LECTURES ON

INTRODUCTION TO QUANTUM STATISTICAL MECHANICS OF DEGENERATE BOSE SYSTEMS

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THE INSTITUTE OF MATHEMATICAL SCIENCES, MADRAS-20 (INDIA)
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OF DEGENERATE BOSE SYSTEMS

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LECTURE I.

Free Bose Gas

Historically, the first known example of a Bose system was the photon gas. In 1924, S.N. Bose\textsuperscript{1}) first showed that one could understand Planck's equation for the energy-density of black-body radiation from a "quantum statistical" point of view. His basic assumption was that many light quanta could occupy the same quantum mechanical element $\hbar^3$ of phase space. This led him, with the aid of a simple statistical mechanical argument, to the important result for the average number of quanta in a single state,

$$\langle N_\omega \rangle = \frac{e^{-\beta \omega}}{1 - e^{-\beta \omega}}$$

(1)

where $\omega = p^2/2m$ is the energy corresponding to the momentum state and $\beta = (kT)^{-1}$. By a simple state was meant an element of phase space $\Omega \delta^3 P$, which equals $\hbar^3$ ($\Omega$ = volume of system). This simple formula could then be used to derive the thermodynamical properties of black-body radiation by elementary means.

The important assumption which has entered into the Bose derivation of equation (1) is that more than one light quantum can occupy a single quantum state. The applicability of this assumption can be generalized to include the quantum statistical analysis of any system of Bose quanta, or particles. Thus, a Bose particle is defined to be any particle which can occupy
a quantum state independently of how many other (identical) Bose particles are already in that state. A Fermi particle is one which cannot occupy a quantum state if another (identical) Fermi particle is already in that state. One refers to this property of elementary particles by saying that they obey either Bose-Einstein statistics or Fermi-Dirac Statistics. One can easily show that the generalization of equation (1) to the case of Free Bose particles is
\[
\langle N_i \rangle = \frac{e^\beta (\mathcal{g} - \omega_i)}{1 - e^\beta (\mathcal{g} - \omega_i)} \tag{2}
\]
where \( \omega_i = \frac{\hbar^2 k_i^2}{2M} \) and \( \mathcal{g} \) is the chemical potential, or thermodynamic potential per particle, of the gas. The significant difference between equations (1) and (2) is the presence in (2) of the quantity \( \mathcal{g} \) which is zero for light quanta. This quantity enters into the derivation of equation (2), because of the extra constraint that the number of Bose particles (Bosons) must be conserved in the system. Of course, this constraint is not present for black-body radiation.

**Bose-Einstein Condensation.**

The ideal Bose gas exhibits an unusual (theoretical) phenomenon, called Bose-Einstein condensation\(^2\), which can be understood by computing the density \( \eta \) of the gas using equation (2). Now, at very high temperatures, the denominator of the expression for \( \langle N_i \rangle \) can be set equal to unity, and one finds the result
\[
\eta = \frac{1}{\mathcal{g} - \omega} \sum_i \langle N_i \rangle \xrightarrow{\eta, \mathcal{T} \to \infty} \lambda_{\mathcal{T}} e^{-\beta \mathcal{g}} \tag{3}
\]
where the thermal wave length \( \lambda_T \) is given by

\[
\lambda_T = \left( \frac{2 \pi \hbar^2}{MKT} \right)^{\frac{1}{2}}
\]

Since \( \eta \lambda_T^3 \ll 1 \) at high temperatures one sees from equation (3) that \( g \) is quite negative in that region. Moreover, it increases towards zero as the temperature is decreased.

An important temperature region for examination occurs when the chemical potential \( g \) approaches zero, i.e., when

\[
\eta \lambda_T^3 \ll 1.
\]

In this case, one must use the full expression (2) to compute the density. One finds that

\[
\eta \lambda_T^3 = 2.612 - 2\sqrt{\pi} (\beta g)^{\frac{1}{2}} + O (\beta g)
\]  

(5)

Clearly, the expression (5) becomes meaningless when

\[
\eta > (2.612) \lambda_T^3.
\]

In fact, the number (2.612) is the upper limit of the series (5) for \( \beta g \leq 0 \) would lead to negative average values for the lowest momentum states, according to (2). It is obvious that higher densities (or lower temperatures) than those allowed by the limit \( \eta > (2.612) \lambda_T^3 \) should be possible for the ideal Bose gas. Therefore, equation (5) presents an inconsistency. (This inconsistency does not occur for the photon gas, because the photon density is not an independent variable).

The resolution to the above inconsistency is achieved by observing that one may isolate a single term in the sum (3), before going to the limit \( -\Omega \rightarrow \infty \) and converting the sum to an integral. The single term is of course, the number of Bosons in the lowest quantum state. One then obtains inste-
of equation (5),

$$n = n_0 + (2.612) \lambda_T^3$$

for \( T \leq T_c \) \hspace{1cm} (6)

where the critical temperature \( T_c \), for a given density of the ideal Bose gas, is defined by

$$n \left( \frac{8 \pi \hbar^2}{M k T_c} \right)^{3/2} = 2.612.$$ \hspace{1cm} (7)

The density \( n_0 \) of zero momentum particles below the critical temperature is found, by solving equations (6) and (7) together, to be

$$n_0 = n \left[ 1 - \left( \frac{T}{T_c} \right)^{3/2} \right].$$ \hspace{1cm} (8)

From the above analysis, one can see that for the ideal Bose gas one is forced to consider the "condensation" of Bosons into the zero momentum state below a critical temperature determined by (7). There is, therefore, a macroscopic occupation of the zero momentum state, so that one can speak of the separation of two phases in equilibrium with each other, not in position momentum space. This phenomenon is called Bose-Einstein condensation.

It is not important for the present exposition to go into the full thermodynamic discussion of the ideal Bose gas in the region of the critical temperature\(^4\). However, it is important to observe that the momentum space ordering which occurs in a Bose gas below the critical temperature is a completely quantum mechanical phenomenon. It occurs in a temperature-density region for which the thermal wave length \( \lambda_T \) of the
Bosons is greater than their interparticle spacing \( l = \frac{n}{\sqrt[3]{3}} \)
Thus, when \( \lambda_{\perp} > l \), the wave functions of the particles
overlap in position space and their Bose statistics causes ex-
change effects to become very important. The contribution of
exchange effects is a major difference between a classical and a
quantum mechanical many-body system.

For a real system one says when \( \lambda_{\perp} \sim l \), and
when the kinetic energy of the system is the same order of mag-
itude (or greater than) the potential energy that the system
is degenerate or strongly degenerate. Degenerate systems can
only be understood on a microscopic basis by using the laws of
quantum mechanics. They are quantum mechanical! (Note that the
term degenerate, as used here, has little to do with energy level
degeneracy -- it is phase space degeneracy).

It is behaved that there is only one strongly de-
genrate Bose system in nature. This is liquid Helium. If one
computes the critical temperature with equation (7), using the
known density of Helium \( (n = 0.146 \ g/w/\text{cm}^3) \), then one
finds a critical temperature \( T_c = 3.13 \, {^\circ}K \). Thus is reason-
ablely close to the observed value of the \( \lambda \) point in liquid
Helium, \( T_{\lambda} = 2.18 \, {^\circ}K \), below which the liquid exhibits
its superfluid properties. The correlation is probably fortuitous.
Nevertheless, it is now generally believed that the theoretical
phenomenon of Bose-Einstein condensation has its manifestation
in nature in the formation of liquid Helium II.
DEGENERATE BOSE SYSTEM WITH INTERACTIONS

There still does not exist a microscopic theory of Helium II, which explains its basic properties quantitatively, including the transition temperature $T_\lambda$. The theory of Feynman\textsuperscript{5)} has had a partial success by qualitatively yielding the observed excitation curve of Helium II, which was first postulated by Landau\textsuperscript{6)}. Beyond this there are model calculations and various hydrodynamical calculations which have only shed limited light on the microscopic behavior of Helium II. Of course, there is also the extensive work of London, Landau, and others towards the development of a microscopic, or thermodynamic, understanding of liquid Helium. To a large extent, the role of a microscopic theory is merely to provide a rigorous basis for the models of the macroscopic theories. Thus, one of the most important features of the macroscopic theories of Helium II is the two-fluid model, first introduced by Tisza\textsuperscript{7)}. The microscopic interpretation of this model, for a system at rest, is that the "superfluid" is composed of those Bosons which occupy the zero momentum state (macroscopically), whereas the "normal fluid" is composed of all the remaining Bosons in non-zero momentum states. This interpretation is based on the ideal Bose gas phenomenon of Bose-Einstein condensation discussed above.

In order to study the detailed aspects of a microscopic extremum theory of liquid Helium II, it is useful to consider simpler, model systems of interacting Bosons. A particularly popular model system in the contemporary literature is the dilute Bose gas of
hard spheres, because it is believed that the hard cores of the Helium atoms must play an essential role in any correct microscopic theory of Helium II. Recently, Lee and Yang have explicitly demonstrated that Bose-Einstein condensation occurs in the dilute gas of hard sphere Bosons. Their calculation has therefore placed the two-fluid model of Tisza on a firmer theoretical basis. Moreover, their thermodynamic results for a model Bose system now provide one important check on the validity of any new theory.

From the preceding paragraph one can see that there is considerable interest in the theory of a general degenerate Bose fluid and not only in the theory of liquid Helium II. Consider now, how the development of a microscopic theory of a general degenerate Bose system can proceed. One first writes down the many-body Hamiltonian, which in second quantized form is:

$$H = \sum_k a_k^+ a_k \omega_k + \frac{i}{\alpha} \sum_{k_1, k_2} a_{k_1}^+ a_{k_2}^+ \langle k_1, k_2 | V | k_4, k_3 \rangle$$

where $$\langle k_1, k_2 | V | k_4, k_3 \rangle$$ is a matrix element in momentum space of the elementary two-particle interaction. The quantities $$a_k$$ and $$a_k^+$$ are the annihilation and creation operators, respectively, of the free Bosons, and these satisfy the usual commutation relations. One next observes that each of the momentum state sums includes a contribution from the zero momentum state, which when considered from the point of view of deviations from the free particle condition may be macroscopically occupied. In order to investigated the grand state ($T = 0$) of the Bose system, it is therefore necessary to treat the zero momentum state specially.
The difficulty presented by the zero momentum state can be most easily seen when attempting to calculate the deviations from the free Bose gas condition by applying many-body perturbation theory in a straightforward manner. One assumes in first approximation that the operators $a_o$ and $a_o^+$ may each be replaced by the number $\langle N_o \rangle^{1/2}$, and one then separates from the interaction part of the Hamiltonian the resulting diagonal terms. Finally, a detailed study of the perturbation treatment of the off-diagonal interaction terms shows that the perturbation theory for the ground state energy diverges in the limit $\langle N \rangle$, $\hbar \to \infty$ (keeping $\gamma = \langle N \rangle / \hbar$ finite). It is the macroscopic occupation of the zero momentum state; i.e., the fact that $\langle N_o \rangle \sim \langle N \rangle$ which causes this divergence.

The off-diagonal interaction terms in (9) which give the dominant contribution to the ground state energy are those for which both of the annihilation (or creation) operators are $a_o$ ($a_o^+$). These "leading" off-diagonal terms, which involve the momentum state pairs $(k, -k)$, can be incorporated into the diagonal part of $\mathcal{H}$ (by a transformation first introduced by Bogoliubov). This transformation consists of introducing two new annihilation and creation operators $\xi^o_k$ and $\xi^i_k$ by the equations

$$\begin{align} 
\frac{\partial}{\partial \psi_k} &= \left(1 - \alpha^2_k\right)^{1/2} \left(a_k + \alpha_k a_{-k}\right), \\
\frac{\partial}{\partial \xi_k^i} &= \left(1 - \alpha^2_k\right)^{-1/2} \left(\frac{\partial}{\partial \psi_k} + \alpha_k a_{-k}\right), \\
\frac{\partial}{\partial \xi_k^o} &= \left(1 - \alpha^2_k\right)^{-1/2} \left(\frac{\partial}{\partial \psi_k} + \alpha_k a_{-k}\right),
\end{align}$$

(10)
where $\alpha_k^\prime$ is a complex number which depends only on the magnitude of $k$ and is determined by the condition of diagonalization. By using this procedure one finds that the dominant off-diagonal terms of the interaction Hamiltonian result (after diagonalization) in the expression for the ground state energy per particle

$$\frac{\langle E_0 \rangle}{\langle N \rangle} = 4\pi \hbar a_s^\prime \left( \frac{\hbar^2}{2m} \right) \left\{ 1 - \left( \frac{12\pi}{15} \right) \left[ n(a_s^\prime)^3/\pi \right] \right\}^2 + O \left[ n(a_s^\prime)^3 \right]$$

(11)

where

$$a_s^\prime = \left( \frac{4\pi \hbar^2}{m} \right)^{-1} \int d^3r \Psi^*(\chi) \Psi(\chi)$$

for a local potential such that $a_s^\prime > 0$.

The result (11) and (12) becomes meaningless when one considers its application to a low density gas of real Bose particles. The reason is that real particles always include a repulsive core and such an interaction produces an infinite number for $a_s^\prime$. The obvious solution to this difficulty is to replace $a_s^\prime$ in (11) by the two-particle scattering length $a_s$ a suggestion due to Landau.\textsuperscript{11} Actually, the first explicit calculation of the result (11) was performed by the Lee and Yang\textsuperscript{12} for the dilute hard sphere Bose gas (characterized by $\gamma > 3/4$) in which case the scattering length is simply the diameter of the hard spheres. Lee, Huang, and Yang\textsuperscript{10},\textsuperscript{13} have shown how to obtain the result (11) and (12) with the aid of the pseudopotential method, and this method (which cannot be directly applied to a bound system) yields (11) with $a_s^\prime$ replaced by $a_s$.

Further discussion of these various methods has been given by
Lieb\textsuperscript{14}). If may be fairly said that none of the existing methods for deriving the result (11) has a straightforward generalisation to the real and important degenerate Bose fluid, Helium II.

**Quantum Statistical Theory of the Degenerate Bose System.**

Perhaps the most promising starting point for the development of a microscopic theory of Helium II is the use of the grand position function \( Z_G \) of quantum statistical mechanics. This quantity can be written as

\[
Z_G = \sum_{N=0}^{\infty} \left( e^{\beta g} \right)^N T_N \left( e^{-\beta H} \right)
\]

where the symbol \( T_N \) indicates that the trace of \( e^{-\beta H} \) is to be taken over a complete set of \( N \)-particle state vectors. The many-body Hamiltonian \( H \) is given in the Fock, or number, representation by equation (9), in which \( V \) is the Helium twoparticle interatomic potential. The quantity \( \frac{\partial}{\partial} \) is called the grand potential, and it is an intensive quantity \( \mathcal{C} \), i.e., the limit of \( \frac{\partial}{\partial} \) as \( \beta \to \infty \) exists.

In the application of equation (13) to a general degenerate Bose system, one finds that the ordinary Ursell method of analysis fails completely to yield a well-defined expression for the grand potential. That is, the grand potential, which equals the pressure divided by \( (kT) \), seems not to be an intensive quantity as it should be. Lee and Yang\textsuperscript{15}) have shown that the reason for this failure is the macroscopic occupation of the zero momentum state (in a system at rest). They observe that if \( \mathcal{L} \) is the number of Bosons in the zero momentum state in any given term of the trace...
in equation (13), then each of the \( L \) \((\text{quantum mechanical})\) exchange terms corresponding to this given term gives an identical contribution. It is the proliferation of identical exchange terms when \( \langle L \rangle \sim \langle N \rangle \) \(\gg 1\) that causes the break-down of the usual Ursell method for determining the grand potential.

To be sure, it is this same proliferation of exchange terms which causes Bose-Einstein condensation, as indicated below equation (8). There is, therefore, not necessarily anything wrong with equation (13) for the grand partition function. Rather, attention is focussed on one's inability to apply equation (13) to the microscopic understanding of a degenerate Bose system.

Lee and Yang\(^{15}\) have also shown how to overcome the difficulty presented by equation (13) with their x-ensemble formulation of the grand partition function. In this formulation, the use of the grand canonical ensemble includes the introduction of a parameter \( X \) which is the density of zero momentum particles in the degenerate Bose system \( \sum \langle X \rangle = \hbar \). \(^{17}\) of equation (8)

Thus, in the "x-ensemble" formulation, the grand partition function is given by

\[
\mathcal{Z}_{x} = \mathcal{Z}_{x} = \sum_{N=0}^{\infty} \sum_{L=0}^{N} \frac{(xL)^{L}}{L!} T_{X}^{N_{L}} L_{N_{L}} e^{-\beta H} (14)
\]

instead of by equation (13). In this new expression \( T_{X}^{N_{L}} \) means that the trace is to be taken over those N-particle state vectors in which \( L \) (and only \( L \)) particles have zero momentum.

In their proof of equation (14), Lee and Yang have shown that if
\[ \frac{\partial f_x}{\partial x} = 0 \quad \text{at} \quad x = \langle x \rangle = \frac{\langle L \rangle}{\Omega} > 0, \] (15)

then \( f_x = f \) in the limit \( \Omega \to \infty \). If equation (15) is not satisfied, then \( f_x = f \) at \( \langle x \rangle = 0 \) and equation (14) reduces to equation (13) for all practical purposes. It can be seen that in the \( x \)-ensemble formulation the macroscopic occupation of a single quantum state \( \langle k = 0 \rangle \) is allowed for from the very beginning, although it is not required that \( \langle x \rangle > 0 \).

The use of eq. (14) for the grand partition function is somewhat analogous to the replacement of the operators \( q_q^+ \) and \( q_q^- \) by \( \langle N_q \rangle^{1/2} \) in the many-body perturbation theory discussed below eq. (9).

It is easy to show how the \( x \)-ensemble expression (14) is obtained from eq. (13), although the following discussion does not constitute a formal proof of eqs. (14) and (15). The motivating step is to eliminate the troublesome factor \( \binom{L}{1} \) from the \( T_{V_N, L} \) (in eq. (13)!). One next observes that when the average number \( \langle L \rangle \) of zero momentum Bosons is \( \sim \langle N \rangle \) then the dominant terms in the grand partition function must be those with

\[ L \sim \langle L \rangle. \] 

One can see this by making an a posteriori argument to show that the fluctuation \( \langle (\Delta L)^2 \rangle \) in the number of zero momentum particles, calculated by using equation (14), is \( \langle L \rangle \).

Then \( \langle L \rangle^{-1} \langle (\Delta L)^2 \rangle^{1/2} = \langle L \rangle^{-\eta \epsilon} < \ll \) \( \ell \) for \( \langle L \rangle \gg \).
One next multiplies the $T X^N, L$ in the grand partition function (13) by the ratio $\left(\langle L \rangle^!\right) (L !)^{-1}$, which is essentially unity for important $L$ values, and this eliminates the troublesome $(L !)$ factor. To arrive at eq. (14), one has finally to use Stirling's approximation for $\langle L \rangle^!$, a step which is valid because $\langle L \rangle >> 1$ and then to replace $\langle L \rangle \approx \frac{\langle x \rangle \Omega}{L}$ by $\langle x \rangle \Omega = L$. In this final step the density $x$ is treated as a variable whose average value can be obtained by the maximum condition (15). This step is necessary in order that one can have a method for calculating $\langle x \rangle$.

With the grand partition function (14) one can apply the Ursell method to arrive at an explicit expression for the grand potential $f_X$. It is not the purpose of the present discussion to go through the details of this subsequent analysis; it has been carried through in a straightforward manner by Lee and Yang\(^{15}\) and, more recently, by Mohling\(^{16}\). For the free Bose gas it is fairly easy to derive from eq. (14) the expression

$$f_X = -\Omega^{-1} \sum_{p \pm 0} \ln \left(1 - e^{\beta (q - \omega_p)}\right) - x + x e^{\beta q}$$

(16)

This agrees with the expression which one would derive from eq. (13), because when $\langle x \rangle > 0$, i.e., when $T < T_c$ then $q = 0$ (see eq. (5) and subsequent discussion).

In order to clarify how eq. (14) is to be used in an actual calculation, it is useful to exhibit the relation between the grand potential and various thermodynamics quantities.Treating
\[ \beta, \varrho \quad \text{and} \quad x \quad \text{as independent variables one can derive from eq. (13) the following expressions} \]

\begin{align*}
\text{Pressure,} & \quad P = \beta^{-1} \frac{\partial}{\partial \omega} (n_f) \quad (17) \\
\text{Particle density,} & \quad n = \omega^{-1} \langle N \rangle = \beta^{-1} \frac{\partial f}{\partial \varrho} \quad (18) \\
\text{Energy per particle,} & \quad \frac{\langle E \rangle}{\langle N \rangle} = \varrho - \beta^{-1} \frac{\partial f}{\partial \beta} \quad (19) \\
\text{Entropy,} & \quad S = \frac{\partial}{\partial f} (\beta^{-1} n_f) \quad (20) \\
\end{align*}

Upon substituting eq. (16) into eq. (18), one finds for the density of the free Bose gas

\[ n = \omega^{-1} \sum_{\varrho \neq 0} \left[ e^{\beta (\varrho - \omega x)} \right] + x e^{\beta \varrho} \quad (21) \]

This agrees with eqs. (6) and (7), because when \( \langle x \rangle > 0 \) then eq. (15) yields for the free Bose gas

\[ \frac{\partial f_x}{\partial x} = 0 = -1 + e^{\beta \varrho} \quad (22) \]

which implies that \( \varrho = 0 \) as pointed out below eq. (16). It is important to observe that the determination of \( \langle x \rangle \) when \( \langle x \rangle > 0 \) has required in this case the use of both eqs. (15) and (18), and not merely eq. (15) alone; this is true quite generally, other thermodynamic expressions for the free Bose gas can readily be derived from eqs. (16), (17), (19) and (20).
As a concluding remark, it is of interest to observe that Equation (13) by arguing that the factor \( e^{-\Omega(x)} (xN)^L (L!)^{-1} \) is just the Poisson distribution of \( L \) about the average value \( \langle xN \rangle \). Since \( \langle xN \rangle \gg 1 \), and the fluctuations in \( L \) are small, equation (13) will be essentially unchanged if each term \( T_N^L (\ldots) \) in the sum over all \( N \) and \( L \) is multiplied by this Poisson distribution function. This observation is due to Professor L. Rosenfeld, Chairman of the Symposium.
LECTURE II

Development of x-Ensemble. Formulation of Quantum Statistics

In the first lecture the principal result which we obtained was Equation (14) for the grand partition function in the ensemble formulation of quantum statistics. In this lecture, our objective is to show how the grand potential may be expressed in terms of the basic two-particle interactions of a Bose system.

It is useful to begin by introducing the interaction representation into equation (14) by defining the operator

$$W_N(\beta) \equiv e^{\beta H_0} e^{-\beta H}$$

(23)

where $H_0$ is the free particle or kinetic energy, term in Equation (9). The operator $W_N(\beta)$ is, of course, unity for free particles. If equation (23) is solved for the operator $\exp (-\beta H)$ and then substituted into eq. (14), one obtains for the grand partition function

$$e^{\Omega_f x} = e^{-\Omega} x \sum_{N=0}^{\infty} \frac{(e^{\beta g})^N}{N!} \sum_{\sum_{i=1}^{N} \omega_i} e^{-\beta \sum_{i=1}^{N} \omega_i} W(x)^{(s)}(k_i \cdots k_N)$$

(24)

where

$$W_x^{(s)}(k_1 \cdots k_N) \equiv \frac{(x \Omega_x^L)}{L!} x^L$$

(25)

$$\left\{ \sum_{P'} \sum_{m'n' \cdots n'} W_N^{(s)}(k_1 \cdots k_N) \right\}$$
In equation (25) the $\sum'_{\mathcal{P}'}$ denotes the sum over all permutations of the primed indices, and after setting $k_i' = k_i$, $l$ of the $k_i$ are zero $[0 \leq l \leq n]$. We have used the free particle representation in eq. (24) to evaluate the trace which appears in eq. (14), and the operator $\exp(-\beta H_0)$ is diagonal in this representation. We henceforth drop the subscript $\times$ from the grand potential $f_x$.

**Ursell Method.**

The Ursell method\(^{17}\) enables one to express the grand potential directly in terms of certain cluster integrals

$$b^{(s)}_N(x, \beta, g, n)$$

by the equation

$$f(x, \beta, g, n) = \sum_{N=1}^{\infty} b^{(s)}_N(x, \beta, g, n) - x$$  \hspace{1cm} (26)

The method consists of defining "cluster functions" in terms of the $W^{(s)}_{N, x}$ of equation (25) by the following set of equations:

$$W^{(s)}_{x}(1) = U^{(s)}_{x}(1)$$

$$W^{(s)}_{x}(1 \ 2) = U^{(s)}_{x}(1) U^{(s)}_{x}(2) + U^{(s)}_{x}(1 \ 2)$$  \hspace{1cm} (27)

$$W^{(s)}_{x}(1 \ 2 \ 3) = U^{(s)}_{x}(1) U^{(s)}_{x}(2) U^{(s)}_{x}(3) + U^{(s)}_{x}(1) U^{(s)}_{x}(2 \ 3) + U^{(s)}_{x}(1 \ 2) U^{(s)}_{x}(3) + U^{(s)}_{x}(1 \ 2 \ 3) + U^{(s)}_{x}(2 \ 3) U^{(s)}_{x}(3) + U^{(s)}_{x}(1 \ 2) U^{(s)}_{x}(12) + U^{(s)}_{x}(1 \ 2 \ 3)$$
These equations are such that the $N$th equation connects with all of the $U_{1,x}^{(s)}, U_{2,x}^{(s)}, \ldots, U_{N,x}^{(s)}$. The equations, which are independent of representations have the significance that they represent all possible ways in which $N$ particles can be grouped into clusters which are both noninteracting and have nonoverlapping wave functions. Thus, the $U_{x,N}^{(s)}$ are indeed "physical cluster functions". One can show by substituting equations (27) into equation (24) and relabelling identical terms that the grand potentials is given by (26) with the cluster integrals defined by

$$B_{N}^{(s)}(x, \beta, g, \Omega) = \sum_{k_{1}}^{N} \frac{(N!)^{-1}}{e^{-\beta g N} \sum_{k_{1}}^{N}} e^{-\beta \sum_{i=1}^{N} \omega_{i}^{(s)}(k_{i}) \sum_{i=1}^{N} \omega_{i}^{(s)}(k_{i})} \times \sum_{k_{1}}^{N} \times U_{x,N}^{(s)}(k_{1}, \ldots, k_{N}).$$

One has to be quite careful in the treatment of the zero momentum state when working out the combinatorial problem in the derivation of equation (26). In particular, just as the $\left( \sum_{k=0}^{N} \right)^{-1}$ factor in equation (25) divides out all but one of the identical exchange terms, so must such a dividing factor be included in each of the $U_{x,N}^{(s)}$.

One can gain insight into the meaning of the Ursell equations (27) by considering their application to the position representation. In this case, the quantity which is a measure of the spread of the particle wave functions is the thermal wavelength $\lambda_{T}$ of equation (4). To see this explicitly, consider the off-diagonal one-particle cluster-function in the Heisenberg, representation. This quantity is given simply by the expression.
\[ U_x(\gamma') = \langle \gamma | e^{-\beta H_0} | \gamma' \rangle = \lambda^{-3} \frac{e^{-\pi (\gamma - \gamma')^2}}{\lambda T} \to \delta^3 (\gamma - \gamma') \quad \lambda T \to 0 \]

The role played by such an off-diagonal matrix element can be better understood when one separates the effect of particle interactions from that of overlapping wave functions, i.e., from statistics, in the \[ U_{x,N}^{(s)} \]. For this purpose one defines with equations (27) the corresponding set of "unsymmetrized cluster functions" \[ U_{x,N} \] of Boltzmann statistics. Now, the \[ U_{x,N} \] contain only the effect of particle interactions, since they are defined with unsymmetrized wave functions. Moreover, one can express the \[ U_{x,N}^{(s)} \] in terms of the \[ U_{x,M}^{[u \Lambda, M \leq N]} \] by combining the two sets of equations (27) with equation (25). One finds that the sum over all exchange terms \[ \sum_{P'} \] in equation (25), i.e., the effect of statistics, leads to the appearance of off-diagonal \[ U_{x,N} \] of which (29) is the one-particle case into the expression for the \[ U_{x,N}^{(s)} \].

There is one final point to make in connection with the cluster-functions \[ U_{x,N}^{(s)} \] of quantum statistics. If one considers the functions \[ T_{x,N} \], defined to be symmetrized combinations of the \[ U_{x,N} \],

\[ T_x \left( l_1, l_2, \ldots, N \right) = \sum P' U_x \left( l_1', l_2', \ldots, N' \right) \]
then the difference \[ U_{x,N}^{(s)} - T_{x,N} \] is not zero except for special cases. This is quite clearly demonstrated by eq. (39) below for the case \( N = 2 \).

**Determination of the** \( U_{x,N}^{(s)} \)**

The explicit determination of the \( U_{x,N}^{(s)} \) by first relating them to the \( T_{x,M} \) of eq. (30) \( M \leq N \) and by then deriving expressions for the \( T_{x,M} \) has been carried through by Mohling \(^{18}\) for the case \( \langle x \rangle = 0 \). The physical insight correlated with this approach has been discussed above.

It is instructive to consider a simpler derivation which leads directly to expressions for the \( U_{x,N}^{(s)} \) in terms of the basic two-particle interactions of the system. In this derivation, one begins by considering the differential equation, in the temperature variable \( \beta \), satisfied by the operator \( \hat{W}(\beta) \) of eq. (23). This equation is

\[
\frac{\partial}{\partial \beta} \, \hat{W}(\beta) = -\hat{V}(\beta) \, \hat{W}(\beta)
\]

(31)

where

\[
\hat{V}(\beta) = e^{\beta \hat{H}_0} \hat{V} e^{-\beta \hat{H}_0}
\]

(32)

and \( \hat{V} \) is the second, or interaction term, in equation (9).

One can easily show by using eq. (9) that a more explicit expression for \( \hat{V}(\beta) \) is:

\[
\hat{V}(\beta) = \frac{1}{4} \sum_{\alpha_1 \alpha_2} h^{\dagger}_{\alpha_1} a^\dagger_{\alpha_2} \langle \omega_1 \omega_2 | V^{(s)} | \omega_3 \omega_4 \rangle a_{\alpha_3} a_{\alpha_4} e^{\beta (\omega_1 + \omega_2 - \omega_3 - \omega_4)}
\]

(33)
where $\langle k_1 k_2 \mid V^{(z)} \mid k_3 k_4 \rangle$ is a symmetrized matrix element of the two-particle interaction $V$.

By using the "initial" condition $W(0) = 1$, one can convert equation (31) to an integral equation.

$$W(\beta) = 1 - \int_0^\beta dt \; V(t) \cdot W(t)$$

$$= 1 - \int_0^\beta dt \; V(t) + \int_0^\beta dt_2 \int_0^{t_2} dt_1 \; V(t_2) V(t_1)$$

$$- \int_0^\beta dt_3 \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 \; V(t_3) V(t_2) V(t_1) + O(V^3)$$

The principle by which expressions for the $U^{(s)}_{x, N}$ can now be derived is to compute matrix elements of the iterated form of (34) using the normalization of equation (25) and then to place the resulting equations in one-to-one correspondence with the Ursell equations (27). It should be observed from equations (27) that in the $N$th equation $U^{(s)}_{x, N}$ is the only completely "connected" term, in the sense that in all of the other terms the variables separate into at least two factors. This observation enables one to identify an expression for each of the $U^{(s)}_{x, N}$ in the explicit derivation of the matrix elements (25).

Rather than give a derivation of the general expression for the $U^{S}_{x, N}$, we shall exhibit this derivation for the simplest cases $N = 1$ and $N = 2$. For the case $N = 1$, only the
The first term in equation (34) contributes and one easily shows that

\[ W_x^{(s)} \left( \frac{K}{K'} \right) = U_x^{(s)} \left( \frac{K}{K'} \right) = \begin{cases} \delta_{K, K'} & \text{if } K = 0 \\ (x, \Omega) \delta_{K, 0} & \text{if } k = 0 \end{cases} \]  

(35)

We see that the two possibilities \( k = 0 \) and \( k \neq 0 \) must be considered separately in equation (35), and this situation occurs for all \( N \). If leads us to adopt the convention that whenever \( k \) does not take the value zero it will be represented by \( P \). (see also equations (16) and (21)).

We next discuss the case \( N = 2 \), and we consider first the possibility that \( K_i = P \) for both \( i = 1 \) and \( i = 2 \). One can show from equation (25) and the second line of (34) that

\[ W_x^{(s)} (P_1, P_2) = U_x (P_1, P_2) + U_x (P_1, P_2) + \int_0^\beta dt \oint \frac{P_1 P_2}{P_1 P_2} \]  

(36a)

where the bracket function in the third term of (36a) is defined by the equation

\[ t_2 \begin{bmatrix} k_1 \\ k_3 \\ k_2 \\ k_4 \end{bmatrix} \equiv \text{pair function} \equiv \begin{pmatrix} \langle k_1 k_2 \mid R(t_2, t_1) \mid k_3 k_4 \rangle + \langle k_1 k_2 \mid R(t_1, t_2) \mid k_4 k_3 \rangle \end{pmatrix} \]  

(37)

with the operator \( R(t_2, t_1) \) given by

\[ R(t_2, t_1) = -\frac{1}{2} \sum_1^t \left[ \mathcal{H}_0 (t_2) e^{-(t_2-t_1) H_0} e^{-(t_2-t_1) H_0} \right] \]  

(38)
The first line of equation (38) is obtained by writing the iterated form of equation (34) with all of the -integrations performed last. It is then a straightforward procedure to verify the second line of eq. (38). The subscripts c and superscripts (2) have been attached to the operators on the RHS of (38) in order to emphasize that the \( R(\xi_2, \xi_1) \) operator occurs in the theory only as a two-body operator. Its symmetrized matrix elements which are the pair-functions of eq. (37), are the interaction representation version of the binary collision kernel first introduced by Lee and Yang^{19}.

The pair-function is the fundamental two-body function of the theory of Mohling^{16}. For a weak interaction, the first line of (38) shows how the perturbation expansion of the pair-function is obtained. An extremely important point is that the pair-function is well-defined (finite) even for strong, or singular, interactions such as a repulsive core, as can easily be seen from the second line of (38). In fact, using the second line of (38) the pair-function can be expressed in terms of two-particle wave-functions or, equivalently, in terms of two-particle reaction matrices. This is shown in reference 18.

When either of the \( \xi \) in \( W_{x,z}^{(s)} \) is zero, then one obtains instead of (36) the expression

\[
W_{x}^{(s)}(0\ P\ 0\ P) = U_{x}^{(s)}(0\ 0) U_{x}^{(s)}(P\ P) + (x\Omega) \int_{0}^{\beta} \left[ \begin{array}{c} 0 \\ 0 \\ P \\ P \end{array} \right] (36a)
\]
It is important to observe here that both of the \( W_{x,n}^{(s)} \) and the \( U_{x,n}^{(s)} \) are invariant under any permutation of their columns, as can be shown by using equations (25) and (27) and the fact that the Hamiltonian (9) is symmetric under particle interchanges. Therefore, the case \( \omega_{1} = \omega_{3}, \omega_{2} = 0 \) is also included in equation (36b).

We finally consider the case in which both \( \omega_{1} = 0 \) and this gives

\[
W_{x}^{(s)}(0,0) = \left[ U_{x}(0,0) \right]^{2} + \frac{1}{2} \left( x, \Omega \right)^{2} \int_{0}^{\beta} dt \left[ \begin{array}{cc}
0 & 0 \\
0 & 0
\end{array} \right]_{t} \tag{36c}
\]

Note that the factor of \( \frac{1}{2} \) from equation (25), which appears in the second term of (36c), in the first term by the equal exchange term. Thus, the exchange term which occurs in (36a) does not appear in (36c).

By comparing equations (36a), (36b) and (36c) with the second of the Ursell equations (27), one finds for the following result:

\[
U_{x}^{(s)}(K_{1}, K_{2}) = U_{x}(P_{1}, P_{2}) U_{x}(P_{2}, P_{1}) + \]

\[
+ \int_{0}^{\beta} dt \left[ \begin{array}{cc}
P_{1} & P_{2} \\
P_{2} & P_{1}
\end{array} \right]_{t} \text{ if } \omega_{1} = P_{1}
\]

\[
= \left( x, \Omega \right) \int_{0}^{\beta} dt \left[ \begin{array}{cc}
0 & P_{1} \\
0 & P_{2}
\end{array} \right]_{t} \text{ if } \omega_{1} = 0, \omega_{2} = P_{2}.
\]
\[ (x, \Omega) \int \beta \left[ \begin{array}{ccc} P & 0 \\ \frac{P}{w} & 0 \end{array} \right] \frac{dt}{t} \quad \text{if} \quad K_1 = P, \quad K_2 = \phi \]

\[ = \frac{1}{2} (x, \Omega)^2 \int \beta \left[ \begin{array}{cc} 0 & 0 \\ 0 & 0 \end{array} \right] \frac{dt}{t} \quad \text{if} \quad K_1 = 0 \]

The method by which \( \bigcup_{x, N}^{(5)} \) has been obtained can be generalized to yield an expression for \( \bigcup_{x, N}^{(6)} \). We shall not give this general derivation here, but shall merely note that the derivation is greatly facilitated by the use of the diagrammatic, or graphical, notation which we shall now introduce.

**INTRODUCTION OF DIAGRAMS**

The diagrams which we shall now introduce are called linkedpair \((\mu, \nu)\)-graphs. They are a set of vertices, which represent the pair-functions (37), linked together by two kinds of lines, wiggly and solid. We shall introduce these diagrams in order that the explicit expression for the \( \bigcup_{N, x}^{(5)} \), or, rather, the grand potential (26) can be written down concisely in terms of the (calculable) two-body functions (37).

In order to facilitate the prescription for performing temperature integrations in the theory, the vertex-functions of \((\mu, \nu)\)-graphs are defined to be slightly generalized versions of the pair-functions (37):
\[ t_1 t_2 \begin{bmatrix} k_1 & k_2 \\ k_3 & k_4 \end{bmatrix} = \theta(t_1 - t_2) \begin{bmatrix} k_1 & k_2 \\ k_3 & k_4 \end{bmatrix} \theta(t_2 - t_0) + \theta(t_2 - t_1) \begin{bmatrix} k_1 & k_2 \\ k_3 & k_4 \end{bmatrix} \theta(t_1 - t_0) \]

where \( \theta(x) \) is a step-function defined by \( \theta(x) = 1 \) if \( x > 0 \)
and \( \theta(x) = 0 \) if \( x < 0 \). A vertex function is represented by a cluster-function, as shown in Fig. 1. It is important to
observe that the lines emanating from a cluster-vertex are directed and that they may be either wiggly or solid. Only the wiggly lines can represent a zero-momentum state. An "upper" temperature variable of a pair-function is either $\beta$ for a solid or a missing line or the temperature variable at the head end vertex for a wiggly line. Missing lines always represent the zero momentum state.

**Linked-pair ($\mu$, $\nu$)-Graphs.**

A $Q^{th}$ order linked-pair ($\mu$, $\nu$)-graphs is a collection of $Q$ cluster-vertices which are entirely interconnected by $m_s$ solid lines and $m_w$ wiggly lines. In addition to these internal lines there are also $\mu$ outgoing external solid lines and $\nu$ incoming external solid lines. The rules for connecting the $Q$ cluster-vertices by the $(m_s + m_w)$ internal lines and the procedures for determining the corresponding the expression are as follows:

(i) It must not be possible to complete a loop in a linked-pair ($\mu$, $\nu$)-graph by following the arrows on wiggly lines. Two wiggly lines may not connect the same two vertices; such a forbidden structure is called a wiggly-line double-bound [see Fig.2 and the associated discussion].

(ii) Associate with each missing (zero-momentum) outgoing line a factor of $\left(\times \Omega\right)^{\nu/2} e^{\beta g}$ and with each missing incoming line a factor of $\left(\times \Omega\right)^{\mu/2}$. For each pair of missing incoming (or outgoing) lines which occurs at the same vertex a factor of $\frac{1}{2}$ must be included in the corresponding expression for the graph.
(iii) External lines are associated with pre-given momenta $P_i$, such that external lines carrying different momenta are regarded as being distinguishable. When an external momentum is zero, then there is no corresponding external line.

(iv) Two linked-pair ($\mu, \nu$)-graphs are different if their topological structures, including internal line types, time directions, and external lines, are different.

(v) Associate with each internal line a different integer $i (= 1, 2, \ldots, m_w + m_\rho)$ and a corresponding momentum $P_i$ or $K_i$ according to whether the line is solid or wiggly.

(vi) Associate with the entire graph a product of $Q$ vertex-functions (40) corresponding to the $Q$ cluster-vertices and explicitly determined by the temperature variables $t_\rho$ of the cluster-vertices and the momentum variable assignment of (iii) and (v). Conservation of momentum at each of the cluster-vertices may then require that some of the wiggly line momenta become zero identically. Graphical structures in which this can occur must be included in any sum over all ($\mu, \nu$)-graphs$^{20}$.

(vii) Assign a factor $S^{-1}$ to the entire graph, where

$$S \equiv \text{Symmetry number},$$

The symmetry number is defined to be the total number of permutations of the $m_s$ integers associated with the solid internal lines that leave the graph topologically unchanged (including the positions of these numbers relative to the $m_s$ solid internal lines, but not necessarily respect to the wiggly line labels).
(viii) Assign a factor \( \nu(p) \) to each solid internal line, where

\[
\nu(p) = \frac{\frac{e^{\beta (g - \omega_p)}}{1 - e^{\beta (g - \omega_p)}}}{(41)}
\]

(ix) Finally, sum over all of the \((m_3 + m_\omega)\) internal momentum coordinates and integrate each of the \(Q\) temperature variables from 0 to \(\beta\).

We observe here that the solid internal lines of linked-pair \((\mu, \nu)\)-graphs arise directly from the particles statistics, i.e., from exchange terms in (25), whereas the wiggly lines are due to the particle interactions, or dynamics.

In order to illustrate the use of the above rules we give below some examples of simplest linked-pair \((0, 0)\)-graphs and their corresponding expressions.

\[
t = \frac{1}{4} (\sum e^{\beta q})^2 \int_0^\beta dt \sum \left[ \begin{array}{c} 0 \\ 0 \\ 0 \end{array} \right]_t
\]

This graph occurs when the last line of (39) is substituted into Equations. (26) and (28).

\[
t \circ \nu = (\sum e^{\beta q}) \int_0^\beta dt \sum \nu_p \left[ \begin{array}{c} 0 \\ P \end{array} \right]_t
\]

This graph occurs when the second and third lines of (39) are substituted into equations (26) and (28) and combined.
This graph occurs when the second term in the first line of (39) is substituted into equations (26) and (28).

\[
1 = \frac{1}{4} \left( x \Omega e^{B(t)} \right)^2 \int_0^\beta \int_0^\beta d t_2 d t_1 \times t_2
\]

where

\[
k_2 = -P_1
\]

\[
1 = \frac{1}{8} \int_0^\beta d t_2 d t_1 \sum_i \sum_j \sum_k \sum_l \left[ P_{j k} P_{l i} \right] t_2 \left[ P_{l i} P_{j k} \right] t_1
\]

This last graph, which has a symmetry number \( S = 8 \), illustrates well rule (vii) above. It is instructive to show that the following two \((0, 0)\)-graphs have symmetry numbers \( S = 6 \) and \( S = 24 \), respectively.

**Linked-Pair Expansion of Grand Potential:**

The expression which one obtains for the grand potential after substituting the general expression for \( \mathcal{U}_x^{(5)} \) into equations (28) and (26) is
\[ \Omega F(x, \beta, q, \Omega) = - \sum_{F} \lambda^{F} \left[ 1 - e^{\beta (q - \omega F)} \right] - x \Omega \]
\[ + x \Omega e^{\beta q} + \sum_{Q \neq 1} [\text{all different } Q \text{ in } \text{order linked pair (0,0) graphs}]
\]

It will be recognized that the first three terms in this equation are the free-particle terms of equation (16). Moreover, if one expands the logarithm of the first term in eq. (43), then it is easy to show that the first two terms in the resulting series arise from the first lines of equations (35) and (39). The third term in eq. (43) arises from the second line of eq. (35) and the second term is due to the \( \exp(-\Delta x) \) factor in eq. (24).

In the limit \( x \to 0 \), eq. (43) reduces to the \( \langle x \rangle = 0 \) expression which one would derive from eq. (13). One can use this fact to show explicitly how eq. (13) leads to a meaningless expression when \( \langle x \rangle \neq 0 \), as discussed below eq. (13). Thus, the missing (zero-momentum) lines of (\( \mu, \nu \))-graphs do not occur in a formalism derived from eq. (13), because they are due to the \( \left( \mathcal{L}_0^\dagger \right)^{-1} \) factors multiplying the \( \text{Tr}_N \) in eq. (14). Instead, when one starts from eq. (13) for the grand partition function, one concludes that the solid line factors \( \nu(P) \), (of eq. (41) and rule (viii)), also apply to the zero momentum state. But we have seen in lecture I, see eq. (5) and below that we must set \( g = 0 \) and \( \nu(0) = \langle N_o \rangle = \langle x \rangle \Omega \) when \( \langle x \rangle > 0 \). Therefore, the volume...
dependence of an arbitrary \((0,0)\)-graph in the formalism is the number of zero-momentum solid lines and \(Q\) is the number of pair-function (37) contributes a volume factor \(\Omega^{-1}\) to the \((0,0)\)-graph. But it is always possible to have \((0,0)\)-graphs with \(l_0 = 2Q\). For such graphs the volume dependence will be \(\Omega^Q\), which leads to a divergent expression for the grand potential \(\Omega\) in the limit \(\Omega \to \infty\) when \((0,0)\)-graphs with \(Q > 1\) are considered. Thus, one is forced to use the Lee-Yang x-ensemble expression (14) for the grand partition function.

**Linked-Pair expansion of Momentum Distribution.**

In the third lecture of this series, we shall devote considerable attention to a study of the momentum distribution

\[
\langle n(\mathbf{k})\rangle
\]

which is the average number of particles with momentum \(\mathbf{k}\) in the Bose system. When \(\mathbf{k} = 0\), then one can show directly from eq. (14) that

\[
\langle n(0)\rangle = \langle L \rangle = \langle x \rangle \Omega
\]

(44)

where we have set \(\mathbf{x} = \langle x \rangle\) in accordance with the statement of eq. (15). The result (44) is not surprising.

When \(\mathbf{k} = \mathbf{p} \neq 0\) then one derives

the following expression for the momentum distribution

\[
\langle n(\mathbf{p})\rangle = \nu(\mathbf{p}) + \nu(\mathbf{p})[1 + \nu(\mathbf{p})] \sum_{Q=1}^{\infty} \sum_{\text{all different \(Q^{\text{th}}\) order \(Q\)-linked-pair \((1,1)\)-graphs}}
\]

\(\times\) derived from eq. (13) will be \(\Omega^{-Q} l_0\). Where \(l_0\) + of vertices. Here we have used the fact that each...
where the function \( \nu(\vec{p}) \) is given by (41). The external
lines in the \((1, 1)\)-graphs of eq. (45) both carry the momentum
\( \vec{p} \) because of conservation of momentum. The first term of
eq. (45) is the free-particle momentum distribution, previously
encountered in eqs. (2) and (21). In fact, the generalization
of eq. (21) to the interacting Bose system is readily seen to
be (for \( \Omega \to \infty \)).

\[
\eta = \langle x \rangle + (2\pi)^{-3} \int d^3 \vec{p} \langle \nu(\vec{p}) \rangle
\]  

(46)

This last equation is equivalent to eq. (18) for the determi-
nation of the density.

It should be clear that in the study of distribution
functions, one requires linked-pair \((\mu, \nu)\)-graphs for \( \mu, \nu = 0, 1, 2, \ldots \) in addition to the \((0, 0)\)-graphs required for
eq. (43). Moreover, in the following lectures we shall encounter
\((\mu, \nu)\)-graphs with \( \mu \neq \nu \). In fig. (2) we give some
examples of simple linked-pair \((1, 1)\)-graphs. The symmetry num-
ber of the third \((1, 1)\)-graph
is $S = 2$, and the symmetry number of each of the other $(1, 1)$-graphs is $S = 1$. It is important to observe that the next-to-last $(1, 1)$-graph does not occur, according to rule (i) above, and this is a consequence of the sum performed in eq. (38).

Thus, the sum over all "wiggly-line double-bounds" which can occur when the cluster-vertices represent the symmetrized matrix element $\left< \overline{K}_1 \overline{K}_2 | \sqrt{(5)} | \overline{K}_1 \overline{K}_3 \right>$ of eq. (33) results in the interaction of the pair-functions (37). After these sums have been performed wiggly-line double-bonds can no longer occur, as is the case in the linked-pair $(\mu, \nu)$-graphs which we have defined above.
LECTURE III.

SELF-ENERGY PROBLEM, MOMENTUM SPACE ORDERING AND QUASI-PARTICLES

It is the purpose of this lecture to indicate, both qualitatively and quantitatively, how the study of the momentum distribution (45) can provide considerable insight into the main point is that the momentum space ordering discussed below into the zero momentum state. There is also an important effect on the non-zero momentum particles, for these are subject to both dynamical (due to the interactions) and statistical (due to the Bose statistics) effects which determine their microscopic behaviour. From the point of view of the quantum statistical theory these effects are called self-energy effects. Consider, for example, the following structures which can occur in the linked-pair (μ, ν)-graphs defined below Eq. (40).

These are called self-energy structures, and the second and third kinds can occur because it is possible for two particles in momentum states \( \vec{P} \) and \( -\vec{P} \) to interact virtually with the zero momentum state, or to have exchange effects with the zero momentum state.
One finds that the iteration of the self-energy structures (when they are placed end-to-end) produces extremely large terms at very low temperatures in the grand potential (43) and the momentum distribution (45). For the dilute gas of hard sphere Bosons near $T = 0$, the parameter which characterizes a self-energy structure to first approximation is $\eta \alpha \lambda^2 \gg 1$.

The iteration of the self-energy structure therefore leads to high powers of $\eta \alpha \lambda^2$. It is clearly necessary to analyze such large terms in detail, wherever they can occur in the theory, and this is the self-energy problem. Furthermore, it should be clear that the solution to the self-energy problem must be intimately associated with the complete understanding of momentum space ordering in the degenerate Bose system. What this understanding must then imply physically can only be suggested, at present, as follows.

Momentum space ordering in a degenerate Bose system (and also in a degenerate Fermi system) produces the quantum mechanical normal modes of the system. These normal modes are called quasi-particles, because they are associated with definite energy-momentum relations. Thus, each "free" non-zero momentum particle, becomes a quasi-particle (hence, the use of the terminology "self-energy effects"). It is believed that if one has once established the quasi-particle theory of a quantum system on a microscopic basis, then it is a straightforward matter to calculate or to deduce the observable physical properties of the system.
This, then, is the specific object of the quantum statistical theory: To deduce the quasi-particle model of the degenerate Bose system from microscopic considerations. This quasi-particle model can only be derived by studying the self-energy problem or, equivalently, by studying the momentum space ordering of the system. The investigation of these questions in greater detail will now be discussed.

The Functions $N_{\nu}(\mathcal{P})$.

It has been emphasized by Lee and Yang$^{15)}$ expression (43) is completely useless for only calculation of the thermodynamic properties of a real degenerate Bose gas for this is associated with the fact that the difference $[\mathcal{N}(\mathcal{P}) - \nu(\mathcal{P})]$ as given by eq. (45) becomes extremely large as $T \to 0$. Moreover, the function $\nu(\mathcal{P})$ of eq. (41) has an unphysical singularity at $\omega P = q$, where for a gas of hard spheres, for example, $q > 0$ at very low temperatures. Thus, the solid line weighting factors in linked-pair $(\mu, \nu)$-graphs are completely unphysical and, therefore, the associated thermodynamics predictions must also be unphysical when in (43) only a few $(0, 0)$-graphs are considered.

The solution to the above dilemna is to regroup the terms in the linked-pair expansion (43) so as to exhibit more physical weighting factors. The hope is that the thermodynamic properties of the Bose system can then be correctly calculated by considering only a "few terms". Lee and Yang$^{15)}$ have taken
the first important step in this direction by their analysis of the momentum distribution. We shall now give some of the results of their analysis, as adopted to the interaction representation.

The starting point of this analysis is to introduce a function \( N_{1,1}(P) \), defined by

\[
N_{1,1}(P) = e^B (g - \omega P) \left[ 1 + \langle n(P) \rangle \right] \tag{47}
\]

\[
= \nu(P) \left\{ 1 + \nu(P) \sum_{Q=1}^{\infty} \frac{\text{all different } Q^{th} \text{ order}}{\text{linked-pair } (1,1)-\text{graphs}} \right\}
\]

where the second line of this equation follows from (45). The program will now be to analyze the self-energy structure of the \((1, 1)\)-graphs in (47), as discussed above. Why must one introduce the function \( N_{1,1}(P) \), instead of considering the momentum distribution \( \langle n(P) \rangle \) directly? The reason is the factor \( [\nu(P)]^2 \) which multiplies each \((1, 1)\)-graph in (47) makes possible the derivation of an integral equation for \( \nu(P) \) which occur as internal solid time factor

\[
N_{1,1}(P) \text{ which the factors } \text{in the iterated solution (47).}
\]

The possibility of doing this will be demonstrated below. On the other hand, the factor \( \nu(P) [1 + \nu(P)] \) which multiplies each \((1, 1)\)-graph in (45) prohibits the derivation of an integral equation for \( \langle n(P) \rangle \) except via the first first line of (47).

When \( \langle x \rangle = 0 \), and there is no macroscopic occupation a single quantum state, then the analysis of self-energy graphs is completely equivalent to the analysis of \( N_{1,1}(P) \).
eq. (47). When $\langle x \rangle \neq 0$, however, $(0, 2)$- and $(2, 0)$-graphs must also be considered in the analysis of self-energy graphs, because they also have only two external lines. Thus, we are led to consider the quantities $N_{0,2}(P)$ and $N_{2,0}(P)$, defined by

$$N_{0,2}(P) = \sum_{\text{all different } Q^{th} \text{ order}} \sum_{Q=1}^{\infty} \left[ \text{linked-pair (0,2)-graphs} \right] = N_{0,2}(-P)$$

$$N_{2,0}(P) = \sum_{\text{all different } Q^{th} \text{ order}} \sum_{Q=1}^{\infty} \left[ \text{linked-pair (2,0)-graphs} \right] = N_{2,0}(-P)$$

We shall first analyze the self-energy graphs only with respect to their solid lines. Then, when this aspect of the problem has been completed, we shall analyze the remaining wiggly-line self-energy graphs. We next define proper and improper graphs as follows:

A linked-pair $(\mu, \nu)$-graph is called improper if by cutting any one of its solid internal lines open the entire graph can be separated into two disconnected graphs. Otherwise the $(\mu, \nu)$-graph is called proper.

With these definitions in mind we next define three functions $K_{\mu, \nu}(P)$ for $\mu + \nu = 2$.

$$K_{\mu, \nu}(P) = \sum_{Q=1}^{\infty} \left[ \text{all different } Q^{th} \text{ order proper linked-pair } (\mu, \nu)\text{-graphs} \right]$$
In these definitions the momenta associated with the external lines are both \( \frac{P}{\omega} \) in the case of the \((1, 1)\)-graphs, and \( \frac{P}{\omega} \) and \( -\frac{P}{\omega} \) in the case of the \((0, 2)\)- and \((2, 0)\)-graphs. It should be clear that \( K_{\mu, \nu}(-\frac{P}{\omega}) = K_{\mu, \nu}(\frac{P}{\omega}) \) for \((\mu, \nu) = (1, 1)\) \((\mu, \nu) = (2, 0)\), but this identity is true for \((\mu, \nu) = (1, 1)\) only in the case of an isotropic system.

We next write down a set of algebraic equations which relate the \( N_{\mu, \nu}(P) \) and the \( K_{\mu, \nu}(P) \). We shall give these equations in diagrammatic form, because our purpose here is only to present the important features of the subsequent analysis. The many details of this analysis are given more carefully in reference 16. The three algebraic equations are as follows:

\[
N_{1,1}(P) = \begin{array}{c}
\frac{P}{\omega} \\
\frac{P}{\omega}
\end{array} = \begin{array}{c}
\frac{P}{\omega} \\
\frac{P}{\omega}
\end{array} + k_{1,1} + k_{0,2} + k_{2,0} + k_{1,1}
\]

\[
N_{1,1}(P) = \begin{array}{c}
\frac{P}{\omega} \\
\frac{P}{\omega}
\end{array} = \begin{array}{c}
\frac{P}{\omega} \\
\frac{P}{\omega}
\end{array} + k_{1,1} + k_{0,2} + k_{2,0} + k_{1,1}
\]

where

\[
\nu(P) = \begin{array}{c}
\frac{P}{\omega} \\
\frac{P}{\omega}
\end{array}
\]

\[
\nu(P) = \begin{array}{c}
\frac{P}{\omega} \\
\frac{P}{\omega}
\end{array}
\]
\[ N_{0,2}(P) = N_{2,0}(P) = \begin{cases} \text{Diagram} \end{cases} \]
These equations appear in Fig. 9 of reference 21, and it is interesting to note that Beliavsky has obtained a similar set of equations in his treatment of the ground state of a degenerate Bose gas using the method of Green's functions. The argument for verifying the first line of eq. (51) is as follows. Consider the incoming external line to be the function $\nu (\underline{p})$. Then the first proper function which will be encountered will be either $K_{1,1} (\underline{p})$ or $K_{0,2} (\underline{p})$ except for the inhomogeneous term. The most general function which can attach to the either $N_{1,1} (\underline{p})$ or $N_{2,0} (\underline{p})$, respectively. Q.E.D. Alternatively, if the outgoing external line is taken to be the function $\nu (\underline{p})$, then one will derive the second line of (51). In a similar manner, one can verify each of the two lines of eqs. (53) and (54).

Having dealt with the case of proper and improper graphs, one next considers the internal structure of the functions $K_{\mu,\nu} (\underline{p})$. This internal structure may include many "improper parts" in the sense that cutting any two solid lines may separate a proper graph into two parts. This leads us to introduce the concept of reducible and irreducible graphs.

A $(\mu, \nu)$-graph is called reducible if by cutting any two of its solid lines open the entire graph can be separated into two (or more) disconnected parts, at least one of which is a $(1, 1)-$, $(0, 2)-$, or $(2, 0)$-graph. A $(\mu, \nu)$-graph which is not reducible is called irreducible. With each of its
internal solid lines representing a factors \( N_{1,0} (P) \), 
\( N_{0,2} (P) \), or \( N_{2,0} (P) \). An irreducible 
(\( \mu, \nu \))-graph, which is clearly also a proper graph, is 
called a dual graph because each of its solid lines now carries 
two arrows, as in eqs. (51) – (54). Some examples of irreducible 
dual (\( \mu, \nu \))-graphs are given in Fig. 3 of reference 16.

One can show in a straightforward manner\(^{16}\) that the 
functions \( K_{\mu,\nu} (P) \) of Eq. (50) are also given by the 
extpression.

\[
K_{\mu,\nu}(P) = \sum_{Q=1}^{\infty} \left[ \text{all different } Q^{th} \text{ order irreducible dual} \right. \\
\left. (\mu, \nu) \right. \left. \text{-graphs.} \right] \sum_{P} 
\]

where (\( \mu + \nu \) = 2. With the introduction of eq. (55) the en-
tire self-energy structure, with respect to solid lines, of the 
functions \( N_{\mu,\nu}(P) \) has been collected together in the 
functions \( N_{\mu,\nu}(P) \) themselves. That is to say, the in-
ternal solid lines of irreducible dual (\( \mu, \nu \))-graphs are 
associated with the line factors \( N_{\mu,\nu}(P) \) and eqs. (51) – (54) have become a set of coupled integral equations. One may 
also express the grand potential (43) in terms of irreducible 
dual (\( \mu, \nu \))-graphs, but we shall not repeat the expression 
here. It is given in reference 16.


The above analysis of the self-energy structure with 
respect to solid lines can be viewed as an analysis of the self-
energy problem in so far as the Bose statistics of the particles is considered. But there is also an aspect of the self-energy problem which is due to the dynamics, or interactions, of the particles. This part of the problem is given by the wiggly-line self-energy structure.

In rule (vi) for linked-pair (μ, ν)-graphs, we have observed that conservation of momentum may require that some of the wiggly-line momenta in these graphs become identically zero. It is easy to see whenever this occurs that the (μ, ν)-graph can be separated into two parts by cutting the wiggly line. Such structures contributed to the zero-momentum self-energy problem, which has only a dynamical aspect there being no zero-momentum solid lines. See below eq. (43). A discussion of the zero-momentum self-energy problem will not be included here. Rather, we shall concentrate our attention on the wiggly-line self-energy structure of the functions Kμ,ν (P̅μ) eq. (55), which occurs for all momenta.

Corresponding to each irreducible dual (μ, ν)-graph, we next define an irreducible, dual (μ, ν)-graph with exactly the same structure and expression, but subject to the condition that we do not integrate over the temperature variables at the vertices to which the incoming external lines (if any) attach. Thus, we define

\[ L_{μ,ν}(t, t', K) = \sum_{Q=1}^{\infty} \left[ \text{all different } Q \text{-th order irreducible, dual } \right]_{L - \text{graphs}} \]

(56)
for \((\mu, \nu) = (1, 1), (0, 2), \text{ or } (2, 0)\). The generalization is such that the external lines of \((\mu, \nu)\) L-graphs may be either wiggly or solid, and this generalization to the case of external wiggly lines is important in the following development.

We adopt the convention that the temperature variable \((\text{in the position }) \ t_2\) is always to be associated with the momentum \(-K\), so that in the case of \((0, 2)\) and \((2, 0)\) L-graphs the temperature variable \(t_1\) is to be associated with the momentum \(-K\). It should be clear that \(L_{\mu, \nu}(t_2, t_1, K)\)

\[
= L_{-\mu, -\nu}(t_2, t_1, -K)
\] when \((\mu, \nu) = (0, 2)\) or \((2, 0)\) \(\text{ see also equations (48) and (49)}\). We note that there are \((0, 2)\) L-graphs in which both incoming lines attach at the same vertex and with these L-graphs we must include a \(\delta\)-function factor \(\delta(t_2 - t_1)\). Also, the \((\mu, \nu)\) L-graphs with external wiggly lines can have \(K = 0\) as well as \(K = P\).

In the particular case where both of the external lines are solid, then \(K = P\) only and equation (55) can be written in terms of the \(L_{\mu, \nu}(t_2, t_1, K)\) functions as follows.

\[
K_{1,1}(P) = \int_0^P dt_1 L_{1,1}(\beta, t_1, P)
\]

\[
K_{0,2}(P) = \int_0^P dt_2 \int_0^P dt_1 L_{0,2}(t_2, t_1, P)
\]

\[
K_{2,0}(P) = L_{2,0}(\beta, \beta, P)
\]
We now study the wiggly-line self-energy structure of the functions \( L_{\mu, \nu} (t_2, t_1, K) \) instead of the functions \( K_{\mu, \nu} (P) \). One can say somewhat loosely that the definition (56) has "fixed" this structure for study, because the wiggly lines "carry" temperature variables at their ends (See Fig. 1). In analogy with the definition of proper and improper graphs, above equation (50), for the study of the functions \( N_{\mu, \nu} (P) \) we now define regular and irregular graphs.

An irreducible dual \((\mu, \nu)\)-graph (or \(D\)-graph) is called \textit{irregular} if by cutting any one of its wiggly internal lines open the entire graph can be separated into two disconnected graphs. Otherwise, the \((\mu, \nu)\)-graph is called \textit{regular} (provided that the zero-momentum self-energy structure has already been grouped into zero momentum factors\(^{20}\)).

With these definitions in mind, we define three functions \( K_{\mu, \nu} (t_2, t_1, K) \) as follows (compare with equation (50))

\[
K_{\mu, \nu} (t_2, t_1, K) = \sum_{Q=1}^{\infty} \left[ \text{all different } q^{th} \text{ order regular } L\text{-graphs} \right] K
\]

We may now write down a set of simple integral equations which relate the functions of equations (56) and (58) by means of their temperature variables. These can be written down in complete analogy with the eqs. (51) - (54), and they are given as eqs. (56) - (59) and in Figs. 5 - 7 in reference 16. An alternate,
and more useful to the subsequent development, form of these integral equations can be given as follows. When \( \langle X \rangle = 0 \), then \((\mu, \nu)\)-graphs with \( \mu \neq \nu \) do not occur in the theory and one can "generate" all wiggly-line self-energy structures with the following two equations.

\[
L(t_2, t_1, K) = \delta(t_2 - t_1) + L(t_2, t_1, K)
\]

(59)

where the temperature variable \( S \) on the RHS of (59) is to be integrated from \( \sigma \) to \( \beta \), and where

\[
G(t_2, t_1, K) = \delta(t_2 - t_1) + L(t_2, t_1, K)
\]

(60)

But, for \( \langle X \rangle \neq 0 \), we are not interested so much in the function \( L(t_2, t_1, K) \) as in the \( L_{\mu, \nu}(t_2, t_1, K) \). Nevertheless, the function \( L(t_2, t_1, K) \) enter 3 into our considerations. Defining

\[
G_{1,1}(t_2, t_1, K) = \delta(t_2 - t_1) + L_{1,1}(t_2, t_1, K)
\]

(61)

in analogy with eq. (60), one can show graphically that the integral equations for \( L_{\mu, \nu}(t_2, t_1, K) \) when \( (\mu, \nu) = (0, 2) \) and \((2, 0)\) are
where the temperature variables $S_1$ and $S_2$ are each to be integrated from $0$ to $\beta$. The functions $K^{(1)}_{0,2}(t_2, t_1; K)$ and $K^{(1)}_{2,0}(t_2, t_1; K)$ are quantities which must be subtracted in the special case that the external lines form a wiggly-line double-bond \textit{[see rule (i) for linked-pair $(\mu, \nu)$-graphs\textsuperscript{[22]}].}

Note that the forms of equations (62) and (63) in which $G$ and $G_{11}$ are interchanged are also valid.
The integral equation for $L_{1,1}(t_2, t_1, K)$ can be written down in analogy with equation (59) as

\[ L_{1,1}(t_2, t_1, K) = G_{1,1}(t_2, t_1, K) \]

(64)

where one can show graphically that the function $P(t_2, t_1, K)$ must be given by

\[ P(t_2, t_1, K) = K_{1,1}(t_1, K) + K_{2,0}(t_1, K) + G(t_2, t_1, K) \]

(65)
Equations (59) - (65) are the basic integral equations which govern or group together, the wiggly-line self-energy structure. Complete Self-Energy Problem.

We have no yet dealt with the internal structure of the functions $K_{\mu, \nu}(t_2, t_1, k)$, defined by eq. (58). This internal structure may include many "irregular (\(\mu, \nu\))-parts" in the sense that cutting any such resulting part for which \((\mu + \nu) = 2\). The sum over all possible irregular (\(\mu, \nu\))-parts is defined to be a function $\mathcal{O}_{\mu, \nu}(t_2, t_1, k)$.

An argument similar to that given for eq. (51) can be made to verify the following expression for

\[
\mathcal{O}_{1,1}(t_2, t_1, k) \equiv t_1 = G_{1,1} + G_{1,0} N_{1,1} + G_{1,0} N_{1,2} + G_{1,0} L_{1,0} + G_{1,0} L_{2,0} + G_{1,0} L_{2,0}
\]
where \( k \rightarrow p \) for the terms in which \( k \neq 0 \). One can also write down explicit expressions for the functions

\[
G_{0,2}(t_2, t_1, K) \equiv \begin{array}{c}
\frac{1}{k - k} \\
K
\end{array}, \quad G_{2,0}(t_2, t_1, K) \equiv \begin{array}{c}
\frac{1}{k} \\
K - k
\end{array}
\]

Such expressions are given in reference 16.

It is important to emphasize that the complete self-energy problem involves the grouping together of all possible self-energy structures into the functions \( G_{\mu, \nu}(t_2, t_1, K) \). In these functions the effects of statistics (solid lines) and dynamics (wiggly lines), which have been treated separately until now, are completely mixed together. One can proceed in the analysis to show that the functions \( K_{\mu, \nu}(t_2, t_1, K) \) and the grand potential may be written in terms of master \((\mu, \nu)\)-graphs. In these graphs there is only one kind of line, the double arrowed solid lines of equa. (66) and (67) which represent the functions \( G_{\mu, \nu}(t_2, t_1, K) \). Master \((\mu, \nu)\)-graphs are also irreducible i.e., topologically, they are the class of irreducible, dual graphs which have no wiggly lines [See above eq. (55)]. We shall not pursue the analysis of the master-graph formulation of quantum statistics further here, because our
primary interest is now to discuss the integral equations (59) - (65). Suffice it to say that the master-graph formulation represents the final step in the combinatorial analysis of the self-energy problem 16).

*Fundamental Integral Equations.*

Although the integral equations (59) - (65) are a set of coupled integral equations in the temperature variables, the discussion which we shall now give requires the consideration of only eq. (64). This equation can be written in terms of functions as

\[ \mathcal{L}_{1,1} (\tau_2, \tau_1, \kappa) = \int_0^\beta \, ds \, G_{1,1} (\tau_2, s, \kappa) \mathcal{P} (s, \tau_1, \kappa) \]  

where \( G_{1,1} (\tau_2, s, \kappa) \) is defined by eq. (61) and \( \mathcal{P} (\tau_2, \tau_1, \kappa) \) is defined by eq. (65). Now, when \( \langle X \rangle = 0 \), eqs. (68) and (61) reduce to eqs. (59) and (60), respectively. In this case, the analysis which we shall now outline 23) becomes much simpler. It has been given by Mohling 24). For the problem of a degenerate Fermi system, as well as for a degenerate Bose system with \( \langle X \rangle = 0 \).

We consider now a special class of terms which occurs in the function \( \mathcal{P} (\tau_2, \tau_1, \kappa) \), and we shall define the sum of these terms to be \( \mathcal{P}_o (\tau_2, \tau_1, \kappa) \). The general form of \( \mathcal{P}_o (\tau_2, \tau_1, \kappa) \), for the case when the two-particle interaction does not include an infinite repulsive core 25), is then
\[
\begin{align*}
P_{o}(t_{2}, t_{1}, k_{\omega}) &= \left[ A(k_{\omega}) + C(k_{\omega}) \right] \Theta(t_{2} - t_{1}) + \\
&\quad C(k_{\omega}) e^{(t_{2} - t_{1})D(k_{\omega})} \Theta(t_{1} - t_{2}) - C(k_{\omega}) e^{-t_{1}D(k_{\omega})}
\end{align*}
\]  

where the functions \( A, C, \) and \( D \) may have a dependence on \( \beta \), although this has not been explicitly indicated in (16). It is unimportant for \( T \approx 0 \). One may demonstrate the existence of each of the terms in eq. (69) by a simple lowest order calculation\(^{23}\) of each of the functions \( K_{\mu, \nu}(t_{2}, t_{1}, k_{\omega}) \) which contribute to eq. (65).

Consider next the consequence of substituting eq. (69) for \( P_{o}(t_{2}, t_{1}, k_{\omega}) \) into the integral eq. (68). We shall define the corresponding solution to this integral equation to be

\[
L_{o}(t_{2}, t_{1}, k_{\omega})
\]

Then

\[
L_{o}(t_{2}, t_{1}, k_{\omega}) = \int_{0}^{\beta} ds \, G_{o}(t_{2}, s, k_{\omega}) \, P_{o}(s, t_{1}, k_{\omega})
\]

\[
G_{o}(t_{2}, t_{1}, k_{\omega}) = \delta(t_{2} - t_{1}) + L_{o}(t_{2}, t_{1}, k_{\omega})
\]

The solution to the integral equation (70) is of the form, suppressing the \( k_{\omega} \)-dependence in the notation,

\[
G_{o}(t_{2}, t_{1}) = \begin{cases} \\
\delta(t_{2} - t_{1}) + \Delta_{+} C^{(\times)}_{+}(t_{2}) e^{-t_{1}\Delta_{+}} & \text{for } t_{2} > t_{1} \\
- \Delta_{-} C^{(\times)}_{-}(t_{2}) e^{-t_{1}\Delta_{-}} & \text{for } t_{2} < t_{1} \end{cases} + \begin{cases} \\
\Delta_{+} C^{(<)}_{+}(t_{2}) e^{-t_{1}\Delta_{+}} & \text{for } t_{2} > t_{1} \\
- \Delta_{-} C^{(<)}_{-}(t_{2}) e^{-t_{1}\Delta_{-}} & \text{for } t_{2} < t_{1} \end{cases} \Theta(t_{1} - t_{2})
\]
Explicit expressions for the coefficients $\mathcal{C}_{\pm}(t_2)$ and $\mathcal{C}_{\pm}(t_1)$ are derived in reference 23, and the functions $\Delta_{\pm}(K)$ are given by

$$\Delta_{\pm} = \frac{1}{2}(A+D) \mp \frac{1}{2} \left[ (D-A)^2 - 4 \ C \ D \right]^{1/2}$$

(72)

Equation (70) is the fundamental integral equation of the theory. We shall indicate below how the solution (71) to this integral equation can be used to transform the entire quantum statistical theory to a form which is amenable to a perturbation treatment. It is extremely important to observe that at very low temperatures it is necessary to derive the solution (71). For this solution involves temperature exponential factors $\exp(t_1, K)$, where $\Delta_{\pm}(K)$ is well-defined in the limit $P \to \infty$.

Then, at very series expansion of this temperature exponential is valid. Moreover, since each of the functions $A, C,$ and $D$ enters into the expression (72) for $\Delta_{\pm}$ it is necessary to include all of the selected terms in the function

$$P_{\pm}(t_2, t_1, K)$$

of (69). Other terms in $P(t_2, t_1, K)$ eq. (65), do not lead to temperature exponential solutions (71),
i.e., to a divergent power series in the iterated form of (70) or (68).

It is, perhaps, not completely clear how the solution (71) must be used in the calculation of thermodynamic quantities and distribution functions for a degenerate Bose system. The method of calculation is to use this solution and a corresponding dominant solution to equation (59) in a first approximate calculation of the functions $L_{\mu,\nu}(t_2, t_1, \omega)$ of equations (62) and (63), and of the functions $G_{\mu,\nu}(t_2, t_1, K)$ of equations (66) and (67). But, in the master-graphs, mentioned below eq. (67), these latter functions are line factors which cannot the vertex-functions (40) of the theory. Thus, except for overall multiplying factors which one must introduce, one is to consider integrals of the following type.

$$\begin{bmatrix} K_1 & K_2 \\ K_3 & K_4 \end{bmatrix} = \int t_1 t_2 G_0 G_0 S_2 S_1$$

In the graphical equation (73) one must perform two temperature integrations over the variables $S_2$ and $S_1$ which are the "upper"
temperature-variables of a vertex-function (40). The function (73) is called a transformed pair-function.

One finds that the integral (73) has the effect of introducing more terms of the type $P_o(t_2, t_1, k)$ into the theory, in addition to those which one starts with in the explicit computation of eq. (69). In other words, the solution (71) does not include all of the dominant terms of the theory, because in the application of this solution one obtains more terms of the same "order of magnitude". Clearly, one is dealing with a "circular path, and it would seem to be impossible to complete circle" with one step. In fact, it is possible to complete the circle, by using the $\Lambda$ -transformation which we discuss next.

$\Lambda$ -Transformation.

The $\Lambda$ -transformation is an integral transformation of the entire quantum statistical theory (in the master-graph formulation) which insures that the integrals (73). The $\Lambda$ -transformation also insures that all "large" terms, of the form

$$\Lambda (t_2, t_1, k)$$

instead of

$$P_o(t_2, t_1, k)$$

are subtracted from the self-energy structures of the theory. These substracted terms then appear elsewhere in the theory, in the expressions for physics quantities.

The emphasis in the $\Lambda$ -Transformation is on the function $G_o(t_2, t_1, k)$, eq. (71), whose coefficients are to be determined after the $\Lambda$ -Transformation instead of before. In other words, the various quantities in the function $G_o(t_2, t_1, k)$ become unknowns and the role of the function
is eliminated. In order to see how these statements can be true, it is best to proceed directly with the equations of the $\Lambda$-transformation.

One first defines two auxiliary quantities $\mathcal{S}(t_2, t_1, k)$ and $\mathcal{E}(t_2, k)$ as follows:

$$
\mathcal{S}(t_2, t_1, k) \equiv e^{-t_2 \mathcal{E}(k)} \int_0^{\beta} dt_1 \mathcal{G}_0(t_2, t_1, k) \tag{74}
$$

$$
= e^{-t_2 \mathcal{E}(k)} \left[ C_+(t_2, k) - C_-(t_2, k) \right]
$$

$$
\mathcal{E}(t_2, k) \equiv \omega(t_2, k) + \Delta^0 \tag{75}
$$

where we have used eq. (71) to derive the second line of (74). The quantity $-\Delta^0$ is a self-energy which arises from the treatment of the zero-momentum self-energy problem. See discussion above eq. (56). It is introduced here, because in the formal development of reference (23) all single-particle energies are expressed relative to the zero-momentum particle energies.

The basic equation of the $\Lambda$-transformation when $\langle x \rangle \neq 0$ is

$$
\mathcal{G}_{ij}(t_2, t_1) = \mathcal{S}(t_2) e^{t_2 \mathcal{E}} \int_0^{\beta} ds \mathcal{G}_{ij}(t_2, s) \mathcal{S}^{-1}(s) e^{-s \mathcal{E}} \mathcal{G}_0(s, t_1) \tag{75}
$$
in which a new function \( G_{1,1}'(t_2, t_1, K) \) is defined and the momentum variable \( K \) has been suppressed in the notation. Disregarding the factors \( \mathcal{S} e^{t_1 \xi} \), the graphical representation of this equation is:

\[
\begin{align*}
G_{0,2} & = G_{1,1}'(t_2, t_1, K) \quad (76a)
\end{align*}
\]

The significance of eq. (76) is or (76a) is that since \( G_0 \) is supposed to contain all of the large terms of the self-energy structures, when one realizes that the function \( G_{1,1}' \) and the difficulties presented by \( G_{0,2} \) and \( G_{1,1}' \) are merely technical in nature, \( \mathcal{J} \) occurs along all of the internal lines of master-graphs.

It can easily be shown that eq. (76) leads to a striking result by the following manipulations. If one defines

\[
L_{1,1}'(t_2, t_1, K) \quad \text{by the equation}
\]

\[
G_{1,1}'(t_2, t_1, K) \equiv \delta(t_2 - t_1) + L_{1,1}'(t_2, t_1, K) \quad (77)
\]

then eq. (76) can be rearranged to the form

\[
L_{1,1}'(t_2, t_1) = \mathcal{J}(t_2) e^{-t_2 \xi} \mathcal{L}_{1,1}(t_2, t_1) \mathcal{J}(t_1) e^{t_1 \xi} - \int_0^\beta ds G_{1,1}'(t_2, s) \Lambda(s, t_1) \quad (78)
\]
where eq. (61) has been used and where the function \( \Lambda(t_2, t_1, \kappa) \) is defined by the equations,

\[
G_\Delta(t_2, t_1) = \delta(t_2 - t_1) + e^{t_2 - t_1} \int_s F(t_2) \Lambda(t_2, t_1) G(t_1) e^{-t_1 \kappa} \tag{79}
\]

one next substitutes eq. (76) into eq. (68) to obtain

\[
L_{1,1}(t_2, t_1) = \delta(t_2) e^{t_1 \kappa} \int_0^\beta ds \int_s G'_{1,1}(t_2, s) P(s, t_1) G^{-1}(t_1) e^{-t_1 \kappa} \tag{80}
\]

where

\[
P'(t_2, t_1) = G^{-1}(t_2) e^{-t_1 \kappa} \int_0^\beta ds \int_s G_\Delta(t_2, s) P(s, t_1) G(t_1) e^{-t_1 \kappa} \tag{81}
\]

The significance of the function \( P'(t_2, t_1, \kappa) \) is that it is related to the transformed pair-functions (73) in precisely the same manner as the function \( P(t_2, t_1, \kappa) \) eq. (65) is related to the "untransformed" vertex-function (40).

Thus, the \( \Lambda \) -transformation has the effect of replacing the entire set of untransformed functions, introduced prior to eq. (69), into a set of transformed functions. For the many details of this \( \Lambda \) -transformation one must refer to reference 23, but one can understand the fundamental importance of the \( \Lambda \) -transformation by performing one further manipulation. One substitutes eq. (80) into (73) to arrive at the result.

\[
L_{1,1}'(t_2, t_1) = \int_0^\beta ds \int_s G'_{1,1}(t_2, s) P'(s, t_1) \tag{82}
\]
where

\[ P'(t_2, t_1) = G'(t_2, t_1) - \Lambda(t_2, t_1) \]  \hspace{1cm} (83)

Equation (83) allows for the subtraction from \( G'(t_2, t_1) \) of all of those terms which, when iterated, would give large contributions to \( L_{1,1}(t_2, t_1) \) at very low temperatures. Clearly, the function \( \Lambda(t_2, t_1) \) is related to \( G'(t_2, t_1) \) in the same manner as the function \( P_o(t_2, t_1) \) of eq. (69) is related to \( P(t_2, t_1) \). The major difference is that the \( \Lambda \) transformation has permitted us to complete the circle as discussed below eq. (73).

Equation (82), which is analogous to the untransformed eq. (68), can now be solved by iteration because the function \( P'(t_2, t_1, k) \) includes only "small" terms. The explicit form of the "large" terms \( \Lambda(t_2, t_1, k) \) is found by combining eqs. (71) and (79) to be:

\[ \Lambda(t_2, t_1) = \mathcal{J}^{-1}(t_2) \mathcal{J}(t_1) \left\{ \left[ \Delta_+ A_+^{(>)}(t_2) \right] e^{t_1 \varepsilon_+} - \Delta_- A_-^{(<)}(t_2) e^{t_1 \varepsilon_-} \right\} \Theta(t_2 - t_1) \]

\[ + \left[ \Delta_+ A_+^{(<)}(t_2) - \Delta_- A_-^{(>)}(t_2) e^{t_1 \varepsilon_-} \right] \Theta(t_1 - t_2) \]

where

\[ A_\pm^{(<)}(t) = e^{-t \varepsilon} C_\pm^{(<)}(t) \]

\[ A_\pm^{(>)}(t) = e^{-t \varepsilon} C_\pm^{(>)}(t) \]

(85)
and
\[
\mathcal{E}_\pm (k_m) = \mathcal{E}(k_m) - \Delta_\pm (k_m) = \omega(k_m) - \Delta_\pm (k_m) + \Lambda \omega(k_m) \tag{66}
\]

As indicated above eq. (74), the functions \(
\Delta_\pm, A_{\pm}^{(\leq)}(t_2)\)
and \(A_{\pm}^{(\geq)}(t_2)\) are treated as unknowns in the \(\Lambda\) transformation. They are determined by the requirement that all large terms in \(\mathcal{G}'(t_2, t_1)\) eq. (81), be of the form of eq. (84). In application this requirement seems to be a completely consistent one, although consistency has not been rigorously proved.

The two energies \(\mathcal{E}_\pm (k_m)\) which have now appeared in the theory include three terms. The first term is the free-particle kinetic energy \(\omega(k_m)\). The second term is a self-energy \(-\Delta_\pm (k_m)\) which is due to the interaction of a particle having momentum \(k_m \neq 0\) with the rest of the degenerate Bose system. The third term is the zero-momentum eq. (75). One would like to interpret the energies \(\mathcal{E}_\pm (k_m)\) as quasi-particle energies (see discussion at the beginning of this third lecture), but the reason why two energies \(\mathcal{E}_+(k_m)\) and \(\mathcal{E}_-(k_m)\) have appeared is not yet understood. It is interesting to note that for a dilute gas of hard sphere Bosons, one obtains the expression
\[
\mathcal{E}_\pm (k_m) = \pm \frac{\hbar^2}{2M} \left( k^2 + 4\pi n \frac{\xi^2}{2} \sigma \right)^{\frac{1}{2}} k \tag{87}
\]
where \( \zeta_\nu(\sim \eta^{-1}\langle x \rangle) \) gives rise to the fraction of Bosons in the zero-momentum state at any temperature. This result is well-known for the positive energy case. Using eq. (87) one can see that the temperature exponentials of eq. (84), for \( \kappa \sim (\hbar \alpha) \sqrt{2} \) involve the large parameter \( \eta \alpha \sqrt{2} \gg 1 \) mentioned at the beginning of this lecture.

The \( \Lambda \) -Transformation also transforms the function \( \nu(P) \) of eq. (41) into a function \( \nu'(P) \) which is given by

\[
\nu'(P) = \frac{\mathcal{F}(\beta, P)}{1 - \mathcal{F}(\beta, P)}
\]

where \( \mathcal{F}(\beta, P) \) is given by eq. (74). We return now to the discussion above eq. (47). It is still true, even after the \( \Lambda \) -Transformation, that the difference \( \langle \nu(P) \rangle - \nu'(P) \) is a not small function. But this fact is now not associated with a series of divergent terms. Rather, it is due to the mixing of the functions \( N_{\mu, \nu}(P) \) by the set of eqs. (51) - (54), which occurs when one solves for \( N_{\mu, \nu}(P) \) and substitutes the result (after the \( \Lambda \) -Transformation) into eq. (47). In fact, the function \( \nu'(P) \) is well-defined for all \( P \), having only a simple \( P^{-2} \) singularity as \( P \to 0 \).

One may say, quite generally that the \( \Lambda \) -Transformation has succeeded in bringing the quantum statistical theory to a well-defined form. That is, it has achieved a complete regrouping of entire infinite series. So that a simple perturbation theory can be applied in terms of the graphs of the transformed theory. One has every reason to believe, therefore, that a simple microscopic quasi-particle picture of the degenerate Bose system can
be derived from the transformed theory, although this has not yet been done. This is the conviction which has been expressed in the introduction to this third lecture.

As a concluding remark, we state a remarkable theorem which has been proved by Lee and Yang. The theorem (in the interaction representation) states that if, as \( \mathcal{J} \to \infty \) the solution to eq. (15) yields \( x = \langle x \rangle \) for \( \langle x \rangle \) real and positive, then at \( x = \langle x \rangle \) the solution to the integrals eqs. (51) - (54) satisfies the identities

\[
\lim_{P \to 0} \left[ N_{11}^{-1}(\mathcal{P}) \right] = 0
\]

\[
\lim_{P \to 0} \left[ N_{11}^{-1}(\mathcal{P}) N_{0,2}(\mathcal{P}) e^{\beta g} \right] = -1
\]

(89)

The first of these identities shows that the momentum distribution \( \langle \mathcal{N}(P) \rangle \), eq. (47), exhibits a singularity at \( P = 0 \) when \( \langle x \rangle > 0 \). This consequence is consistent with the interpretation of the x-ensemble formulation in which \( \langle x \rangle \neq 0 \) corresponds to a macroscopic occupation of the zero-momentum state. The \( \Lambda \) transformation modifies these identities in only a minor way without changing this consequence.
REFERENCES

1. S.N. Bose, Zeits fur Phys. 26, 178 (1924); 27, 384 (1924).
4. See reference 3, pp. 40-53, for a complete analysis of the thermodynamics near and below $T_c$.
8. See reference 3, pp. 30-35, for an excellent discussion of this point.

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REFERENCES.


20. See Sec. 5 of reference 16.


22. See below Equation (59) in reference 16.


25. The expression (69) is valid for an arbitrarily strong, but finite, repulsive core. When one considers an infinite repulsive core, then correction terms enter into the pair-function (37) (see reference 187), which account for the fact that the two-particle wave-functions no longer form a complete set over all position space. Thus, these correction terms are excluded volume terms, and for a dilute gas their effect is negligible.

26. See sec. 6 of reference 23.

27. In this connection, see E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963); E. H. Lieb, Phys. Rev. 130, 1616 (1963). In which a "double" quasi-particle spectrum is obtained for a one-dimensional interacting Bose gas. These authors, incidentally, do not allow for a multiple occupation of the lowest momentum single-particle state in the ground state of the system, and this fact throws some doubt on the validity of their results.
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