# Condensation of the Ideal Bose Gas as a Cooperative Transition

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The thermodynamic properties of the noninteracting Bose gas in the neighborhood of its transition are examined in detail. The order parameter is a complex extensive variable, but the thermodynamic properties depend only on its amplitude under simple boundary conditions. As the dimensionality or the single-particle energy spectrum is varied, the critical singularity displays a variety of forms. The equation of state has a simple structure, different from the homogeneous form often discussed for critical systems but asymptotically reducing to the latter except when logarithmic singularities are involved. The correlation function in the critical region is a homogeneous function of the distance and a correlation length. Only for a quadratic energy spectrum is the Ornstein-Zernike theory result valid at the critical temperature. A precise correspondence is noted between the asymptotic properties of the ideal Bose gas transition and those of the spherical model of ferromagnetism.

### I. INTRODUCTION

'HE ideal Bose gas is one of the few systems which possess a thermodynamic transition and whose properties can be calculated exactly. While in many ways unphysical, particularly in the low-temperature region, it has nevertheless proved a useful model system for studies of the superfluid state. In this paper we examine the neighborhood of the transition itself as a model of a cooperative transition. To do this, we introduce explicitly the dynamical variable which achieves a long-range order in the condensed state. The thermal average of this variable we call the Bose moment; its properties are in complete analogy with those of the magnetic moment for a system which undergoes a ferromagnetic transition. The Bose 6eld is the intensive variable thermodynamically conjugate to the Bose moment and a transition occurs only in zero field.

The thermodynamic properties can be determined exactly in any number, d, of dimensions. In particular, the asymptotic functional forms near the "critical point" are found for the coexistence curve, the "susceptibility," the critical isotherm, the specific heat, etc.; these are listed in Tables I and II. The exponent  $\beta$ characterizing the coexistence curve has, for all  $d$ , the "classical" value  $\beta = \frac{1}{2}$ . The properties on the lowtemperature side of the transition are rather uninteresting because of the unphysical nature of this region, but on the high-temperature side a rich variety of functional singularities is displayed for different values of  $d$ . The equation of state for the order parameter can be expressed as a function of one variable only. Its asymptotic form in the region of a transition point reduces to the homogeneous structure proposed by Widom except when logarithmic singularities are involved, that is, in four dimensions. Everywhere in the asymptotic region the correlation function is a homogeneous function depending only on the distance and a single correlation length, the latter being a function of state. This structure is simpler than the form proposed by Kadanoff. The distance dependence of the correlation function conforms to the Ornstein-Zernike theory.

In Sec. V we discuss the precise correspondence that exists between the asymptotic properties of the ideal Bose gas transition and those of the spherical model of the ferromagnetic transition. The relationship between the condensation of the ideal Bose gas and the  $\lambda$  transition in liquid helium is similar to that between the spherical model and a real ferromagnet.

In the concluding section the homogeneity properties of the Bose transition and the thermodynamic inequalities involving critical exponents are discussed. We do not discuss here flow properties or properties related to inhomogeneous fields.

### II. STATISTICAL MECHANICS OF THE IDEAL BOSE GAS

#### A. Discussion of the Bose Moment

Consider a system composed of a number  $N$  of noninteracting Bose particles of mass  $m$  enclosed in a stationary, simply connected volume V. We introduce the<br>set of pairs of dynamical variables<br> $\psi_k = V^{-1/2} a_k$ ,  $\psi_k^{\dagger} = V^{-1/2} a_k^{\dagger}$ set of pairs of dynamical variables

$$
\psi_{\mathbf{k}} = V^{-1/2} a_{\mathbf{k}}, \quad \psi_{\mathbf{k}}^{\dagger} = V^{-1/2} a_{\mathbf{k}}^{\dagger}
$$

which are linear combinations of the pairs of Hermitia operators

$$
V^{-1/2}(a_{\mathbf{k}}+a_{\mathbf{k}}^{\dagger}), \quad iV^{-1/2}(a_{\mathbf{k}}^{\dagger}-a_{\mathbf{k}}).
$$

The operators  $a_k^{\dagger}$ ,  $a_k$  are the creation and annihilation operators for the single-particle state k, of the energy  $\epsilon_k$ , with  $k=0$  as the ground state. Let  $\Psi_k$ ,  $\Psi_k^*$  be the thermodynamic averages of  $\psi_{k}, \psi_{k}^{\dagger}$ , respectively, with  $v_k$ ,  $v_k^*$  the corresponding intensive thermodynamic variables. Thus defined,  $V\Psi_k$  is a complex, extensive variable. The particular one  $V\Psi_0$ , which we will call the total Bose moment, is of special interest here, as it is the order parameter for the stationary, simply connected ideal Bose gas.<sup>1</sup> We will refer to  $\Psi_0$  as the Bose moment per unit volume or, more briefly, the Bose moment, in complete analogy with the magnetic mo-

<sup>&</sup>lt;sup>1</sup> One or more of the other variables  $\Psi_k$  could play the role of an order parameter under a different choice of conditions, such as equilibrium in a rotating system.

ment for a system displaying magnetic properties. Just as the conjugate variable in the latter case is called the magnetic field, we will call  $\nu_0$  the Bose field. The complex-valued  $\Psi_0$  represents two real thermodynamic variables, which could be taken as the amplitude  $\Psi$  and phase  $\theta$  of the Bose moment,

$$
\Psi_0{=}\Psi e^{i\theta}\,.
$$

Similarly, we will write  $\nu$  for the amplitude of  $\nu_0$ . As we shall see, the free energy for the above system in a homogeneous field depends only on  $|\Psi_0|^2$ , so that there will be no loss of generality for our present purposes in eventually choosing  $\nu_0$  (and hence  $\Psi_0$ ) as real.

In the same way as for the ferromagnetic system and other systems developing long-range order, the ideal Bose gas can be characterized in. the vicinity of a transition point by such functions as a coexistence curve (relating the "spontaneous Bose moment" in zero field to the temperature difference,  $T-T_c$ , from the transition temperature,  $T_c$ ) a critical isotherm (relating  $\Psi$ and  $\nu$  at  $T_c$ ), an isothermal "Bose susceptibility,"  $kT(\partial \Psi/\partial \nu)_T$ , and other quantities discussed in detail in Sec. II C.

We now wish to consider the statistical mechanics problem of calculating the properties of the Bose moment. In general when dealing with a system undergoing a cooperative transition which is characterized by an order parameter, it is useful to introduce a generating function to facilitate the calculation of its properties. Thus for a system whose Hamiltonian is  $H$  and whose dynamical order parameter<sup>2</sup> is  $X$ , one introduces the generating function  $Z(\beta, \xi)$  which is the thermal average of  $[\exp(\beta \xi X)]$ , with  $\beta = 1/kT$ . Thus

$$
Z(\beta,\xi) = \mathrm{Tr} \, \exp[-\beta(H-\xi X)].
$$

Then the thermodynamic order parameter

$$
\langle X\rangle = \lim_{\xi\to+0} \langle X\rangle_{\xi},
$$

where  
\n
$$
\langle X \rangle_{\xi} = \lim_{V \to \infty} \{ \text{Tr} X \exp[-\beta (H - \xi X)] / \sigma \}
$$
 (The thermodynamic "free er

**Hence** 

$$
\langle X \rangle = \lim_{\hbar \to 0} \lim_{N \to \infty} \beta^{-1} [\partial \ln Z(\beta, \xi) / \partial \xi]
$$

and  $\xi$  plays the role of the thermodynamic variable The thermodynamic properties are determined by conjugate to  $X$ . In general one finds for an order the differential relation (the Gibbs-Duhem equation) parameter that

$$
\langle X \rangle = 0, \quad T > T_c
$$
  

$$
\langle X \rangle \neq 0, \quad T < T_c
$$

where  $T_c$  is the "critical" temperature characterizing the onset of long-range order. The usefulness of this

generating function stems from the fact that if one calculates

$$
\bar{X} = \lim_{\alpha \to 0} \{ \text{Tr} X \, \exp(-\beta H) / \text{Tr} \, \exp(-\beta H) \}
$$

one finds

 $\bar{X}=0$ 

for all temperatures. The value zero for  $T < T_c$  is, however, achieved by the system possessing exactly balanced contributions from each side of the coexistence curve. This is a reflection of a basic symmetry property of  $H$  associated with the order parameter for a particular system. The term  $-\xi X$  is just such as to break this  $s$ ymmetry.<sup>3</sup> The most familiar example of this procedure is for magnetic systems, where  $X$  is the magnetic moment and  $\xi$  is the magnetic field. Our present example is the ideal Bose gas, for which  $X$  and  $\xi$  correspond to the Bose moment and the Bose Geld. The Hamiltonian commutes with the particle number operator  $N$  and is invariant under the gauge transformation ( $\exp iN\phi$ ), where  $\phi$  is the phase. This gauge invariance leads to a zero value for the total Bose moment for all temperatures, a property which is removed by the symmetrybreaking term.

#### B. Partition Function

The grand canonical partition function for a gas of noninteracting Bose particles in a homogeneous Bose field<sup>4</sup>  $\nu_0$  is therefore

$$
\Xi = \mathrm{Tr} \, \exp\{-\beta \left[H - \mu N - V(\nu_0 \psi_0 + \nu_0^* \psi_0^{\dagger})\right]\}, \quad (1)
$$

where  $\psi_0 = V^{-1/2} a_0$ , with

$$
H = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} a_{k}^{\dagger} a_{k},
$$
  
\n
$$
N = \sum_{\mathbf{k}} a_{k}^{\dagger} a_{k},
$$
\n(2)

and where the value of the chemical potential,  $\mu$ , must satisfy where satisfy satisfy the satisfying  $\sim$  satisfying  $\sim$  satisfying  $\sim$  satisfying  $\sim$ 

$$
\epsilon_0 - \mu \geq 0. \tag{3}
$$

The thermodynamic "free energy" for this partition  $Tr \exp[-\beta (H - \xi X)]$ . function is just the pressure,

$$
p = p(T, \mu, \nu_0) = \lim_{V \to \infty} (\beta V)^{-1} \ln \mathbb{E}(T, \mu, \nu_0).
$$
 (4)

the differential relation (the Gibbs-Duhem equation)

$$
d\mathbf{p} = s dT + \rho d\mu + \Psi_0 d\nu_0 + \Psi_0^* d\nu_0^*,\tag{5}
$$

where  $\rho$  is the mean number density and s and  $\Psi_0$  the

<sup>&#</sup>x27;This procedure is, of course, suitable for calculating the thermal average of any dynamical variable, whether or not it is an order parameter.

<sup>&</sup>lt;sup>3</sup> N. N. Bogoliubov [Physica 26 (Suppl.), S1 (1960)] used the term "quasiaverage" for the thermodynamic mean  $\langle X \rangle$  defined above.

<sup>&</sup>lt;sup>4</sup> We could easily consider the general case where the symmetrywe could easily consider the general case where the symmetry<br>breaking term is  $-V\sum_{k}(\nu_{k}\psi_{k}+\nu_{k}*\nu_{k}^{*})$ , instead of the particular<br>choice made for the purposes of our present discussion.

entropy and Bose moment per unit volume. Thus

$$
s = \frac{\partial p}{\partial T}, \quad \rho = \frac{\partial p}{\partial \mu}, \quad \Psi_0 = \frac{\partial p}{\partial \nu_0}.
$$
 (6)

The partition function (1) can be evaluated exactly by making the canonical transformation

$$
b_0 = a_0 - V^{1/2} \nu_0^* / (\epsilon_0 - \mu), \quad b_0^{\dagger} = a_0^{\dagger} - V^{1/2} \nu_0 / (\epsilon_0 - \mu)
$$
  

$$
b_k = a_k, \quad b_k^{\dagger} = a_k^{\dagger}, \quad k \neq 0.
$$
 (7)

$$
\Xi = \operatorname{Tr} \exp[\beta V \nu_0 \nu_0^* / (\epsilon_0 - \mu) - \beta \sum_{\mathbf{k}} (\epsilon_k - \mu) b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}]
$$
(8)

$$
= \exp[\beta V \nu_0 \nu_0^*/(\epsilon_0 - \mu)] \mathrm{Tr} \exp \left(-\beta \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \mu) b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}.\right)
$$
 (9)

As the transformation is canonical, the eigenvalues of the operators  $(b_k^{\dagger}b_k)$  are the positive integers and zero. Thus we see that the trace remaining in (9) is just the partition function of the ideal Bose gas in zero field. Inserting the explicit single-particle spectrum,  $\epsilon_k = \hbar^2 k^2$  $2m, \epsilon_0=0$ , we thus find that<sup>5</sup>

$$
p = \lim_{V \to \infty} (\beta V)^{-1} \ln \Xi = -\nu_0 \nu_0^* / \mu + (\beta \lambda^d)^{-1} F_{d/2+1}(-\beta \mu), \quad (10)
$$

where

$$
\lambda^2 = 2\pi \hbar^2 / mkT \tag{11}
$$

and the function

$$
F_{\sigma}(x) = \sum_{n=1}^{\infty} n^{-\sigma} e^{-nx}, \quad x \ge 0.
$$
 (12)

The thermodynamic extensive quantities are, from (6),

$$
\Psi_0 = -\nu_0^*/\mu\,,\tag{13}
$$

$$
\rho = \nu_0 \nu_0^* / \mu^2 + \lambda^{-d} F_{d/2}(-\beta \mu) , \qquad (14)
$$

$$
s = (\frac{1}{2}d + 1)\lambda^{-d} F_{d/2+1}(-\beta\mu) - \beta\mu\lambda^{-d} F_{d/2}(-\beta\mu). \quad (15)
$$

The expression  $(14)$  is a conservation equation for the density, with the first term on the right corresponding to the contribution  $N_0/V$  of the single-particle ground state; using  $(13)$ , we have

$$
\rho = \Psi_0^* \Psi_0 + \lambda^{-d} F_{d/2} (\beta \nu_0^* / \Psi_0).
$$
 (16)

The contribution of the remaining single-particle states is specified by the usual set of zero field occupation numbers

$$
N_{\mathbf{k}} = {\exp[\beta(\epsilon_{\mathbf{k}} - \mu)] - 1}^{-1}.
$$
 (17)

Ily inspection of (10) and (11) we see that  $(p+v_0v_0^*/\mu)$  is a homogeneous function of kT and  $\mu$ , of degree  $(\frac{1}{2}d+1)$ . Further, as p depends on  $\nu_0$  and  $\nu_0^*$ only through the factor  $\nu_0 \nu_0^*$ , we choose  $\nu_0$ , without any loss of generality for our present purposes, to be real. We therefore set  $v=v_0=v_0^*$ ;  $\Psi=\bar{\Psi}_0=\bar{\Psi}_0^*$ .

Let us define a critical temperature  $T_c(\rho) = 2\pi \hbar^2$ /  $mk\lambda_c^2$ , for  $d>2$ , with

$$
\lambda_c{}^d = \rho^{-1} F_{d/2}(0), \quad d > 2. \tag{18}
$$

We can now write  $(14)$  in the form

$$
\rho^{-1}(\nu/\mu)^2 + (T/T_c)^{d/2} F_{d/2}(-\beta \mu)/F_{d/2}(0) = 1. \quad (19)
$$

This has a solution for  $\mu(\rho, T)$  which is an *analytic* function of  $\rho$  and T so long as  $\nu \neq 0$ . It is easy to see that for  $T < T_c$  a finite contribution must come from the first term in (19) (corresponding to the ground-state contribution), since the coefficient of  $(T/T_c)^{d/2}$  is  $\leq 1$ for all  $\mu \leq 0$  [Eq. (3)]. [The functions  $F_{d/2}(x)$  are finite monotonically decreasing functions of x, for  $x \geq 0$ ,  $d > 2$ . Since this is still true for  $\nu=0$ ,  $\mu$  must vanish for all  $T < T_c$ , whereas it does not vanish for  $T > T_c$ . Thus for  $\nu=0$ ,  $\mu$  is *not* an analytic function of T. That is, a transition occurs only for  $\nu=0$ , at a temperature  $T_c(\rho)$ . For  $d \leq 2$  there is no transition.

We now use the thermodynamic equations obtained above to calculate various properties of the Bose system in the vicinity of the transition. From (16) we find an equation of state  $\nu(\Psi, T)$  given by the solution of

$$
F_{d/2}(\nu/kT\Psi)/F_{d/2}(0) = (T_c/T)^{d/2}(1-\rho^{-1}\Psi^2).
$$
 (20)

1) Let us define the function  $G_d(x)$  by

$$
F_{d/2}(x)/F_{d/2}(0) = 1 - G_d(x) \tag{21}
$$

and introduce its inverse function  $H_d(x)$  such that if

$$
z = G_d(x),
$$
  
\n
$$
x = H_d(z).
$$
\n(22)

Then the equation of state is a function of one vari able, i.e.,  $\nu/kT\Psi = H_d(z)$ 

with

$$
z=1-(T_c/T)^{d/2}(1-\rho^{-1}\Psi^2). \tag{23}
$$

We now introduce, for a given density, the dimensionless temperature variable

$$
t = T/T_c(\rho) - 1
$$

with the transition point characterized by the value zero for t, v,  $\mu$ , and  $\Psi$ . Indeed, by (13),  $\nu/\Psi$  also vanishes and therefore in the neighborhood of the transition point, with  $|t| \ll 1$  and  $\nu/kT\Psi \ll 1$ , we can readily expand (23). Thus

$$
\nu/kT_c\Psi \sim H_d(\frac{1}{2}dt + \rho^{-1}\Psi^2). \tag{24}
$$

The equation of state has a particularly simple structure:  $\nu/kT_c\Psi$  in the asymptotic region around the transition point is a function only of the variable  $(\frac{1}{2}dt+\rho^{-1}\Psi^2)$ . Further, using the expansion<sup>6</sup> of  $G_{d}(x)$  it is easy to show that the functions  $H_d(x)$  have the

<sup>&</sup>lt;sup>5</sup> The term  $V^{-1} \ln(1-\exp\beta\mu)$  which corresponds to the groundstate contribution for  $v_0=0$  vanishes in the limit  $V \to \infty$  for  $v_0 > 0$ , as  $-\mu > 0$ .

<sup>&</sup>lt;sup>6</sup> J. E. Robinson, Phys. Rev. 83, 678 (1951).

asymptotic forms,<sup>7</sup> for  $x \rightarrow 0$ ,

$$
H_d(x) \sim \hat{H}_d(x) = A_d \times x^{2/(d-2)}, \quad 2 < d < 4
$$
  
  $\times x/\ln x^{-1}, \quad d = 4$   
  $\times x, \quad d > 4$ 

so that, for the same ranges of  $d$ ,

$$
\begin{array}{ll}\n\mathbf{v}/k \cdot \mathbf{T}_c \sim A_d \Psi \times (\frac{1}{2} dt + \rho^{-1} \Psi^2)^{2/(d-2)} \\
& \times (2t + \rho^{-1} \Psi^2) / \ln(2t + \rho^{-1} \Psi^2)^{-1} \\
& \times (\frac{1}{2} dt + \rho^{-1} \Psi^2),\n\end{array} \tag{25}
$$

where the number  $A_d$  depends only on d (a similar notation is used in the sequel for other numerical factors). In the special cases where the function is a simple power  $(d\neq 4)$ , these asymptotic expressions are examples of the homogeneous structure first proposed by Widom. ' In general, however, the form is diferent from Widom's proposal  $(d=4)$ . This distinction is not trivial and is discussed in Sec. VI.

From (25) it is clear that for  $t>0$  the condition  $\nu=0$ has, as expected, the one solution  $\Psi=0$ ; i.e., the Bose moment is identically zero above the transition temperature in zero field. For  $t<0$  the condition  $\nu=0$  has the solutions  $\Psi = 0$  (which is unphysical) and

$$
\Psi = \pm \left( -\frac{1}{2} d\rho t \right)^{1/2}, \quad d > 2 \tag{26}
$$

which defines the coexistence curve.

The critical isotherm  $t=0$ , is given by

$$
\begin{array}{ccc}\n\nu/kT_c \sim B_d(\rho) \times \Psi^{(d+2)/(d-2)}, & 2 < d < 4 \\
\times \Psi^3/\text{ln}\Psi^{-1}, & d = 4 \\
\times \Psi^3, & d > 4\n\end{array} \tag{27}
$$

and the isothermal "Bose susceptibility,"  $x=kT$  $\times (\partial \Psi/\partial \nu)_T$ , is given for  $t>0$  and the same ranges of d by

$$
\begin{array}{c}\n \chi \sim C_d \chi t^{-2/(d-2)}, \\
 \chi \ln t^{-1}/t, \quad \Psi = 0. \\
 \chi t^{-1},\n\end{array} \tag{28}
$$

On the low-temperature side  $(t<0)$ ,  $\chi$  is infinite everywhere on the coexistence curve. This property reflects the unphysical nature of this region and the nonexistence of a metastable state for the ideal Bose gas (see Sec. V and the discussion by Langer<sup>9</sup> for the spherical model).

#### C. Critical Exponents

It is a straightforward matter to calculate the behavior of other thermodynamic functions, such as the specific heats  $c_{v,r}$ ,  $c_{p,r}$ . The behavior of these and other functions in the neighborhood of the transition is described in Table II in terms of the corresponding critical exponents defined in Table I. These exponents, with extensions discussed below, are defined in the usual way: We say that the quantity f with variable x has

TABLE I. Definition of critical exponents.

Quantity	Variable	Exponent	Region <sup>a</sup>
Ψ			Coexistence curve
v	Ψ		$T = T_c$
υ	Ψ	δs	$S = S_{\alpha}$
x			$\nu = 0$
$c_p, v$		– E	$\dot{\phi}$ constant, $\nu = 0$
$c_v$ , $\nu$		$-\alpha_{\rm s}$	$\rho$ constant, $\nu = 0$
$S_c-S$	Ψ	$1 + r$	$T = T_c$
$T-T_c$	Ψ	â	$S = S_{c}$
C(r)		$\frac{(d-2+\eta)}{-\hat{p}}$	$T = T_c$ , $\nu = 0$
$R_0$			$T = T_c, \nu = 0$
$R_0$	υ	— к	$T = T_c$

<sup>a</sup> Except for  $\beta$  all exponents are defined for  $T > T_c$  and, with the exception  $\xi$ , for constant density.

TAsLE II. Critical exponents of the noninteracting Bose gas. (Single-particle energy  $\sim k^{\sigma}$ , in d dimensions.)

Exponent	$1 < d/\sigma < 2$	$d/\sigma = 2$	$d/\sigma > 2$
$\delta = \delta_S$ $\alpha_s$ $1 + \zeta = \hat{\sigma}$ κ	$\frac{d+\sigma}{d-\sigma}$ $\sigma/(d-\sigma)$ $(2\sigma-d)/\sigma$ $-(2\sigma-d)/(d-\sigma)^b$ $2\sigma/(d-\sigma)$ $2-\sigma$ $1/(d-\sigma)$ $2/(d+\sigma)$	31 1ı 01 0 Żι $2-\sigma$ $\sigma \hat{\nu} = 1_{L}$ $\sigma \kappa = (\frac{2}{3})_l$	$-(d-2\sigma)/\sigma^{\rm a}$ $-(d-2\sigma)/\sigma^{\rm a}$ $2-\sigma$ $1/\sigma$ $2/3\sigma$

**4** When  $d/\sigma = 2 + n$ , with *n* a positive integer, the first derivative of the specific heat to diverge is the *n*th, with the divergence being logarithmic.<br>
<sup>b</sup> For values of  $d/\sigma$  between 1 and 2 such that  $(2\sigma - d)/(d - \sigma)$ 

an exponent  $\eta$  if

$$
\lim_{x\to 0}\ln f(x)/\ln x=\eta.
$$

Whether a quantity vanishes or diverges is indicated by the sign  $(+ \text{ or } -)$  in the third column of Table I.

The extensions to this notation are as follows. We distinguish logarithmic factors by "exponents" with suffix l. Thus  $f(x)$  is said to have exponent  $\eta_i$  or  $\eta'$ respectively, if

$$
f(x) \sim x^{\eta}/\ln x^{-1}
$$
 or  $k^{\eta} \ln k^{-1}$ .

(The entry  $0^l$  for the index  $\alpha_s$  means that  $c_{v,\nu}$  – const  $\sim 1/t^{0} = 1/\ln t^{-1}$ .) The specific heat  $c_{v,r}$  for the ideal Bose gas remains finite<sup>10</sup> as  $t \rightarrow \pm 0$ , but one of its temperature derivatives may diverge as  $t \rightarrow +0$  (the same remarks hold for  $c_{p,\nu}$  for  $d>4$ ). We can characterize this behavior by defining an exponent  $(m+\alpha_s)$ such that the *m*th derivative of  $c<sub>v</sub>$  diverges like

$$
\partial^m c_n / \partial T^m {\sim} t^{-(m+\alpha_s)}
$$

The with many asymptotic expansions, these asymptotic forms and hence (25) are in many cases *extremely bad* as approximations over any practical interval. See Sec. VI.<br>
<sup>8</sup> B. Widom, J. Chem. Phys. 43, 3898 (1965).<br>
<sup>9</sup> J

<sup>&</sup>lt;sup>10</sup> This behavior is by no means a special property of the Bose<br>gas. In fact, it is quite general. Thus, for example, for a ferro-<br>magnetic system with finite compressibility, an infinity in  $c_{p,H}$ <br>is associated with a Eairbank, in *Progress in Low-Temperature Physics*, edited by C. J.<br>Gorter (North-Holland Publishing Co., Amsterdam, 1961), Vol.<br>Gorter (North-Holland Publishing Co., Amsterdam, 1961), Vol.<br>III.] The notation for this case

If  $\alpha_s$  is positive, the above corresponds to the usual definition of the exponent for the specific heat. However, this definition also allows one to give an explicit, consistent meaning to negative  $\alpha_s$  so as to characterize the dominant singularity in the specific heat. We are only interested in the first diverging derivative; i.e., in the smallest value of *m* for which  $(\alpha_s+m) > 0$ . The negative values of  $\alpha_s$  and  $\xi$  which occur in Table II are to be interpreted in this fashion.

We conclude this section by noting the behavior of the density for the Bose gas.<sup>11</sup> Although for a cooperative transition the behavior of that extensive parameter which becomes long-range ordered (in this case  $\Psi_0$ ) is of primary interest, any other parameter in general also has nonanalytic behavior. It can be shown<sup>10</sup> that any system possessing an infinite specific heat,  $c_p$ , on a line of finite slope in the  $P-T$  diagram has also a singular thermal expansion coefficient and isothermal compressibility and moreover that the asymptotic form of the singularity in both these properties is the same as that of  $c_p$  itself. Thus each of these quantities for the Bose gas is characterized by the critical exponent  $\xi$  given in Table II. <sup>A</sup> further property of interest is the shape of the isotherms on the pressure-density diagram. These approach a point on the transition line  $(p_c, \rho_c)$  like

$$
\begin{array}{ll}\np-p_c \sim (\rho_c - \rho)^{2/(d-2)}, & 2 < d < 4 \\
& \sim (\rho_c - \rho)/\ln(\rho_c - \rho)^{-1}, & d = 4 \\
& \sim (\rho_c - \rho), & d > 4\n\end{array} \tag{29}
$$

for  $\rho \leq \rho_c$ .

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## III. IDEAL BOSE GAS WITH MODIFIED SINGLE-PARTICLE ENERGY SPECTRUM

It is a simple matter to extend the above results to the case where the single-particle energy spectrum, instead of being quadratic, is given by  $\epsilon_k = ck^{\sigma}$ . The effect of this extension of the model is precisely to replace d in the results of the last section by  $(2d/\sigma)$ , since the spectrum only affects the density of states.

### IV. BOSE MOMENT CORRELATION FUNCTION

The correlation function for the set of dynamical variables  $\{\psi_{k}, \psi_{k}^{\dagger}\}\)$  is

$$
C_{\mathbf{k}1} = \langle \psi_{\mathbf{k}}^{\dagger} \psi_{1} \rangle = (N_{\mathbf{k}} / V) \delta_{\mathbf{k}1}.
$$
 (30)

The equivalent correlation function in coordinate space, obtained via a transformation to the particle-field operators

 $C(\mathbf{r}_1-\mathbf{r}_2)=\sum_{\mathbf{k},\mathbf{l}} C_{\mathbf{k}\mathbf{l}} \exp[i(\mathbf{k}\cdot\mathbf{r}_1-\mathbf{l}\cdot\mathbf{r}_2)].$  $\psi(r) = \sum_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{r})\psi_{\mathbf{k}}$ 

Thus

$$
C(\mathbf{r}) = \sum_{\mathbf{k}} \exp(i\mathbf{k}\cdot\mathbf{r}) (N_k/V).
$$
 (31)

Using the expressions (16) and (17) for  $(N_k/V)$  and converting the sum (31) into an integral, it is easy to show that the dimensionless correlation function

$$
g(\mathbf{r}) = \lambda^d [C(\mathbf{r}) - \Psi^2]
$$
 (32)

is isotropic and given by

$$
g(r) = g(|r|) = D_d'' R^{-d} G(R, R_0), \qquad (33)
$$

$$
G(R, R_0) = \int_0^\infty \frac{x^{d/2} J_{d/2-1}(x) dx}{\exp(x^2/R^2 + R_0^{-2}) - 1}
$$
(34)

and

where

$$
R=r/\lambda
$$
,  $R_0 = (-\beta \mu)^{-1/2}$ , (35)

and where  $\lambda^2 = \lambda^2/4\pi$ .

The function  $J_n(x)$  is a Bessel function of the first kind.

It is for large r, that is,  $R \gg 1$ , and in the neighborhood of the transition, where  $R_0 \gg 1$ , that we are primarily interested in the correlation function. It can easily be shown that in this region the function  $G(R, R_0)$ approaches

$$
R^{2} \int_{0}^{\infty} \frac{x^{d/2} J_{d/2-1}(x) dx}{x^{2} + (R/R_{0})^{2}}
$$
  
=  $D_{d}^{\prime} R^{2} (R/R_{0})^{d/2-1} K_{d/2-1} (R/R_{0}),$  (36)

the integral being a Hankel transform, where  $K_n(x)$ is a modified Bessel function of the third kind. Thus, when  $R$  and  $R_0$  are both large,

$$
g(r) \sim D_d R^{-(d-2)} (R/R_0)^{d/2-1} K_{d/2-1} (R/R_0) \qquad (37)
$$

which reduces to the limiting forms

$$
g(r) \sim R^{-(d-2)} \qquad R/R_0 \ll 1 \qquad (38)
$$

and

$$
g(r)
$$
 ~  $R^{-\frac{1}{2}(d-1)}R_0^{-\frac{1}{2}(d-3)}$  exp $(-R/R_0)$ ,  $R/R_0 \gg 1$ . (39)

Summarizing the above results, we first note from (33) the simple and exact result that the dimensionless correlation function  $g(r)$  is a function only of R and  $R_0$ . The only dependence of  $g(r)$  on the thermodynamic variables is contained in the correlation length,  $R_0$ , which itself is a function of state, equal to  $(-\beta\mu)^{-1/2}$ . Further, in the vicinity of the transition point,  $R_0$  becomes large and for  $R$  large,  $g(r)$  then reduces to the homogeneous function of degree  $[-(d-2)]$  given by (37). Physically, then, there is only one scaling length,  $R_0=R_0(t, \nu, \rho)$ . This result is simpler than that obtained by Kadanoff<sup>12</sup> using general "scaling" arguments for a

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<sup>&</sup>lt;sup>11</sup> More details may be found in J. D. Gunton, thesis, Stanford University, 1966 {unpublished).

<sup>&</sup>lt;sup>12</sup> L. P. Kadanoff, Physics 2, 263 (1966). His equation (28) can be written in the form  $g(r) \sim R^{-n}G(R/R_t; R/R_s)$  where  $R_t$  and  $R_s$  are inverse powers of t and v respectively. The (second moment) correlation length  $R_0$  is a homogeneous function of t and  $\nu$  such that as  $\nu \to 0$ ,  $R_0 \to R_t$  and as  $t \to 0$ ,  $R_0 \to R_{\nu}$ .

thermodynamic singularity. The asymptotic dependence of  $R_0$  on the intensive variables (the temperature  $t$  and the Bose field  $\nu$ ) is listed in Table II. Finally, it can be seen from (38) and (39) that the dependence of  $g(r)$ on the distances large and small compared to the correlation length, conforms to the Ornstein-Zernike theory.

In the extended model, where  $\epsilon_k = ck^{\sigma}$ , a similar analysis can be made; the results are listed in Table II. The correlation function in the neighborhood of the transition remains homogeneous, but now of degree  $[-(d-\sigma)]$ . It should be noted that except for  $\sigma = 2$  the results are not those of the Ornstein-Zernike theory.

## V. CORRESPONDENCE BETWEEN CRITICAL EXPONENTS OF THE IDEAL BOSE GAS AND THE SPHEMCAL MODEL OF FERROMAGNETISM

The spherical model of ferromagnetism was introduced by Berlin and Kac'4 and has since been discussed by many authors. We briefly summarize here some results for this model, to show the correspondence which exists between it and the ideal Bose gas. Consider a lattice of  $N$  sites, labeled by the index  $l$ , each occupied by a spin  $\mu_l$ . The Hamiltonian in a magnetic field B is

$$
H = -\frac{1}{2} \sum_{l,\,l'} v_{l,\,l'} \mu_l \mu_{l'} - B \sum_l \mu_l. \tag{40}
$$

The spin variables are allowed to take on all real values  $-\infty < \mu<+\infty$  subject to the "spherical constraint"

$$
\sum \mu_i^2 = ND \tag{41}
$$

where  $D^{1/2}$  is the mean "spin" per particle. Let z denote the thermodynamic intensive variable conjugate to the extensive variable ND.

The partition function

$$
\Xi_s = \prod_l \int_{-\infty}^{\infty} d\mu_l \exp(-\beta H + \beta z ND) \tag{42}
$$

can be evaluated exactly $9,14$  and reduces to

$$
N^{-1} \ln \Xi_s \approx \frac{\beta B^2}{2(2z - v_0)} - \frac{1}{2N} \sum_{\mathbf{k}} \ln(2z - v_0 + \gamma k^2) \quad (43)
$$

in the transition region. The terms  $v_0$  and  $(\gamma k^2)$  are the first terms in the expansion for small  $k$  of the Fourier transform of the finite range interaction  $v_{l,l'}$ .

Returning to the ideal Bose gas, it can easily be

shown that Eq. (9) for the partition function reduces to

$$
V^{-1}\ln\Xi_B \cong -\frac{\beta\nu^2}{\mu} - \frac{1}{V} \sum_{\mathbf{k}} \ln(-\beta\mu + \lambda^2 k^2)
$$
 (44)

in the transition region, where  $\lambda^2 k^2$  is just the singleparticle energy  $\epsilon_{k}$  divided by  $kT$ . Thus it can be seen that a simple transformation identifying equivalent variables shows that the corresponding thermodynamic properties of the two models are the same in the transition region. That is, the corresponding critical exponents are identical.

The case of the spherical model with long-range The case of the spherical model with long-range<br>forces has been discussed by Joyce.<sup>15</sup> This model, for which the interaction falls off with distance to the power  $(d+\sigma)$  has a Fourier transform for small k given by

$$
v_k \leq v_0 - ak^{\sigma} + bk^2 + \cdots. \tag{45}
$$

This corresponds for  $\sigma < 2$  to an "ideal Bose gas" whose single-particle energy spectrum is  $\epsilon_k = ck^{\sigma}$  discussed above.

Finally, we remark that a similar correspondence exists between the ideal Bose gas at constant pressure (the above correspondence is with the Bose gas at constant density) and the Gaussian model of ferromagnetism. To see this, we recall that the Gaussian model assigns a distribution  $\exp(-\sum \mu_i^2)$  to the spin values. If we consider a "generalized" Gaussian model with a distribution of spins given by  $\left[\exp-\left(z\sum \mu_i^2\right)\right]$ , the parameter s can be considered as the intensive variable conjugate to the extensive one,  $D$ , given by (41). Thus the free energy at constant  $z$  (i.e., the "Gaussian" model) is just the Legendre transform of the free energy<br>at constant D (i.e., the "spherical" model).<sup>16</sup> at constant D (i.e., the "spherical" model).

### VI. DISCUSSION

The ideal Bose gas is an artificial model because of its lack of molecular interactions and the consequent unphysical nature of its low-temperature behavior. It is even more artificial in an arbitrary number  $d$  of dimensions. (We could, however, restrict ourselves to three dimensions, say, and recover most of the cases considered, by varying the energy spectrum exponent,  $\sigma$ .) However, its properties are not without interest for the general problem of cooperative transitions,

To begin with, we have found that the equation of state given exactly by Eq. (23), reduces in the critical region to (24). The right-hand side of (24) further reduces to the asymptotic form  $\hat{H}_d$  given by Eq. (25). As noted above this asymptotic form for the equation of state is not, in general, of the homogeneous structure

<sup>&</sup>lt;sup>13</sup> L. S. Ornstein and F. Zernike, Proc. Acad. Sci. Amsterdam **17, 793** (1914). This result is apparent from the small *k* dependence of (30), which is just  $(k^{\sigma}-\mu)^{-1}$ , corresponding to the Ornstein-Zernike behavior only for  $\sigma = 2$ , <sup>14</sup> T. H. Berlin and M. Kac, Phys. Rev. 86, 8

<sup>&</sup>lt;sup>15</sup> G. S. Joyce, Phys. Rev.  $146$ ,  $349$  (1966). "This mathematical correspondence was, in effect, pointed out by H. %'. Lewis and G. H. Kannier, Phys. Rev. 88, <sup>682</sup> (1952). The implication that the spherical and Gaussian models describe the same physical system does not seem to have been generally appreciated.

proposed by Widom,<sup>8</sup> because of the logarithmic structure in the case  $d=2\sigma$ . This lack of homogenity may have relevance to the general problem of cooperative transitions, where experimental evidence<sup>10,17</sup> suggests that logarithms are involved, at least in the specific heats. Indeed, the model considered in this paper (including the spherical model) is the only one possessing a logarithmic singularity in the specific heat for which an exact solution in terms of all variables has been obtained,<sup>18</sup> and for this case the equation of state is not homogeneous. This would suggest generalizing Widom's proposal to encompass the possibility of logarithmic factors.<sup>19</sup> logarithmic factors.

The equations of state also provide examples of a problem of importance in the experimental or numerical analysis of critical behavior. This concerns the accuracy and domain of validity of approximations of the type involved in obtaining (24) and (25) respectively. The second is an asymptotic approximation whose accuracy depends on the function involved. An example will suffice to make the point. The case  $d=3$ ,  $\sigma=5/3$  (which gives  $\gamma = 5/4$ ) results in (24) being accurate to 2% for values of the argument less than  $10^{-2}$ . However,  $(25)$ has the same accuracy only for arguments less than about  $10^{-8}$ .

The precise relationship of the structure of the correlation function to that of the free energy in the asymptotic region of cooperative transitions is an interesting and as yet unsolved problem. Thus it is revealing that for the ideal Bose gas the correlation function is always a homogeneous function of distance and a correlation length for all  $d$  and  $\sigma,$  as contraste with the structure of the equation of state discussed above. However the correlation length  $R_0=R_0(t, v)$  is itself a homogeneous function of  $t$  and  $\nu$  only when the equation of state is.

The rigorous thermodynamic inequalities<sup>20</sup> are, of course, satisfied by the Bose gas. Thus  $\beta(\delta+1) \geq 2-\alpha'$ 

<sup>19</sup> A simple example of such a structure has been proposed by M. Azbel, A. V. Voronel, and M. S. Giterman, Zh. Eksperim. i<br>Teor. Fiz. 46, 673 (1964) [English transl.: Soviet Phys.—JETP 19, 457 (1964)].<br><sup>20</sup> R. B. Griffiths, J. Chem. Phys. 43, 1958 (1965).

is satisfied as an inequality for  $d/\sigma < 2$ ,  $\alpha'$  being zero in all cases. (The relation  $2\beta + \gamma' \geq 2 - \alpha'$  is not relevant here since  $\gamma'$  is undefined, but the thermodynamic condition normally leading to this statement is trivially satisfied). It is of interest to note that, recalling the definitions and results of Sec. II, we have in all cases<br> $2-\alpha_s \geq 2\beta + \gamma \geq 2-\alpha',$ 

$$
2-\alpha_s \ge 2\beta + \gamma \ge 2-\alpha',
$$
  

$$
2-\alpha_s \ge \beta(\delta+1) \ge 2-\alpha',
$$

the left-hand relations being equalities for  $d/\sigma < 2$ . Turning to the general relations involving correlatio function indices, $21$ function indices,<sup>21</sup>

$$
d-2+\eta \geq 2d/(\delta+1),
$$
  
\n
$$
\rho d \geq \gamma(\delta+1)/(\delta-1),
$$
  
\n
$$
\kappa d \geq 1+1/\delta,
$$

we see that the equalities hold for  $d/\sigma < 2$ . Furthermore since the correlation function is homogeneous in all cases, we have the expected results

$$
(2-\eta)\hat{v}=\gamma\,;\quad (2-\eta)\kappa=1-1/\delta\,.
$$

As was pointed out in Sec. II, the free energy for the stationary, simply connected ideal Bose gas in a homogeneous field depends on the complex  $\Psi_0$  only through its amplitude. Thus our results here only involve relationships between the amplitudes of the Bose moment and its associated field. A discussion of the phase variable is left for another occasion.

We have also not discussed here the relation between the transition of the ideal Bose gas and the  $\lambda$ -transition in liquid helium. It is of some interest to note that the singular form of the specific heat and the density variations indicated by experimental results are asymptotically those of the ideal Bose gas in three dimensions with energy spectrum index  $\sigma = \frac{3}{2}$ . This is a case in which the accuracy involved in using the asymptotic approximation, Eq. (25) would be even worse than in the example quoted above. It is clear however, in spite of some statements to the contrary, that the  $\lambda$  transition should be regarded as an example of a cooperative transition. It is just as respectable as the ferromagnetic transitions even though the absence of controllable "external Bose fields" is a serious hindrance to the experimenter.

2' J. D. Gunton and M. J. Buckingham, Phys. Rev. Letters (to be published).

<sup>&</sup>lt;sup>17</sup> See, for example, *Critical Phenomena*, edited by M. S. Green and J. V. Sengers (National Bureau of Standards, Washington D. C., 1966).<br><sup>18</sup> The two-dimensional Ising model has a symmetric logarithmic

divergence in the specific heat, but its behavior in a magnetic field is not known exactly. The present model is unsatisfactory, of course, because of its anomalous low-temperature behavior.