in a straightforward way, the ground-state energy involves a divergence. A similar divergence appears also in the 3-D case due to the use of an approximate pseudopotential. As we shall discuss later, the main difference between the spectrum of the soft-potential case and the approximate pseudo-

potential case is in the disappearance of the roton minimum for the latter.

V. PAIR DISTRIBUTION FUNCTION

It is difficult to evaluate analytically the pair distribution function for a soft potential. Therefore, in what follows we report an approximate result retaining only the first term with $J_1(qa)$ in Eq. (3.4):

$$\Delta\rho_2(r) = \rho_2(r) - I(r) \quad (5.1)$$

For the asymptotic expression for the pair distribution function, we retain only the constant term of $u(q)$ and use

$$\Delta\rho_2(r) = n^2 - \frac{n}{2\pi} \times \int_0^\infty dy y J_0(ry) \left[1 - \frac{1}{[y^2 + 2nu(0)]^{1/2}} \right] \quad (5.2)$$

$$\Delta\rho_2(r) = n^2 - \frac{n}{2\pi} \left[\int_0^\infty dy y J_1'(ry) \left[1 - \frac{1}{[y^2 + 2nu(0)]^{1/2}} \right] + \frac{1}{r} \int_0^\infty dy J_1(ry) \left[1 - \frac{1}{[y^2 + 2nu(0)]^{1/2}} \right] \right] \quad (5.4)$$

Integrating by parts we obtain

$$\Delta\rho_2(r) = n^2 - \frac{n}{2\pi} \frac{\alpha}{r} \frac{\partial}{\partial \alpha} \frac{\partial}{\partial r} \int_0^\infty \frac{J_0(ry)}{(y^2 + \alpha^2)^{1/2}} dy \quad (5.5)$$

We can apply the integral formula

$$\int_0^\infty \frac{J_\nu(2ax)}{(x^2 + y^2)^{1/2}} dx = I_{\nu/2}(ay) K_{\nu/2}(ay) \quad (5.6)$$

to arrive at

$$\Delta\rho_2(r) = n^2 - \frac{n}{2\pi} \frac{1}{2} \alpha^2 [K_0(z)I_0(z) - K_1(z)I_1(z)] \quad (5.7)$$

where

$$z = \frac{\alpha r}{2} = \left(\frac{u(0)}{2\pi} \right)^{1/2} \frac{r}{r_0} = \left(\frac{u(0)}{2\pi} \right)^{1/2} \frac{R}{R_0} \quad (5.8)$$

$$\left(R = \frac{r}{a}, R_0 = \frac{r_0}{a} \right)$$

For large arguments, the Bessel functions are given by

$$I_\nu(z) \approx (2\pi z)^{-1/2} e^z \sum_{n=0}^{\infty} (-)^n \frac{(\nu, n)}{(2z)^n} \quad (5.9)$$

$$K_\nu(z) \approx \left(\frac{\pi}{2z} \right)^{1/2} e^{-z} \sum_{n=0}^{\infty} \frac{(\nu, n)}{(2z)^n}$$

$$(\nu, n) = \Gamma(\nu + n + \frac{1}{2}) / n! \Gamma(\nu - n + \frac{1}{2})$$

Therefore, we find the asymptotic result

$$\frac{\Delta\rho_2(R)}{n^2} = 1 - \frac{1}{4} \left(\frac{2\pi}{u(0)} \right)^{1/2} \frac{R_0^3}{R^3} \times \left[1 + \frac{2373}{2^{11}} \frac{2\pi}{u(0)} \frac{R_0^2}{R^2} + \dots \right] \quad (5.10)$$

In terms of the relations between the Bessel functions

$$J_\nu'(z) = J_{\nu-1}(z) - \frac{\nu}{z} J_\nu(z) \quad (5.3)$$

$$y J_1'(ry) = y J_0(ry) - \frac{1}{r} J_1(ry)$$

we can rewrite Eq. (5.2)

This result is subject to the condition

$$R \gg \frac{1}{2^5} \left(\frac{2373\pi}{u(0)} \right)^{1/2} R_0 = Q_1 R_0 \quad (5.11)$$

The factor Q_1 here is approximately 0.21 for the parameters which will be chosen in Sec. VI. The R^{-3} proportionality of the pair distribution function is characteristic of 2-D phonons. It is this decrease which causes the phonon spectrum. For three dimensions, the R^{-4} asymptotic variation of the pair distribution function characterizes the phonon spectrum. The quantity $u(0)$ is dimensionless. This is another 2-D peculiarity.

VI. RESULTS AND DISCUSSIONS

Figure 1 illustrates the Fourier transform $u(q)$ of the soft potential which we adopted. The potential parameters have been chosen so as to be able to fit the same experimental data at the density of 0.0279 \AA^{-2} , as used by Hipólito and Lobo,

$$V_0 = 10.44 \text{ }^\circ\text{K}, \quad \delta = 10.22 \text{ }^\circ\text{K}$$

$$a = 4.1 \text{ } \text{\AA}, \quad m^* = 0.75 m$$

With these parameters, the excitation spectrum was obtained as in Fig. 2. The spectrum is phonon-like for small momenta and roton-like at around q_0 . The roton parameters and the sound velocity are listed in Table I in comparison with what Hipólito and Lobo and also Padmore reported recently.^{3,4}

The small differences in the energy gap and q_0 between Hipólito-Lobo's case and ours may not be seriously considered, but Padmore's calculation indicates that the energy gap decreases for low coverages. The difference in the effective mass is more significant. Padmore's calculation indicates that m^* increases towards low coverages. His value for the

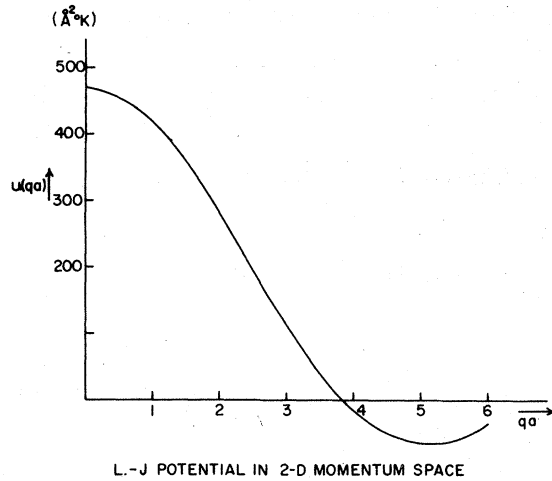


FIG. 1. Fourier transform of a soft potential given by Eq. (3.4).

density of $0.6\rho_0$ is $0.30 m$. Hence, for our low-coverage case, a larger value such as ours may be expected.

From the excitation spectrum we can obtain the condition for superfluidity. We have found that the critical velocity is given by

$$v_c = 50.69 \text{ m/sec} .$$

If the interaction potential is not soft and does not give a solution to

$$q^2 = n(-2u - \frac{1}{2}qu') ,$$

we do not expect a roton dip. Since the left-hand side is positive, the attractive potential and the decrease of the repulsive part are important.

Figure 3 illustrates our theoretical structure factor corresponding to the excitation spectrum of Fig. 2. For small momenta ($q \sim 0.2 \text{ \AA}^{-1}$), the structure factor is proportional to $q/[2nu(0)]^{1/2}$. It reaches a maximum at around $q = 1.05 \text{ \AA}^{-1}$.

The specific-heat data are complex. Around 1970, the low-temperature data showed the essential characteristic of a 2-D Debye model. For instance, an empirical formula could be used, i.e.,

TABLE I. Roton parameters and sound velocity.

	$(10^{-2} \text{ \AA}^{-2})$	Δ/k_B (°K)	q_0 (\AA^{-1})	m^*/m	v_s
Isihara-Um	2.79	4.12	1.02	0.75	164.4
Hipólito-Lobo	2.79	4.37 ^a	0.86 ^a	0.20	157
Padmore	4.69 ^b	6.8	1.25	0.30	

^aRead from the graph.

^bCorresponds to $0.6 \rho_0$.

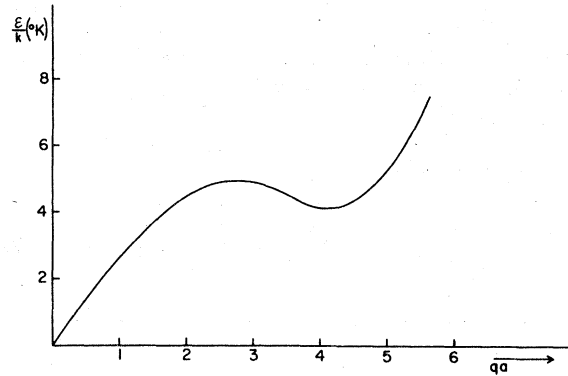


FIG. 2. Excitation spectrum of a helium film evaluated for a soft potential.

$$C_v/Nk = 28.8(T/\Theta_D)^2 .$$

The Debye characteristic temperature varies with the substrates. For instance, it is about $23 \pm 1 \text{ °K}$ for Nuclepor filters and is 56.1 for Grafoil. On the other hand, Cray and Vilches reported recently¹ that helium on argon-plated Grafoil gave an exponent of 3.3 ± 0.2 . Hence, the real films are very complicated and the effects of the substrates are important. Our theoretical model gives approximately the same overall temperature variation as that of Hipólito and Lobo.

We remark that the energy spectrum given by Hipólito and Lobo in their Eq. (3.1) differs from our Eq. (3.8). Their sound velocity is inversely proportional to the hard-sphere diameter [see Eq. (3.3)] in

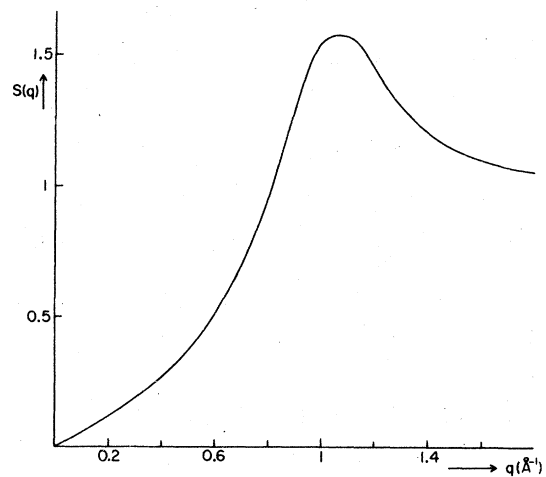


FIG. 3. Structure factor evaluated for a soft potential.

contrast to the Bogolieubov spectrum. However, note that their parameter B is of complex nature. We have not traced their calculation in every detail, but their Eq. (2.5) seems to be not quite correct.

Apart from these points, Hipólito and Lobo's replacement of a two-body distribution function by a product of singlet distribution functions, and the correlation function expressed by Eq. (2.2), ought to be critically examined. The Kirkwood superposition approximation⁸ has been made by Miller and Woo. Since their final results are given numerically for a set of potential and other parameters, it is not easy to find the validity of these approximations in an analytical way. Nevertheless, Hipólito and Lobo's specific-heat result is not very far from experiment except for very low temperatures and near the specific-heat peak. After a correction of a factor of 4, the result of Miller and Woo agrees well with the experimental specific heat. Therefore, their approximations may not be very bad.

Concerning the specific heat, we have chosen the parameters in more or less relation with Hipólito and Lobo. Then, the roton parameters came out close as in Table I. Note that both theories deviate from the specific-heat data at low temperatures. If the quadratic dependence is the case, we could of course fit such a dependence at low temperatures.

The excitation energy spectrum has been evaluated by several authors. In close examination, the curve in Fig. 4 of Miller and Woo seems to show a shoulder at around 0.2 \AA^{-1} . A similar shoulder is clearly seen in their curve for the structure factor. No such shoulder is found in Hipólito and Lobo's and our results. Our overall curve is similar to what Hipólito and Lobo gave. On the other hand, Padmore reported that the roton dip disappears at a low density. The radial part of the Laplacian which he used appears to be three-dimensional rather than two-dimensional, but in any case for a high coverage, his result for the excitation spectrum is not very far from ours as in Table I.

The structure factor reported by Miller and Woo shows a peak at around 1.5 \AA^{-1} with a maximum value of 1.18. The structure factor given by Hipólito and Lobo depends largely on the parameter B which in turn varies with the density. For $B = 225$ for which they evaluated the energy spectrum, the structure factor reaches a maximum value of around 1.5 at around 1 \AA^{-1} . These results are close to what we have reported in Fig. 3.

In Fig. 4 we have illustrated our theoretical normal fluid density given by $\rho_{N\text{ph}} + \rho_{N\text{rot}}$ of Eqs. (4.12) and (4.13). It is normalized by the mass density ρ and T^3 so that the constancy of the normal-fluid density is exhibited at the lowest temperature. A similar curve has been obtained by Washburn, Rutledge and Mochel⁹ who measured the third-sound velocity. Prior to these authors, Scholtz, McLean and Rudnick¹⁰

used a flight time measurement for the third sound. After the initial constancy, the normal-fluid density in Fig. 4 shows a dip at around $0.25 \text{ }^\circ\text{K}$, in agreement with Washburn, Rutledge and Mochel (WRM).

The roton gap Δ is determined by q_0 which in turn is given by Eq. (3.11) as a function of n and the potential. While it is difficult to solve this implicit equation, the gap value can change when different densities are used.

The roton gap has been given by WRM as a function of the film coverage parameter d . Our theoretical value for d can be found by converting the saturated number density $2.18 \times 10^{-2} \text{ \AA}^{-3}$ of bulk helium into two dimensions and then by dividing our surface density $2.79 \times 10^{-2} \text{ \AA}^{-2}$ by thus obtained value, i.e., $7.07 \times 10^{-2} \text{ \AA}^{-2}$. Our theoretical Δ as a function of d is given by Fig. 5 by the black circle. In comparison, the data of WRM are illustrated by white circles. If we connect the three white circles with the black circle, we obtain a dashed curve. Although the meaning of this curve has yet to be investigated, indications are that the roton gap might decrease with the film coverage. This may be so because the roton excitation is a result of boson correlations which may vary with density. We remark also that our result agrees well with the roton gap obtained by Rutledge, McMillan and Mochel¹¹ On the other hand, for the same density the roton gap can be the same as in the bulk liquid as in the experiment of Carneiro *et al.*¹²

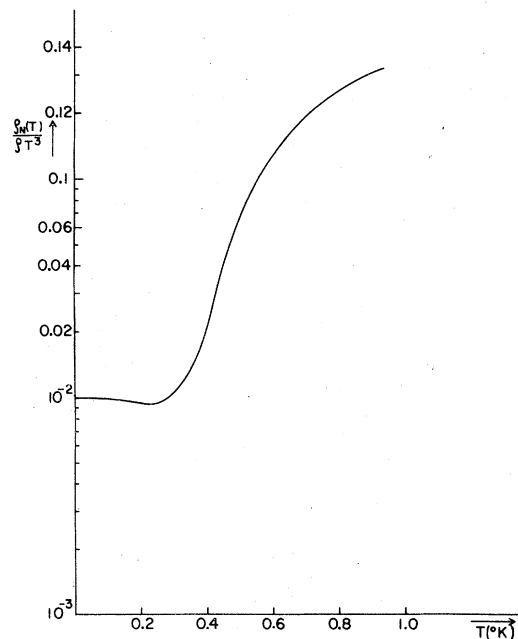


FIG. 4. Normal-fluid density $\rho_N(T)$ as a function of temperature.

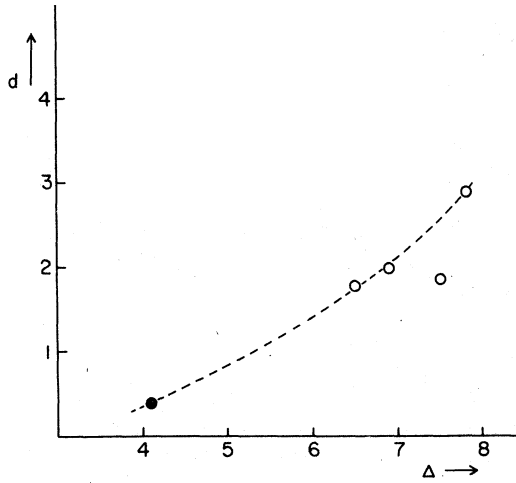


FIG. 5. Roton energy gap as a function of film coverage d in atomic layers. The white circles represent the data by Washburn, Rutledge and Mochel and the black circle is our theoretical point. The dashed curve connects three experimental points with the theoretical point.

Instead of the normal-fluid density, one can evaluate the superfluid density ρ_s as a function of temperature. From Eq. (4.12) we obtain

$$\rho_s/\rho = 1 - \alpha T^3 - (\beta/T^{1/2})e^{-\Delta/T},$$

where α and β are constants. Recently, Bishop, Parpia, and Reppy¹³ fit their data to a theoretical relation similar to the above, except that their second term is quadratic. This seems to be incorrect. Their theoretical curves deviate at higher temperatures. If their quadratic term is replaced by a cubic term as in the above expression, their curves would decrease faster as in the experimental data.

The λ temperature may be determined from the condition that $\rho_{N_{tot}}/\rho = 1$, as in the 3-D case. We then find $T_\lambda = 1.5$ °K. If we adjust this value in proportion to the ratio of the theoretical and experimental values for the 3-D case, we obtain $T_\lambda = 1.2$ °K for the soft potential which has been used.

We have evaluated the ground-state energy analytically as in Eq. (4.21). The parameter δ appearing in the last term is found approximately to be -0.0112 . For the parameters which we have used for the density 0.0279 \AA^{-2} , Eq. (4.21) gives $\epsilon_0 = 3.09$ °K. This value corresponds to $na^2 = 0.47$. Some other values for the produce na^2 will give different energies. On the other hand, if the density alone is changed, readjustment of other parameters such as a has to be made. Therefore, it is not a simple matter to find the energy as a function of density. When na^2 is used as a single variable, nevertheless, our theoretical curve for the energy becomes similar to what Liu, Kalos

and Chester obtained numerically.¹⁴

The ground-state energy expression (4.21) is based on a Taylor expansion. If we simplify the potential such that

$$u(q) = \begin{cases} u_0 = \pi V_0 a^2; & q \leq q_c \\ 0; & q > q_c \end{cases}$$

then the ground-state energy can be obtained analytically as follows:

$$\epsilon_0 = \frac{1}{4}A^2 + \frac{1}{4\pi n} \left[\frac{1}{4}q_c(q_c + A^2)^{3/2} - \frac{1}{8}A^2q_c(q_c + A^2)^{1/2} - \frac{1}{8}A^4 \ln \frac{(q_c^2 + A^2)^{1/2} + q_c}{A} - \frac{1}{4}q_c^4 - \frac{1}{4}A^2q_c^2 \right], \quad (6.1)$$

where $A^2 = 2\pi na^2 V_0$.

In order to simplify this expression, let us consider that

$$q_c = 1/a, \quad na^2 \ll 1, \quad V_0 a^2 \ll 1.$$

Then, the leading terms of the energy are given by

$$\epsilon_0 = \frac{1}{2}\pi na^2 V_0 \left(1 + \frac{1}{8}a^2 V_0 \ln(nV_0 a^4) \right). \quad (6.2)$$

Because of the above conditions, the logarithmic term is negative. Since its factor is being considered

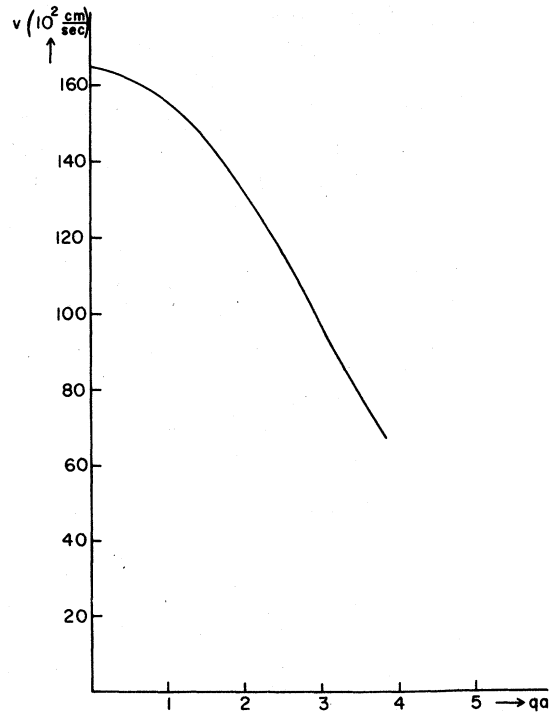


FIG. 6. Sound-wave dispersion.

to be small, the ground-state energy is positive. This positiveness agrees with the well-known 3-D hard-sphere case.¹⁵

The ground-state energy was treated by Schick by a different method.¹⁶ The result given by his Eq. (14) differs from ours in that the energy does not have a term corresponding to our first term, does not depend on V_0 and has a logarithmic factor in the denominator. Although detailed analysis of his approach is beyond the scope of the present paper, there is no condensate in our case. The appearance of our first dominant term is clear. Our logarithmic term is obtained by summing all the graphs including b , d , etc. in Schick's Fig. 1. Since our result depends on V_0 , the energy vanishes when V_0 is brought to zero. This must be so because we have omitted U_0 in Eq. (2.4).

The derivative of the excitation energy with respect

to q yields the sound velocity v_s as a function of momentum. Figure 6 illustrates our theoretical curve for the velocity as a function of qa . The sound velocity at zero momentum depends on the molecular parameters, especially the hard-sphere diameter and density. We have used the previous molecular parameters which have been determined so as to have a specific-heat curve similar to Hipólito and Lobo's. On the other hand, if only the region near absolute zero of the specific heat is concerned, we would obtain a lower sound velocity.

ACKNOWLEDGMENT

This work was based on the thesis submitted by one of the authors (C.U.) to the State University of New York at Buffalo for partial fulfillment of Ph.D. requirements.

-
- ¹Robert L. Elgin and David L. Goodstein, *Phys. Rev. A* **9**, 2657 (1974); M. Bretz, J. G. Dash, D. C. Hickernell, E. O. McLean, and O. E. Vilches, *ibid.* **8**, 1589 (1973); R. L. Siddon and M. Schick, *ibid.* **9**, 907 (1974); S. B. Crary and O. E. Vilches, *Phys. Rev. Lett.* **38**, 973 (1977).
- ²P. C. Hohenberg, *Phys. Rev.* **158**, 383 (1967).
- ³Michael D. Miller and Chia-Wei Woo, *Phys. Rev. A* **7**, 1322 (1973); Timothy C. Padmore, *Phys. Rev. Lett.* **32**, 825 (1974).
- ⁴O. Hipólito and R. Lobo, *Phys. Rev. B* **14**, 3892 (1976).
- ⁵A. Isihara and T. Samulski, *Phys. Rev. B* **16**, 1969 (1977); *Physica (Utr.) A* **82**, 294 (1976).
- ⁶A. Isihara, *Statistical Physics* (Academic, New York, 1971), Chap. 10 & 11.
- ⁷N. N. Bogoluebov and D. N. Zubarev, *Zh. Eksp. Teor. Fiz.* **28**, 129 (1955) [*Sov. Phys. JETP* **1**, 83 (1955)].
- ⁸To a Bose fluid, the product approximation may not be applicable. See, for instance, P. Berdahl, *Phys. Rev. A* **10**, 2378 (1974).
- ⁹T. E. Washburn, J. E. Rutledge, and J. M. Mochel, *J. Low Temp. Phys.* **14**, 372 (1975).
- ¹⁰J. H. Scholtz, E. O. McLean, and I. Rudnick, *Phys. Rev. Lett.* **32**, 147 (1974).
- ¹¹J. E. Rutledge, W. L. McMillan, and J. M. Mochel, in *Quantum Fluids and Solids*, edited by S. B. Trickey, E. D. Adams, and J. W. Dufty (Plenum, New York, 1977), p. 438.
- ¹²K. Carneiro, W. D. Ellenson, L. Passell, J. P. McTauge, and H. Taub, *Phys. Rev. Lett.* **37**, 1695 (1976).
- ¹³D. J. Bishop, J. M. Parpia, and J. D. Reppy, *J. Low Temp. Phys.* **14**, 380 (1975).
- ¹⁴K. S. Liu, M. H. Kalos, and G. V. Chester, *Phys. Rev. B* **13**, 1971 (1976).
- ¹⁵T. D. Lee, K. H. Huang, and C. N. Yang, *Phys. Rev.* **106**, 1135 (1957); A. Isihara and Daniel Yee, *Phys. Rev.* **136**, 618 (1963).
- ¹⁶M. Schick, *Phys. Rev. A* **3**, 1067 (1971).