

$$\times \exp \left[-\rho \left(\frac{1}{gg'x_0} - \frac{g}{g'(x'+1)} - \delta \right) \right] dx', \quad \int_0^\infty Q(x_0) dx_0 = 1. \quad (\text{B32})$$

$$x_0 \geq \frac{1}{g(g+g'\delta)} \quad (\text{B31})$$

and the normalization condition

That is,

$$W = \int_0^\infty Q(x_0) \exp \left(\rho \frac{g}{g'(1+x_0)} \right) dx_0. \quad (\text{B33})$$

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Bose-Einstein Condensation in a One-Dimensional Model with Random Impurities*

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We study the thermodynamics of a one-dimensional system of noninteracting bosons in the presence of random fixed finite-range repulsive potentials. It is shown that a Bose-Einstein condensation into the lowest state occurs. The critical temperature increases with the number of impurities. The specific heat exhibits a discontinuity and is infinitely differentiable from both sides of the critical point. For a suitably defined pressure the isothermals exhibit a flat portion below the "transition length."

I. INTRODUCTION

In this paper we shall study a one-dimensional gas of independent spinless bosons in the presence of random impurities. These impurities are represented by fixed finite-range repulsive potentials. The model is identical to the one studied in the preceding paper,¹ where the structure of the low-lying states and the density of states was investigated. There we found it possible to obtain these levels for an arbitrary finite-range impurity potential. Now we imagine independent bosons occupying these states. In the interest of simplicity the calculations are only carried out for the case where the impurity potential is represented by a δ function of infinite strength. Considerations of the same nature may be made for the general case² (because the structure of the low-lying levels is very similar), but we do not go into these here, as the details prove to be quite complicated.

In Sec. II we show that the Bose-Einstein transi-

tion occurs in the thermodynamical limit. In Sec. III the transition temperature and detailed nature of the transition are investigated. Finally, in Sec. IV, it is shown that our result is not in contradiction with the well-known Bogoliubov inequality,³ which has been used by Hohenberg⁴ to show that there is no condensation into the lowest-momentum state in one-dimensional systems of bosons.

II. EXISTENCE OF BOSE-EINSTEIN TRANSITION

For the case of impurity potentials represented by δ functions of infinite strength, the energy levels can be given explicitly.¹ Let L_j represent the j th-largest distance between δ functions (i. e., the length of the j th-largest "cell"). For $\nu - 1$ impurities, $L_1 \geq L_2 \geq L_3 \cdots \geq L_\nu$.

The levels are

$$E_{j,s} = c^2 s^2 / L_j^2, \quad s = 1, 2, \dots, \infty \quad (2.1)$$

$$c^2 \equiv \hbar^2 \pi^2 / 2m.$$

The number of bosons is given by

$$N = \sum_{j,s} \bar{n}_{j,s} = \sum_{j,s} \frac{1}{\exp[\beta(E_{j,s} - \mu)] - 1}, \quad (2.2)$$

where $\beta = 1/kT$ and μ is the chemical potential of the system. Consider the situation at the absolute zero temperature. Clearly all particles are in the lowest state $E_0 = E_{11} = c^2/L_1^2$:

$$\bar{n}_0 = N = \frac{1}{e^{\beta(E_0 - \mu)} - 1}, \quad \beta \rightarrow \infty. \quad (2.3)$$

Let us define a quantity

$$\zeta = e^{-\beta(E_0 - \mu)}, \quad (2.4)$$

so that $\zeta \rightarrow (1 + 1/N)^{-1}$ as $\beta \rightarrow \infty$ and is (in this limit clearly) independent of the distribution of impurities. The chemical potential, on the other hand, approaches E_0 , which (through L_1) does depend on the impurity distribution. For finite temperatures

$$\bar{n}_0 = \frac{1}{\zeta^{-1} - 1}, \quad (2.5)$$

since $0 \leq \bar{n}_0 \leq N$ and $0 \leq \zeta \leq N/(N+1) < 1$.

In terms of ζ , the expression for N becomes

$$N \equiv N(\zeta) = \sum_{j,s} \frac{1}{\zeta^{-1} e^{\beta(E_{j,s} - E_0)} - 1}. \quad (2.6)$$

By direct differentiation we see that $\partial N(\zeta)/\partial \zeta$ is non-negative, so that $N(\zeta)$ is a monotonically increasing function of ζ varying from 0 ($\zeta = 0$) to ∞ ($\zeta = 1$). Therefore, for any given N , there is a unique ζ solving (2.6).

Now we assert that $N(\zeta)$ in (2.6), for given ζ , is a "self-averaging" function. That is, we shall show that for the right-hand side of (2.6) the fluctuation is negligible compared to its mean, the average being over the ensemble of different possible arrangements of the impurities.

We saw in (I) that the ensemble average of a quantity $A(L_1, L_2, \dots)$ may be calculated from

$$\begin{aligned} \langle A \rangle &= \int_0^\infty A(L_1, L_2, \dots, L_\nu) \bar{P}(L_1, L_2, \dots, L_\nu) dL_1 dL_2 \dots dL_\nu, \\ \bar{P} &= \nu! p^\nu e^{-\rho(L_1 + L_2 + \dots + L_\nu)} \Theta(L_1 - L_2) \Theta(L_2 - L_3) \dots \Theta(L_{\nu-1} - L_\nu), \\ \Theta(x) &= 0, \quad x < 0; \quad \Theta(x) = 1, \quad x > 0; \quad \rho \equiv \nu/L. \end{aligned} \quad (2.7)$$

(For more on this distribution function, see the Appendix.)

Let us first compute $\langle N(\zeta) \rangle$:

$$\begin{aligned} \langle N(\zeta) \rangle &= \left\langle \sum_{s=1}^\infty \frac{1}{\zeta^{-1} e^{\beta(E_{1s} - E_0)} - 1} \right\rangle + \left\langle \sum_{j \neq 1} \sum_s \frac{1}{\zeta^{-1} e^{\beta(E_{j,s} - E_0)} - 1} \right\rangle \\ &= S_1 + S_2, \end{aligned} \quad (2.8)$$

$$S_1 = \frac{1}{\zeta^{-1} - 1} + \sum_{s=2}^\infty \left\langle \frac{1}{\zeta^{-1} e^{\beta(E_{1s} - E_0)} - 1} \right\rangle \equiv \frac{1}{\zeta^{-1} - 1} + S'_1, \quad (2.9)$$

$$\begin{aligned} S'_1 &= \sum_{s=2}^\infty \left\langle \frac{1}{\zeta^{-1} e^{\beta(E_{s1} - E_0)} - 1} \right\rangle \leq \sum_{s=2}^\infty \left\langle \frac{1}{e^{\beta(E_{1s} - E_0)} - 1} \right\rangle \\ &\leq \frac{1}{\beta} \sum_{s=2}^\infty \left\langle \frac{1}{E_{1s} - E_0} \right\rangle, \end{aligned}$$

using the inequality $e^x - 1 \geq x$. Thus

$$S'_1 \leq \frac{1}{c^2 \beta} \left\langle \sum_{s=2}^\infty \frac{1}{s^2 - 1} \right\rangle \langle L_1^2 \rangle. \quad (2.10)$$

It is easy to see (Appendix) that

$$\langle f(L_1) \rangle = \int_0^\infty f(L_1) \nu \rho e^{-\rho L_1} (1 - e^{-\rho L_1})^{\nu-1} dL_1, \quad (2.11)$$

$$\langle L_1^2 \rangle = \nu \rho \int_0^\infty L_1^2 e^{-\rho L_1} (1 - e^{-\rho L_1})^{\nu-1} dL_1. \quad (2.12)$$

This integral is easily evaluated in terms of the Euler Γ function and its derivatives. For $\nu \gg 1$, the leading term is

$$\langle L_1^2 \rangle = (\ln \nu)^2 / \rho^2. \quad (2.13)$$

Since we are only interested in terms of order N (or ν) in (2.8), it follows (since $\sum_{s=2}^\infty 1/s^2 - 1$ is a finite pure number) that S'_1 is negligible, and that

$$S_1 = 1/(\zeta^{-1} - 1). \quad (2.14)$$

For S_2 we proceed as follows:

$$S_2 = \sum_{s=1}^\infty \left\langle \sum_{j=2}^\nu \frac{1}{\zeta^{-1} \exp[c^2 \beta (s^2/L_j^2 - 1/L_1^2)] - 1} \right\rangle. \quad (2.15)$$

This is the average of a quantity of the form

$$\sum_{j=2}^\nu F(L_1, L_j).$$

From the Appendix we have

$$S_2 = \sum_{s=1}^\infty \int_0^\infty dL_1 \int_0^{L_1} dL_2 \nu(\nu-1) \rho^2 e^{-\rho L_1} (1 - e^{-\rho L_1})^{\nu-2} e^{-\rho L_2} \frac{1}{\zeta^{-1} \exp[c^2 \beta (s^2/L_2^2 - 1/L_1^2)] - 1}, \quad (2.16)$$

or

$$\frac{S_2}{\nu} = \sum_{s=1}^\infty \int_0^\infty dL_2 \int_{L_2}^\infty dL_1 \rho e^{-\rho L_2} P_{\nu-1}(L_1) \frac{1}{\zeta^{-1} \exp[c^2 \beta (s^2/L_2^2 - 1/L_1^2)] - 1},$$

where

$$P_{\nu-1}(L_1) = \rho(\nu-1)(1 - e^{-\rho L_1})^{\nu-2} e^{-\rho L_1}. \quad (2.17)$$

Now $P_{\nu-1}(L_1)$ is a normalized (to unity) probability distribution, and has its most probable value at $L_1 = \ln(\nu-1)/\rho$. If we write $L_1 = \ln(\nu-1)/\rho + L'$, then (2.17) becomes

$$P_{\nu-1}(L_1) = \rho[(1 - e^{-\rho L'})^{\nu-2} e^{-\rho L'}]. \quad (2.18)$$

This expression has for large ν the limit

$$\lim_{\nu \rightarrow \infty} P_{\nu-1}(L_1) = \rho e^{-\rho L'} \exp(-e^{-\rho L'}). \quad (2.19)$$

That is, for large ν , L_1 may be replaced by $\ln \nu / \rho$ in the quantity we are averaging in (2.16), which is the same as replacing it by infinity. Therefore, for large ν , the leading term of S_2 is

$$S_2 = \nu \sum_{s=1}^{\infty} \int_0^{\infty} dL_2 \rho e^{-\rho L_2} \frac{1}{\xi^{-1} \exp(c^2 \beta s^2 / L_2^2) - 1}$$

$$= \frac{\nu \rho c}{2} \sum_{s=1}^{\infty} s \int_0^{\infty} dE \frac{e^{-\rho c s / E^{1/2}}}{E^{3/2}} \frac{1}{\xi^{-1} e^{\beta E} - 1}$$

$$= \int_0^{\infty} dE g(E) \frac{1}{\xi^{-1} e^{\beta E} - 1}, \quad (2.20)$$

$$g(E) \equiv \frac{\nu \rho c}{2 E^{3/2}} e^{-\rho c / E^{1/2}} (1 - e^{-\rho c / E^{1/2}})^{-2}. \quad (2.21)$$

$g(E)$ is just the ensemble-averaged density of states for this model, as already discussed in I. [A more complete derivation of (2.20) may be found in Ref. 2.] Finally, therefore,

$$\langle N(\xi) \rangle = \frac{1}{\xi^{-1} - 1} + \int_0^{\infty} dE g(E) \frac{1}{\xi^{-1} e^{\beta E} - 1}. \quad (2.22)$$

Now let us calculate the fluctuation of $N(\xi)$ from its mean. Write

$$N(\xi) = f(L_1) + \sum_{j=2}^{\nu} F(L_1, L_j), \quad (2.23)$$

$$N^2(\xi) = f^2(L_1) + 2f(L_1) \sum_{j=2}^{\nu} F(L_1, L_j) + \sum_{j,i=2}^{\nu} F(L_1, L_j) F(L_1, L_i)$$

$$= f^2(L_1) + 2f(L_1) \sum_{j=2}^{\nu} F(L_1, L_j) + \sum_{j=2}^{\nu} F^2(L_1, L_j) + \sum_{j,i=2; (j \neq i)}^{\nu} F(L_1, L_j) F(L_1, L_i).$$

Using the results of the Appendix once more, we have

$$\langle N^2(\xi) \rangle = \int_0^{\infty} f^2(L_1) P_{\nu}(L_1) dL_1 + \int_0^{\infty} dL_2 \rho \nu e^{-\rho L_2} \int_{L_2}^{\infty} dL_1 P_{\nu-1}(L_1) [2f(L_1) F(L_1, L_2) + F^2(L_1, L_2)] + \int_0^{\infty} dL_2 \rho \nu e^{-\rho L_2}$$

$$\times \int_0^{\infty} dL_3 \rho (\nu-1) e^{-\rho L_3} \int_{\max(L_3, L_1)}^{\infty} dL_1 P_{\nu-2}(L_1) F(L_1, L_2) F(L_1, L_3). \quad (2.24)$$

We wish to show that $\langle N^2(\xi) \rangle - \langle N(\xi) \rangle^2$ is of order less than ν^2 , which means that the fluctuation is a smaller order of magnitude than the mean. Let us write

$$f(L_1) = \frac{1}{\xi^{-1} - 1} + \tilde{f}(L_1), \quad (2.25)$$

$$\tilde{f}(L_1) = \sum_{s=2}^{\infty} \frac{1}{\xi^{-1} e^{\beta(L_1 s - E_0)} - 1}.$$

We saw that

$$\tilde{f}(L_1) \leq \frac{1}{\beta c^2} \left(\sum_{s=2}^{\infty} \frac{1}{s^2 - 1} \right) L_1^2.$$

Since L_1 is of order $\ln(\nu/\rho)$ [by the same analysis as in the discussion of (2.16) with $\nu-1$ replaced by ν], it is quite easy to see that $\tilde{f}(L_1)$ cannot contribute to order ν^2 in (2.24). Dropping \tilde{f} and using (2.19) for the other terms of (2.24), we get for the terms of order ν^2

$$\langle N^2(\xi) \rangle \cong \left(\frac{1}{\xi^{-1} - 1} \right)^2 + 2 \frac{1}{\xi^{-1} - 1} \int_0^{\infty} dL_j \rho \nu e^{-\rho L_j} F(\infty, L_j)$$

$$+ \int_0^{\infty} dL_j \rho \nu e^{-\rho L_j} \int_0^{\infty} dL_2 \rho \nu e^{-\rho L_2}$$

$$\times F(\infty, L_j) F(\infty, L_2)$$

$$= \left(\frac{1}{\xi^{-1} - 1} + \int_0^{\infty} dL_j \rho \nu e^{-\rho L_j} F(\infty, L_j) \right)^2$$

$$= \langle N(\xi) \rangle^2. \quad (2.26)$$

Therefore $\langle N^2(\xi) \rangle - \langle N(\xi) \rangle^2$ is of smaller order than ν^2 . [A more complete discussion of these terms is found in Ref. 2, where it is shown that $\langle N^2(\xi) \rangle - \langle N(\xi) \rangle^2$ is actually of order $\nu^2 / \ln^2 \nu$.] Thus we have shown that, with negligible fluctuation,

$$N = N(\xi) = \frac{1}{\xi^{-1} - 1} + \int_0^{\infty} dE g(E) \frac{1}{\xi^{-1} e^{\beta E} - 1}. \quad (2.27)$$

This equation always has a unique solution for ξ , no matter what N , β , L , and ν are. However, the integral is bounded, at large E because of $e^{\beta E}$, and low E because of the exponential factor $e^{-\rho c / E^{1/2}}$. Hence, as N is increased, a point will be reached

when

$$N - \int_0^{\infty} \frac{g(E)dE}{e^{\beta E} - 1}$$

is greater than zero, and of order N . (The integral is greatest when $\zeta=1$.) This means that the term $1/\zeta^{-1} - 1$ must be of order N . But $\bar{n}_0 = 1/\zeta^{-1} - 1$ is the mean number of bosons in the lowest-energy state; therefore Bose-Einstein condensation into the lowest-energy state occurs. This state is *localized* in the following sense: The wave function is confined to a region of length L_1 . L_1 , however, differs negligibly from $\ln\nu/\rho$. Therefore, although this goes to ∞ as $\nu \rightarrow \infty$, the ratio L_1L (fraction of the line occupied) is $\ln\nu/\nu$, which approaches zero as $\nu \rightarrow \infty$. We see from this discussion that the condensation is actually quite unphysical, and will disappear if there is the smallest (size-independent) repulsive interaction between the bosons. The density of bosons in the ground state will be $\bar{n}_0/L_1 = (\bar{n}_0/L)(L/L_1)$. Below the transition temperature \bar{n}_0/L is of order unity, whereas $L/L_1 = \nu/\ln\nu$ approaches infinity. Clearly if there is the slightest repulsion between the bosons this (essentially infinite) density will be energetically unfavorable and the bosons will "leak out" into the smaller cells.

The condensation occurs when

$$N = \int_0^{\infty} \frac{g(E)dE}{e^{\beta_c E} - 1}, \quad \beta_c = \frac{1}{kT_c}. \quad (2.28)$$

T_c is the critical temperature.

III. THERMODYNAMIC PROPERTIES OF SYSTEM

In this section we consider some of the thermodynamic properties of the phase transition. We will calculate the critical temperature, the specific heat, and the pressure of the system.

A. Critical Temperature

The critical temperature $T_c = 1/k\beta_c$ is given by

$$N = \int_0^{\infty} \frac{g(E)dE}{e^{\beta_c E} - 1} = \frac{L\rho^2 \hbar \pi}{2(2m)^{1/2}} \int_0^{\infty} \frac{dE 1/(E)^{3/2} e^{-\rho \hbar \pi / (2mE)^{1/2}}}{(e^{\beta_c E} - 1)(1 - e^{-\rho \hbar \pi / (2mE)^{1/2}})^2}. \quad (3.1)$$

Put

$$\gamma \equiv \frac{\rho^2 \hbar^2 \pi^2}{2m}, \quad E = xy, \quad (3.2)$$

$$N = \frac{L\rho}{2} \int_0^{\infty} \frac{e^{-1/x^{1/2}} (1 - e^{-1/x^{1/2}})^2 1/x^{3/2}}{(e^{\beta_c \gamma x} - 1)} dx.$$

Equation (3.2) cannot be solved exactly for β_c (or T_c) in terms of ρ . However, the following conclusions can be drawn:

(i) $d\beta_c/d\rho < 0$, or T_c , increases monotonically with ρ . The proof is straightforward differentiation.

(ii) When $\rho \ll 1$,

$$\frac{2N}{\rho L} = \frac{1}{\beta_c \gamma} \int_0^{\infty} \frac{e^{-1/x^{1/2}}}{x^{5/2} (1 - e^{-1/x^{1/2}})^2} dx \equiv \frac{1}{\beta_c \gamma} I_1, \quad (3.3)$$

or

$$T_c = \rho \frac{N \hbar^2 \pi^2}{L k m I_1}. \quad (3.4)$$

It can be shown that what we have neglected in (3.2) is small for small ρ .

(iii) $\rho \gg 1$. We write (3.2) as

$$\frac{2N}{L\rho} = \sum_s \sum_t \int_0^{\infty} \frac{s}{x^{3/2}} e^{-s/x^{1/2}} e^{-\beta_c \gamma x t} dx. \quad (3.5)$$

Put

$$x = \frac{y^2}{(\beta_c \gamma)^{2/3}} = \sum_s \sum_t \int_0^{\infty} \frac{dy}{y^2} \exp[-(\beta_c \gamma)^{1/3} (s/y + ty^2)] dy.$$

For large ρ , $(\beta_c \gamma)^{1/3}$ is a large number, as we will later see. Hence we use the saddle-point method. Also, we need only retain the term $s=t=1$. Therefore,

$$\begin{aligned} \frac{2N}{L\rho} &= \int_0^{\infty} \frac{dy}{y^2} \exp[-(\beta_c \gamma)^{1/3} (1/y + y^2)] dy \\ &\approx 2 \times 2^{2/3} (\frac{1}{3}\pi)^{1/3} (\beta_c \gamma)^{1/6} \exp[-(3/2^{2/3})(\beta_c \gamma)^{1/3}], \end{aligned} \quad (3.6)$$

or

$$T_c = \frac{1}{k} \frac{\rho^2 \hbar^2 \pi^2}{2m} \frac{3^3}{2^2} \frac{1}{[\ln(L2^{2/3}/N)^{1/3} \pi]^3}; \quad (3.7)$$

i. e.,

$$T_c \propto \rho^2 / (\ln\rho)^3.$$

Notice that $(\beta_c \gamma) \propto (\ln\rho)^3$ is indeed large. The dependence of T_c on ρ is shown graphically in Fig. 1.

B. Specific Heat

The internal energy of the system is given by

$$U = \sum_{js} \frac{E_{js}}{\zeta^{-1} e^{\beta(E_{js} - E_{11})} - 1}$$

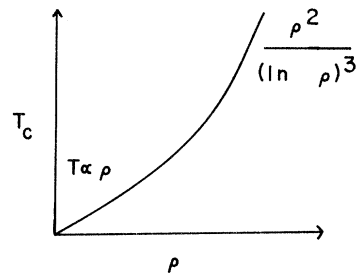
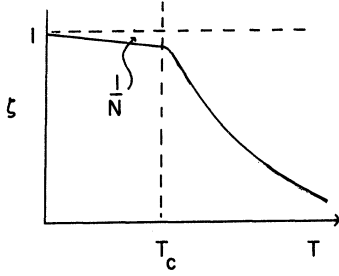


FIG. 1. Variation of critical temperature with density of impurities ρ .

FIG. 2. Variation of ζ with respect to temperature.

$$= \frac{E_0}{\zeta^{-1} - 1} + \sum' \frac{E_{js}}{\zeta^{-1} e^{\beta(E_{js} - E_0)} - 1}. \quad (3.8)$$

Taking the ensemble average, we can neglect the first term, being of order $1/(\ln\nu)^2$. The second term can be treated as in Sec. II, to give

$$\langle U \rangle = \int_0^\infty \frac{Eg(E)dE}{(\zeta^{-1} e^{\beta E} - 1)}. \quad (3.9)$$

Again, the standard deviation is negligible.

We discuss the specific heat at constant length (or one-dimensional volume) below and just above the critical temperature.

(a) $T < T_c$, or $\beta > \beta_c$:

$$N = \frac{1}{\zeta^{-1} - 1} + \int_0^\infty \frac{g(E)dE}{e^{\beta E} - 1}.$$

ζ is obtained by solving this equation. It is very close to 1 ($\zeta^{-1} - 1 \approx 1/N$) (see Fig. 2). Therefore,

$$U = \int_0^\infty \frac{Eg(E)dE}{e^{\beta E} - 1}, \quad (3.10)$$

$$c_L = \left(\frac{dU}{dT} \right)_L = \frac{1}{kT^2} \int_0^\infty \frac{e^{\beta E} E^2 g(E) dE}{(e^{\beta E} - 1)^2},$$

$$\frac{dc_L}{dT} = \frac{1}{k^2 T^4} \int_0^\infty \frac{E^2 g(E) e^{\beta E} dE}{(e^{\beta E} - 1)^3 \beta} [E\beta(e^{\beta E} + 1) - 2e^{\beta E} + 2]. \quad (3.11)$$

The term in the brackets is always non-negative. Therefore, $dc_L/dT > 0$, or c , increases monotonically with T below the transition temperature.

Near $T=0$, U can be evaluated by the saddle-point method:

$$\begin{aligned} U &= \int_0^\infty \frac{\nu c \rho}{2E^{3/2}} e^{-(\beta E + \rho c/E^{1/2})} dE \\ &= \nu c \rho \frac{(2\hbar)^{1/2} 2^{3/2} (\rho c)^{-3/2} \beta^{1/6}}{6^{1/2}} \exp[-(\rho c)^{2/3} \beta^{1/3} \frac{2}{3}] \end{aligned}$$

$$c_L = \frac{1}{kT^2} \left(\int_0^\infty \frac{\zeta^{-1} E^2 e^{\beta E} g(E) dE}{(\zeta^{-1} e^{\beta E} - 1)^2} - \int_0^\infty \frac{Eg(E) dE}{(\zeta^{-1} e^{\beta E} - 1)^2} \zeta^{-2} e^{\beta E} + \int_0^\infty \frac{\zeta^{-1} Eg(E) dE e^{\beta E}}{(\zeta^{-1} e^{\beta E} - 1)^2} / \int_0^\infty \frac{\zeta^{-2} e^{\beta E} g(E) dE}{(\zeta^{-1} e^{\beta E} - 1)^2} \right). \quad (3.17)$$

$$= \frac{\nu A}{T^{1/6}} e^{-\beta/T^{1/3}}. \quad (3.12)$$

Therefore

$$c_L \sim \frac{\nu e^{-\beta/T^{1/3}}}{T^{3/2}}. \quad (3.13)$$

The value of c_L just below the transition temperature is

$$c_L^- = \frac{1}{k\beta T_c^2} \int_0^\infty \frac{E^2 g(E) dE e^{\beta c E}}{(e^{\beta c E} - 1)^2}. \quad (3.14)$$

It is also easy to show that all the derivatives of U exist below the transition temperature:

$$\begin{aligned} \frac{d^n U}{d\beta^n} &= \int_0^\infty Eg(E) dE \frac{d^n}{d\beta^n} \left(\frac{1}{e^{\beta E} - 1} \right) \\ &= \sum \int_0^\infty Eg(E) dE \frac{n! m!}{i! j! h! \dots k!} \frac{(-1)^m}{(e^{\beta E} - 1)^{n+1}} \\ &\quad \times \frac{e^{m\beta E}}{(1!)^i (2!)^j \dots (e!)^k}, \quad (3.15) \end{aligned}$$

where the sum is over all solutions in positive integers of the equations

$$i + j + h + \dots + k = m,$$

$$i + 2j + 3h + \dots + lk = n.$$

Each term in (3.15) is well defined. At low E , $e^{-\beta E/E^{1/2}}$ from $g(E)$ makes contributions small. At large E , $e^{\beta E}$ from the denominator cuts off exponentially. Hence, for $T < T_c$, all the derivatives of U with respect to T exist. In particular, all the derivatives of c_L exist as we approach from below the critical point. No critical exponent exists.

(b) $T > T_c$, $\beta < \beta_c$:

$$U = \int_0^\infty \frac{Eg(E)dE}{(\zeta^{-1} e^{\beta E} - 1)}.$$

ζ is now a function of β and

$$c_L = \frac{1}{kT^2} \int_0^\infty \frac{Eg(E)dE}{(\zeta^{-1} e^{\beta E} - 1)^2} \left(\zeta^{-1} e^{\beta E} E - \zeta^{-2} e^{\beta E} \frac{d\zeta}{d\beta} \right). \quad (3.16)$$

$d\zeta/d\beta$ can be determined from

$$\begin{aligned} N &= \int_0^\infty \frac{g(E) dE}{\zeta^{-1} e^{\beta E} - 1}, \\ 0 &= \int_0^\infty \frac{g(E) dE}{(\zeta^{-1} e^{\beta E} - 1)^2} \left(\zeta^{-1} e^{\beta E} - \zeta^{-2} e^{\beta E} \frac{d\zeta}{d\beta} \right). \end{aligned}$$

Therefore,

As $T \rightarrow T_c^+$, $\xi \rightarrow 1$. Therefore

$$c_L \rightarrow c_L^+ = \frac{1}{kT_c^2} \left[\int_0^\infty \frac{E^2 e^{\beta c E} g(E) dE}{(e^{\beta c E} - 1)^2} - \left(\int_0^\infty \frac{E e^{\beta c E} g(E) dE}{(e^{\beta c E} - 1)^2} \right)^2 / \int_0^\infty \frac{g(E) e^{\beta c E} dE}{(e^{\beta c E} - 1)^2} \right]. \quad (3.18)$$

The first term in (3.18) is just c_L^- . Therefore, there is a discontinuity at T_c , of value

$$\Delta c_L = c_L^+ - c_L^- = - \left(\int_0^\infty \frac{E g(E) e^{\beta c E} dE}{(e^{\beta c E} - 1)^2} \right)^2 / kT_c^2 \left(\int_0^\infty \frac{g(E) e^{\beta c E} dE}{(e^{\beta c E} - 1)^2} \right). \quad (3.19)$$

Notice that the discontinuity is always negative.

Again, we can take higher derivatives c_L at T_c^+ . They are all well defined, because the integral is always limited by the factor $e^{-\rho c/E^{1/2}}$. Hence no critical exponents exist for the specific heat just above T_c .

The variation of c_L as a function of T is seen in Fig. 3.

C. Pressure

We now study the isotherms of the system. The "pressure" that we use is the formal pressure of just the bosons. That is, we imagine squeezing down on the system with a "piston" that is permeable to the impurities, but not the bosons. This keeps the density of impurities (ρ) fixed, but increases the density of bosons. If Ω is the thermodynamic potential of the grand partition function,

$$\Omega = + \frac{1}{\beta} \sum_{j_s} \ln(1 - e^{-\beta(E_{j_s} - \mu)}), \quad (3.20)$$

$$P \equiv - \left(\frac{\partial \Omega}{\partial L} \right)_{\mu, T, \rho}. \quad (3.21)$$

Now, just as in Sec. II, it is not difficult to see that Ω is given by its ensemble average with negligible fluctuation,

$$\Omega = \frac{1}{\beta} \int_0^\infty \ln(1 - \xi e^{-\beta E}) g(E) dE, \quad (3.22)$$

and [using (2.21)]

$$P = - \left(\frac{\partial \Omega}{\partial L} \right)_{\xi, T, \rho}$$

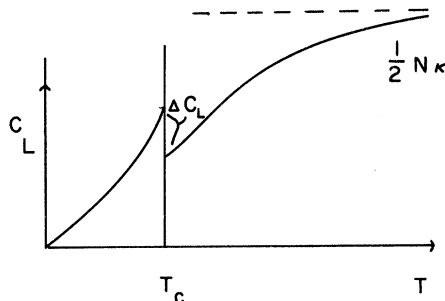


FIG. 3. Specific heat at constant length.

$$= \frac{1}{\beta} \int_0^\infty [-\ln(1 - \xi e^{-\beta E})] \frac{\rho^2 c}{2E^{3/2}} \frac{e^{-\rho c/E^{1/2}}}{(1 - e^{-\rho c/E^{1/2}})^2} dE. \quad (3.23)$$

For a given temperature and ρ , define a critical length L_c by

$$N = L_c \int_0^\infty \frac{1}{e^{\beta E} - 1} \frac{\rho^2 c}{2E^{3/2}} \frac{e^{-\rho c/E^{1/2}}}{(1 - e^{-\rho c/E^{1/2}})^2} dE. \quad (3.24)$$

For $L > L_c$ we have a normal boson gas; for $L < L_c$ we are in the region of Bose-Einstein condensation. For $L < L_c$, $\xi = 1$, and it is clear that P is independent of L and given by

$$P = \frac{1}{\beta} \int_0^\infty -\ln(1 - e^{-\beta E}) \frac{\rho^2 c}{2E^{3/2}} \frac{e^{-\rho c/E^{1/2}}}{(1 - e^{-\rho c/E^{1/2}})^2} dE, \quad (3.25)$$

$L < L_c.$

For $L > L_c$, we easily see that ξ is a monotonically decreasing function of L (ρ , β fixed), so ρ is a monotonically decreasing function of L . Using, for $L > L_c$,

$$N = \int_0^\infty \frac{1}{\xi^{-1} e^{\beta E} - 1} g(E) dE$$

$$= L \int_0^\infty \frac{1}{\xi^{-1} e^{\beta E} - 1} \frac{\rho^2 c}{2E^{3/2}} \frac{e^{-\rho c/E^{1/2}}}{(1 - e^{-\rho c/E^{1/2}})^2} dE, \quad (3.26)$$

we can find $(\partial \xi / \partial L)_{\beta, \rho}$ and therefore $(\partial P / \partial L)_{\beta, \rho}$. Using this we obtain the result that

$$\left(\frac{\partial P}{\partial L} \right)_{\beta, \rho} \Big|_{L=L_c^+}$$

is negative (nonvanishing). Therefore the variation of this pressure with L has the form given in Fig. 4.

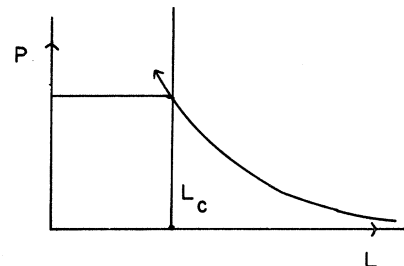


FIG. 4. Pressure at constant temperature.

IV. CONNECTION WITH BOGOLIUBOV INEQUALITY

Hohenberg⁴ has shown, using an inequality due to Bogoliubov,³ that in a one-dimensional system there can be no Bose-Einstein condensation into the zero-momentum state. We now discuss this inequality and show that it may be put into a form that yields the Hohenberg result but gives no contradiction when applied to our problem.

The Bogoliubov inequality reads

$$\frac{1}{2} \langle [C, \tilde{H}], C^\dagger \rangle \langle \{A, A^\dagger\} \rangle \geq kT \langle [C, A] \rangle^2, \quad (4.1)$$

where $[,]$ means the commutator, $\{, \}$ the anti-commutator, \langle, \rangle the thermodynamic average with the grand canonical distribution function, and

$$\tilde{H} = H - \mu N, \quad (4.2)$$

H being the Hamiltonian of the system and μ the chemical potential.

For the Hamiltonian we have

$$H = \sum_i \frac{P_i^2}{2m} + \sum_i V(x_i) + H'. \quad (4.3)$$

$V(x)$ is the potential energy of interaction with the impurities; H' is a symmetry-breaking term added as usual⁵ for convenience. In second-quantized notation,

$$H' = -\alpha(a_0 + a_0^\dagger), \quad (4.4)$$

where a_0^\dagger is the creation operator for the ground state of $P^2/2m + V(x)$. Call this ground-state energy E_0 and wave function ϕ_0 . Now choose

$$C = \sum_j e^{i\kappa x_j},$$

$$A = a_q, \quad (4.5)$$

where a_q is the destruction operator for a plane wave normalized to unity in L of propagation vector q . Straightforward calculation then gives

$$\langle \{A, A^\dagger\} \rangle = \bar{n}_q + \frac{1}{2}, \quad (4.6)$$

$$[[C, \tilde{H}], C] = N\hbar^2 \kappa^2 / m + 2\alpha \bar{n}_0^{1/2}, \quad (4.7)$$

$$\langle [C, A] \rangle = \bar{n}_0^{1/2} \int_0^L \frac{e^{-iqx}}{L^{1/2}} e^{i\kappa x} \phi_0(x) dx. \quad (4.8)$$

We have made use of the fact that, in the presence of the symmetry-breaking term,

$$\langle a_0 \rangle = \langle a_0^\dagger \rangle = \bar{n}_0^{1/2} \quad (4.9)$$

and \bar{n}_0 is the mean occupation number of the ground state.

Using these results, (4.1) becomes

$$\begin{aligned} & (\bar{n}_q + \frac{1}{2}) [(N\hbar^2/m)q^2 + 2\alpha \bar{n}_0^{1/2}] \\ & \geq kT \bar{n}_0 \frac{1}{L} \left| \int_0^L e^{i(\kappa-q)x} \phi_0(x) dx \right|^2. \end{aligned} \quad (4.10)$$

We consider two cases.

(i) No impurities, $V=0$. Further, take $\kappa=q$ in (4.10). Then $\phi_0 = 1/L^{1/2}$ and

$$\bar{n}_q \geq -\frac{1}{2} + \frac{kT \bar{n}_0}{N\hbar^2/m + 2\alpha \bar{n}_0^{1/2}}. \quad (4.11)$$

The total mean number of particles with propagation vector less in magnitude than q_0 is

$$\begin{aligned} \sum_{|q| < q_0} \bar{n}_q & \leq \sum_{|q| \leq q_0} \left(-\frac{1}{2} + \frac{kT \bar{n}_0}{(N\hbar^2/m)q^2 + 2\alpha (\bar{n}_0)^{1/2}} \right) \\ & = \frac{L}{2\pi} \int_{-q_0}^{q_0} \left(\frac{kT \bar{n}_0}{(N\hbar^2/m)q^2 + 2\alpha (\bar{n}_0)^{1/2}} \right) dq = -\frac{L}{2\pi} q_0 + \frac{kT \bar{n}_0 L}{2\pi} \int_{-q_0}^{q_0} \frac{dq}{(N\hbar^2/m)q^2 + 2\alpha (\bar{n}_0)^{1/2}} \\ & = -\frac{L}{2\pi} q_0 + \frac{kTm}{\pi \hbar^2} \frac{n_0 L}{N} \frac{1}{\delta} \tan^{-1} \left(\frac{q_0}{\delta} \right), \end{aligned} \quad (4.12)$$

where

$$\delta \equiv \left(\frac{2\alpha (\bar{n}_0)^{1/2} m}{N\hbar^2} \right)^{1/2}.$$

We choose, as is customary,⁵ $\alpha = aN^{1/2}$, a independent of N , and ultimately take the limit $a=0$. Then

$$\delta = \left[\frac{2m}{\hbar^2} \left(\frac{\bar{n}_0}{N} \right)^{1/2} a \right]^{1/2}. \quad (4.13)$$

The assumption that \bar{n}_0 is of the order of N is the same as δ independent of N but approaching zero as closely as we please. For fixed q_0 , q_0/δ approach-

es infinity and

$$\sum_{|q| < q_0} \bar{n}_q \leq -\frac{L}{2\pi} q_0 + \frac{kTm}{2\hbar^2} \frac{\bar{n}_0}{N} \frac{1}{\delta} L. \quad (4.14)$$

Since the left-hand side of (4.14) cannot exceed $N = L(N/L)$, it is clear that by choosing a small enough we have a contradiction. This is the usual Hohenberg result.

(ii) Now with impurities

$$\phi_0 = \left(\frac{2}{L_1} \right)^{1/2} \sin \left(\frac{\pi}{L_1} x \right) \quad (x \text{ inside largest cell})$$

= 0 (otherwise).

Choose $\kappa = q$ again. Then (4.10) becomes

$$(n_q + \frac{1}{2})[(N\bar{n}^2/m)q^2 + 2\alpha(\bar{n}_0)^{1/2}] \geq kT\bar{n}_0 \frac{1}{L} \left[\frac{8}{\pi^2} L_1 \cos^2 \left(\frac{\pi}{L_1} x_0 \right) \right], \quad (4.15)$$

where x_0 is the starting point of the largest cell. Since $\cos^2(\pi x_0/L_1) \leq 1$, the right-hand side of (4.15) is reduced from the corresponding result in (4.11) by a factor of order of magnitude L_1/L . However, L differs negligibly from $\ln(\nu/\rho)$ = $[\ln(\nu/\rho)]L_1$, and therefore this factor is of order $\ln(\nu/\rho)$. If we now carry out the same operations as we did for the free-particle case, there is no contradiction since the corresponding term inversely proportional to δ in (4.14) is only of order of magnitude of $\ln \nu$ instead of ν , and is negligible in the thermodynamic limit. Therefore, the existence of the Bose-Einstein transition is not in contradiction to the Bogoliubov inequality for our case.

APPENDIX

The probability distribution function for the cell lengths to be L^1, L^2, \dots, L^ν is

$$P(L^1, L^2, \dots, L^\nu) = (\nu-1)!/L^{\nu-1} \delta(L^1 + L^2 + \dots + L^\nu) \quad (A1)$$

for a random system. For large ν , this can be replaced by

$$P(L^1, L^2, \dots, L^\nu) = \rho^\nu \exp[-\rho(L^1 + L^2 + \dots + L^\nu)] \quad (A2)$$

(see Paper I). The normalized probability distribution function for the largest cell to have length L_1 , the second largest cell to have length L_2 , etc., is

$$\bar{P}(L_1, L_2, \dots, L_\nu) = \rho^\nu \exp[-\rho(L_1 + L_2 + \dots + L_\nu)] \nu! \times \Theta(L_1 - L_2) \Theta(L_2 - L_3) \dots \Theta(L_{\nu-1} - L_\nu). \quad (A3)$$

We will derive a few other distribution functions from (A3).

(a) $P_\nu(L_1)$, which is the probability distribution function for the largest cell to have length L_1 , is

$$P_\nu(L_1) = \int \dots \int \bar{P}(L_1, L_2, \dots, L_\nu) dL_2 \dots dL_\nu = \nu \int_0^{L_1} dL_2 \int_0^{L_1} dL_3 \dots \int_0^{L_1} dL_\nu \rho^\nu$$

$$\begin{aligned} \left\langle \sum_{j=2}^{\nu} f(L_1, L_j) \right\rangle &= \nu! \rho^\nu \int_0^\infty dL_1 \frac{e^{-\rho L_1}}{(\nu-1)!} \int_0^{L_1} dL_2 \int_0^{L_1} dL_3 \dots \int_0^{L_1} dL_\nu \exp[-\rho(L_2 + L_3 + \dots + L_\nu)] \sum_{j=2}^{\nu} f(L_1, L_j) \\ &= \nu \rho^\nu \int_0^\infty dL_1 e^{-\rho L_1} \int_0^{L_1} dL_2 e^{-\rho L_2} (\nu-1) f(L_1, L_2) \int_0^{L_1} dL_3 \dots \int_0^{L_1} dL_\nu \exp[-\rho(L_3 + L_4 + \dots + L_\nu)] \\ &= \nu(\nu-1) \rho^2 \int_0^\infty dL_1 e^{-\rho L_1} \int_0^{L_1} dL_2 e^{-\rho L_2} (1 - e^{-\rho x_1})^{\nu-2} f(L_1, L_2) \\ &= \int_0^\infty dL_2 \int_{L_2}^\infty dL_1 \nu \rho e^{-\rho L_2} P_{\nu-1}(L_1) f(L_1, L_2). \end{aligned} \quad (A7)$$

$\times \exp[-\rho(L_2 + L_3 + \dots + L_\nu)] e^{-\rho L_1}$

$$= \nu \rho e^{-\rho L_1} (1 - e^{-\rho L_1})^{\nu-1}. \quad (A4)$$

The average value of the largest cell length

$$\begin{aligned} \langle L_1 \rangle &= \int_0^\infty P_\nu(L_1) L_1 dL_1 \\ &= \nu \rho \int_0^\infty dL_1 L_1 e^{-\rho L_1} (1 - e^{-\rho L_1})^{\nu-1} \\ &= -L \left(\frac{\partial}{\partial t} B(\nu, t) \right)_{t=1}, \end{aligned}$$

where

$$\begin{aligned} B(\nu, t) &= \int_0^\infty dy e^{-ty} (1 - e^{-y})^{\nu-1} \\ &= \frac{\Gamma(\nu) \Gamma(t)}{\Gamma(\nu+t)}. \end{aligned}$$

is the β function. Therefore,

$$\langle L_1 \rangle = -\langle L/\nu \rangle \Gamma'(1) + (L/\nu) \psi(\gamma+1),$$

where

$$\begin{aligned} \psi(m) &= \frac{d}{dm} \ln \Gamma(m) = -\gamma + \sum_{k=1}^{m-1} k^{-1}, \\ \Gamma'(1) &= \psi(1) = -\gamma, \end{aligned}$$

where γ is the Euler number. Therefore

$$\begin{aligned} \langle L_1 \rangle &= \frac{L}{\nu} \sum_{k=1}^{\nu} k^{-1} = \frac{L}{\nu} \left(1 + \frac{1}{2} + \frac{1}{3} + \dots + \frac{1}{\nu} \right) \\ &= \left(\frac{L}{\nu} \right) \ln \nu \quad \text{for large } \nu. \end{aligned} \quad (A5)$$

(b) Consider next averages of the form

$$\begin{aligned} \left\langle \sum_{j=2}^{\nu} f(L_1, L_j) \right\rangle &= \nu! \rho^\nu \int_0^\infty dL_1 \int_0^{L_1} dL_2 \dots \int_0^{L_{\nu-1}} dL_\nu \\ &\times \exp[-\rho(L_1 + L_2 + \dots + L_\nu)] \sum_{j=2}^{\nu} f(L_1, L_j). \end{aligned} \quad (A6)$$

Since

$$\sum_{j=2}^{\nu} f(L_1, L_j)$$

is a symmetric function of L_2, L_3, \dots, L_ν , we may write this as

(c) Finally consider averages of the form

$$\left\langle \sum_{j,i=2,j \neq i} f(L_1, L_i, L_i) \right\rangle. \quad \left\langle \sum_{j,i=2,j \neq i}^{\nu} f(L_1, L_i, L_i) \right\rangle = \nu! \rho^{\nu} \int_0^{\infty} dL_1 \int_0^{L_1} dL_2 \cdots \int_0^{L_{\nu-1}} dL_{\nu} \times \exp[-(L_1 + L_2 + \cdots + L_{\nu})] \sum f(L_1, L_i, L_i) \quad (\text{A8})$$

Exactly the same method that worked in (b) works again here:

Since $\sum f(L_1, L_i, L_i)$ is a symmetric function of $L_2 \cdots L_{\nu}$, we have

$$\begin{aligned} \langle \sum f(L_1, L_i, L_i) \rangle &= \nu \rho^{\nu} \int_0^{\infty} dL_1 \int_0^{L_1} dL_2 \int_0^{L_2} dL_3 \cdots \int_0^{L_{\nu-1}} dL_{\nu} \exp[-\rho(L_1 + L_2 + \cdots + L_{\nu})] \sum f(L_1, L_i, L_i) \\ &= \nu(\nu-1)(\nu-2)\rho^3 \int_0^{\infty} dL_1 \int_0^{L_1} dL_2 \int_0^{L_2} dL_3 f(L_1, L_2, L_3) \int_0^{L_3} dL_4 \cdots dL_{\nu} \rho^{\nu-3} \\ &\quad \times \exp[-\rho(L_1 + L_2 + \cdots + L_{\nu})] \\ &= \nu(\nu-1)(\nu-2)\rho^3 \int_0^{\infty} dL_1 \int_0^{L_1} dL_2 \int_0^{L_2} dL_3 e^{-\rho(L_1+L_2+L_3)} (1 - e^{-\rho L_1})^{\nu-3} f(L_1, L_2, L_3) \\ &= \int_0^{\infty} dL_2 \int_0^{\infty} dL_3 \nu(\nu-1)\rho^2 e^{-\rho(L_2+L_3)} \int_{\max(L_2, L_3)}^{\infty} dL_1 P_{\nu-2}(L_1) f(L_1, L_2, L_3). \end{aligned} \quad (\text{A9})$$

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Theory of the Frank Elastic Constants of Nematic Liquid Crystals*

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It is shown that the Frank elastic constants may be expressed in terms of even-order Legendre polynomials averaged over the one-molecule orientational distribution function. In particular, it is found that $(K_{11} - \bar{K})/\bar{K} = C - 3C'\bar{P}_4/\bar{P}_2 + \cdots$, $(K_{22} - \bar{K})/\bar{K} = -2C - C'\bar{P}_4/\bar{P}_2 + \cdots$, $(K_{33} - \bar{K})/\bar{K} = C + 4C'\bar{P}_4/\bar{P}_2 + \cdots$, where $\bar{K} = (1/3)(K_{11} + K_{22} + K_{33})$, C and C' are constants, which depend on the details of the system, and \bar{P}_m is the weighted average of the m th Legendre polynomial. Higher-order terms in these series involve \bar{P}_6 , etc. The constants C and C' are calculated for the case of rodlike molecules interacting via a hard-core repulsion. The results are in good agreement with experiments on the substance *p*-azoxyanisole.

I. INTRODUCTION

The Frank elastic constants are a measure of the free energy associated with long-wavelength distortions of the nematic state in which the local preferred direction of molecular orientation varies in space. If the local preferred direction at the point \vec{r} is parallel to the unit vector $\hat{n}(\vec{r})$, the free energy associated with the distortion may be written¹

$$\Delta F = \frac{1}{2} \int d^3 r [K_{11}(\nabla \cdot \hat{n})^2 + K_{22}(\hat{n} \cdot \nabla \times \hat{n})^2 + K_{33}(\hat{n} \times \nabla \times \hat{n})^2]. \quad (1)$$

The vector \hat{n} is usually called the director. The distortions corresponding to K_{11} , K_{22} , and K_{33}

are called splay, torsion, and bending, respectively. These three types of distortion are illustrated in Fig. 1.

In the mean-field approximation the free energy of the nematic state can be written as a sum of three terms²:

$$F = E - TS_t - TS_r. \quad (2)$$

Here E is the internal energy, T is the temperature, S_r is the rotational entropy, and S_t is the translational entropy. The translational entropy includes all the entropy of the system not contained in S_r . For a uniaxial system S_r is given by²

$$S_r = -k_B N \int h(\Omega) \ln h(\Omega) d\Omega. \quad (3)$$