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Degenerate Bose System. I. Quantum Statistical Theory*

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The theory of a degenerate system of interacting bosons is developed using the x-ensemble formulation of quantum statistics, previously introduced by Lee and Yang. Particular attention is devoted to the self-energy structure of the graphs of the theory, and it is shown that the complete analysis of this structure involves an intimate mixing of the effects of particle statistics and particle interactions. Therefore, the effect of statistics, which causes Bose-Einstein condensation, becomes mixed with the dynamics in a real system. A prescription is given for the grand potential in which all self-energy effects are included in the line factors of master graphs. An expression for the pair-distribution function of a degenerate Bose system is also derived.

1. INTRODUCTION

THE purpose of the present series of papers is to develop a microscopic theory of liquid helium four below the λ point (helium II). It is true that theories of liquid helium exist in the literature. The objective of the present work is not to replace these theories, but rather to supplement the understanding which they have already provided. For example, there is the extensive work of London, Landau, and others towards the development of a macroscopic or thermodynamic understanding of liquid helium.[1] 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, there is the work of Feynman[2] on the development of a microscopic theory of liquid helium II with the aid of variational calculations of the energy. In particular, the calculations of Feynman and Cohen[3] has produced a qualitative understanding of the elementary excitations in liquid helium II as first postulated by Landau.[4]

We shall only be concerned with the equilibrium properties of liquid helium II, and we shall not deal with the associated gaseous phase which exists when the temperature $T>0$. Moreover, in the present paper, attention is devoted to helium II only insofar as it is a degenerate Bose system. The methods of quantum statistics are applied to such a system with the hope that the generality of this approach will enable us to investigate the properties of helium II for all temperatures *including the transition temperature* T_λ. Thus, it is precisely in the analysis of the transition temperature region that previous theories have been inadequate. Moreover, even the most recent attempts[5] have still not been able to reproduce the experimentally-determined helium II excitation curve in the so-called roton region. These and other questions can be clarified by a correct microscopic theory of helium II.

One of the most important features of the macroscopic theories of helium II is the two-fluid model, first introduced by Tisza.[6] The microscopic interpretation of this model for an ideal 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 of the remaining bosons in nonzero momentum states. Thus, the two fluids represent a separation of two phases in momentum space in equilibrium with each other. This *momentum space ordering* is to be contrasted with the separation of phases in position space which occurs for most systems. The mechanism by which it is achieved is believed to be a Bose-Einstein condensation.

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[1] F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1954), Vol. II.

[2] R. P. Feynman, Phys. Rev. **91**, 1291 (1953); **91**, 1301 (1953); **94**, 262 (1954).

[3] R. P. Feynman and M. Cohen, Phys. Rev. **102**, 1189 (1956).

[4] L. Landau, J. Phys. (USSR) **11**, 91 (1947). See also J. Phys. (USSR) **5**, 71 (1941); **8**, 1 (1944).

[5] H. W. Jackson and E. Feenberg, Rev. Mod. Phys. **34**, 686 (1962).

[6] L. Tisza, Nature **141**, 913 (1938); see also Phys. Rev. **72**, 838 (1947).

Although the theoretical phenomenon of Bose-Einstein condensation is well known for a gas of free bosons, it is only recently that Lee and Yang[7] have explicitly demonstrated that Bose-Einstein condensation can occur for interacting bosons. The results which they have obtained for their model system, a dilute gas of hard-sphere bosons, provide one important check on the validity of any theory. Indeed, one can find many examples in the literature of papers where their zero-temperature expressions are duplicated by different methods.

The pseudopotential method used by Lee and Yang to study the gas of hard-sphere bosons has no simple generalization to the case of helium II.[8] However, another approach developed by Lee and Yang for this problem does lend itself to such a generalization. This is their x-ensemble formulation of quantum statistics,[9] and it is this approach which we shall pursue in the present work. The important new feature of the x-ensemble formulation is that it introduces into the grand partition function from the very beginning the possibility of the macroscopic occupation of a single quantum state. The quantity x is the density of zero-momentum particles for a Bose system at rest.

The use of the x-ensemble formulation of quantum statistics by no means requires that the average value $\langle x\rangle > 0$. Thus, when $\langle x\rangle = 0$, the x-ensemble formulation reduces to the usual grand canonical ensemble of quantum statistics. In Sec. 2, the x-ensemble formulation is reviewed, along with the basic equations of quantum statistics, in order to specify with care the notation and underlying concepts of our work.

In Sec. 3 we make our first departure from the directions indicated by Lee and Yang by deriving the linked-pair expansion of the grand potential. In this expansion, the grand potential is directly expressed in terms of the pair functions defined by Eqs. (18)–(20). The pair function is a quantity closely related to the binary collision kernel introduced by Lee and Yang in an earlier paper.[10] The difference between the present work and that of Lee and Yang is therefore not in the use of a two-particle function, but rather in our emphasis that the theory must be *exhibited* as an expansion in terms of this function. In the work of Lee and Yang[9] the effects of statistics and interactions are treated separately. More specifically, the grand potential is exhibited in terms of cluster functions U_N of Boltzmann statistics (this exhibits the effects of statistics or exchange), and then the U_N are separately expressed in terms of two-body functions (this exhibits the effect of interactions). The *necessity* of treating these two effects together is discussed below.

[7] T. D. Lee and C. N. Yang, Phys. Rev. **112**, 1419 (1958).
[8] See Kerson Huang, Phys. Rev. **115**, 765 (1959); **119**, 1129 (1960).
[9] T. D. Lee and C. N. Yang, Phys. Rev. **117**, 897 (1960). Hereafter referred to as LY V.
[10] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959).

The linked-pair expansion of the grand potential is not yet a major alteration of the expressions derived by Lee and Yang. Therefore, we are able to return to the "Lee-Yang direction" in Sec. 4 by adapting their analysis of the momentum distribution to our notation. This analysis emphasizes the importance of the momentum distribution (to an understanding of momentum space ordering) by expressing the grand potential in terms of three functions $N_{1,1}(\mathbf{p})$, $N_{2,0}(\mathbf{p})$, and $N_{0,2}(\mathbf{p})$. The first of these functions differs from the momentum distribution $\langle n(\mathbf{p})\rangle$ in only a minor way [see Eq. (31)]. The resulting formulation of the theory is called the dual graph expansion of the grand potential, and associated with this expansion is a set of integral equations for the functions $N_{\mu,\nu}(\mathbf{p})$.

The major contribution which is made in this paper starts from the observation that the analysis of the functions $N_{\mu,\nu}(\mathbf{p})$ is only *one* part of a larger problem which is the analysis of all self-energy structures in the graphs of the theory. Thus, the function $N_{\mu,\nu}(\mathbf{p})$ represents that part of a self-energy structure which arises, due to statistics. But there is also an equally important contribution to the self-energy structure which is due to the interactions, and this contribution cannot be omitted from the analysis. In fact, it is demonstrated in Sec. 6 that these two effects are entirely interrelated in the functions $\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{k})$ which represent the sum over all possible self-energy structures. These latter functions are the line factors in the master graph formulation of quantum statistics, where the master graphs are the appropriate generalization of the dual graphs (to the case when the effects of the interactions are explicitly considered). It is the mixing of the effects of statistics and interactions, carefully avoided by Lee and Yang, which results in the transition from a dual graph formulation to a master graph formulation of the theory. Thus, although Bose-Einstein condensation is due to the Bose statistics, the effect of the statistics is mixed with that due to the interactions in a real system.

It is to be emphasized that the final justification of the particular analysis made in this paper can only come from an *a posteriori* examination of the consequences, and this examination will be left to be discussed in the subsequent papers of this series. However, it can be said here that there are serious low-temperature divergences in the theory which have necessitated a regrouping of the terms in the original linked-pair expansions of quantum statistics. In the following paper, we identify the source of these divergences and transform the entire theory, by means of the Λ transformation, to a form in which the divergences no longer give any difficulty. We shall leave to this second paper the definition of the Λ transformation, and only remark here that our physical interpretation of the Λ transformation is that it transforms the theory from an expansion in terms of free-particle quantities to one in terms of quasiparticle quantities. Thus, the quasiparticles are the elementary excitations which are possible in the degenerate Bose system, and the divergent terms mentioned above reappear in the expressions for the quasiparticle interactions and their energy-momentum relations. Here again, we must qualify these remarks by saying that this physical interpretation can only be demonstrated by an *a posteriori* study of the consequences of the theory in an application to a real or model system. Nevertheless, we have given this interpretation now in order to justify the nomenclature "self-energy structures" as used above, for it is precisely these structures which are the source of the divergent terms in the denerate Bose system. Moreover, their treatment by the Λ transformation is certainly a mathematical necessity, and we believe that this treatment can only be successfully achieved in the master graph formulation of quantum statistics.

The discussion of the preceding three paragraphs has been entirely concerned with the nonzero momentum particles of the degenerate Bose system, i.e., with the "normal fluid." There is also a corresponding self-energy analysis which must be performed for the zero-momentum "superfluid," and this analysis is carried through in Sec. 5. To be sure, there can be no self-energy problem with the zero-momentum particles due to their statistics, for the very purpose of the x-ensemble formulation of quantum statistics is to eliminate zero-momentum exchange terms (see Sec. 2). Nevertheless, there is an important effect due to zero-momentum particle interactions, and the analysis of the associated zero-momentum self-energy structures results in the zero-momentum factors of Sec. 5.

As a final matter for this paper, an expression for the pair-distribution function in a degenerate Bose system is derived in Sec. 8. This derivation has been included, not only because it is an interesting application of the methods developed here, but also because the pair-distribution function has been experimentally determined by scattering experiments.[11]

2. x-ENSEMBLE FORMULATION OF QUANTUM STATISTICS

In the theory of the grand canonical ensemble of quantum statistics, one is able to calculate average values and their fluctuations of the energy E, the total particle number N, and other thermodynamic quantities for any given system. Moreover, one may also calculate the momentum distribution $\langle n_{\mathbf{k}}\rangle$, the pair-distribution function $P_2(\mathbf{r},\mathbf{r}')$, and any of the higher order correlation functions in any representation whatsoever. All of these quantities are available from a calculation of the grand partition function,

$$e^{\Omega f}=\sum_{N=0}^{\infty}\exp(\beta gN)\,\mathrm{Tr}_N[\exp(-\beta H^{(N)})]\,, \qquad (1)$$

and its various moments. In Eq. (1), g is the thermodynamic potential, $\beta=(\kappa T)^{-1}$, and Ω is the volume of the system. The symbol Tr_N indicates that the trace of $\exp[-\beta H^{(N)}]$ is to be taken over a complete set of N-particle state vectors. We shall assume that the N-particle Hamiltonian $H^{(N)}$ includes only two-particle interactions and, therefore, that interatomic electron exchanges[12] are completely unimportant for the low-temperature problems of interest in our work. The quantity f is called the grand potential, and it is assumed to be an intensive quantity, i.e., we assume that the limit as $\Omega\to\infty$ of $f(\beta,g,\Omega)$ exists. We shall consider only Bose systems in this paper.

It is characteristic of physics that to only know how to do something *in principle* is to not know how to do it in practice. Thus, in an application of Eq. (1) to the calculation of the grand potential for a degenerate Bose gas, Lee and Yang[9] have shown that ordinary methods of analysis fail completely. The reason for this failure is readily attributed by them to the macroscopic occupation of the zero-momentum state (in a system at rest). That is to say, if L is the number of bosons in the zero-momentum state in any given term of the trace of Eq. (1), then each of the $L!$ exchange terms corresponding to this given term gives an identical contribution. One then finds when $\langle L\rangle\sim\langle N\rangle\ggg 1$, that the normal Ursell expansion of the grand potential does *not* give an intensive quantity, as originally assumed. In fact, the grand potential appears to have horrible divergences in the limit $\Omega\to\infty$, even for a low-density system.

Lee and Yang have given the solution to the above difficulty by their x-ensemble formulation of the grand canonical ensemble,[9] in which the grand partition function is given by

$$\exp(\Omega f_x)=e^{-\Omega x}\sum_{N=0}^{\infty}\exp(\beta gN)\times\sum_{L=0}^{N}(x\Omega)^L(L!)^{-1}\,\mathrm{Tr}_{N,L}[\exp(-\beta H^{(N)})]\,, \qquad (2)$$

instead of by Eq. (1). In this equation, $\mathrm{Tr}_{N,L}$ means that the trace is to be taken only over those N-particle state vectors in which L particles have zero momentum. In their proof of Eq. (2) Lee and Yang have shown that if

$$\partial f_x/\partial x=0 \quad\text{at}\quad x=\langle x\rangle\equiv\Omega^{-1}\langle L\rangle>0\,, \qquad (3)$$

then $f_x(\beta,g,\Omega)=f(\beta,g,\Omega)$ in the limit $\Omega\to\infty$. If Eq. (3) is not satisfied, then $f_x=f$ at $\langle x\rangle=0$, and Eq. (2) reduces to Eq. (1) for all practical purposes. We see from (3) that the quantity x is the density of zero-momentum particles.

It is easy to show how the x-ensemble formulation (2) is obtained. The motivating step is to eliminate the

[11] D. G. Hurst and D. G. Henshaw, Phys. Rev. **100**, 994 (1955).

[12] See M. Girardeau, J. Math. Phys. **4**, 1096 (1963).

troublesome factor $(L!)$ from the $\mathrm{Tr}_{N,L}$. 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 potential must be those with $L\sim\langle L\rangle$. One can, of course, only verify this statement by showing in an *a posteriori* calculation that the fluctuation $\langle(\Delta L)^2\rangle$ in the number of zero-momentum particles is $\sim\langle L\rangle$ [see Sec. 8 or prove directly from Eq. (2)]. One next multiplies the $\mathrm{Tr}_{N,L}$ in the grand partition function by the Poisson distribution of L about its average value $\langle x\rangle\Omega$ (which is essentially unity for important L values). One finally replaces $\langle x\rangle\Omega$ by $x\Omega$, thereby treating x as a variable whose average value can be obtained by the maximum condition (3).

It is now useful to introduce the interaction representation into Eq. (2) by defining the operator

$$W_N(\beta)\equiv\exp(\beta H_0{}^{(N)})\exp(-\beta H^{(N)}), \tag{4}$$

which is unity for free particles. The grand partition function (2) can then be written in the form

$$e^{\Omega f}=e^{-\Omega x}\sum_{N=0}^{\infty}(N!)^{-1}\exp(\beta gN)\times\sum_{\mathbf{k}_1\cdots\mathbf{k}_N}\exp(-\beta\sum_{i=1}^{N}\omega_i)W_x{}^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N\\ \mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N\end{pmatrix}, \tag{5}$$

where the subscript x has now been dropped from the grand potential, and where $\omega_k=\hbar^2k^2/2M$. The matrix elements of $W_N(\beta)$ are given by the symmetrized expression

$$W_x{}^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N\\ \mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N\end{pmatrix}=(x\Omega)^L(L!)^{-1}W^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N\\ \mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N\end{pmatrix}, \tag{6}$$

where

$$W^{(S)}\begin{pmatrix}\mathbf{k}_1\,\mathbf{k}_2\cdots\mathbf{k}_N\\ \mathbf{k}_1'\mathbf{k}_2'\cdots\mathbf{k}_N'\end{pmatrix}\equiv\sum_{P'}P'\langle\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N|W_N(\beta)|\mathbf{k}_1'\cdots\mathbf{k}_N'\rangle, \tag{7}$$

in which $\sum_{P'}$ denotes the sum over all permutations of the primed indices.

In order to caclulate the various distribution functions in position space, one requires not only the diagonal matrix elements (6) but also off-diagonal matrix elements. Thus, for the pair-distribution function, one must be able to calculate the (symmetrized) off-diagonal elements $\langle\mathbf{k}_1\mathbf{k}_2|\rho_2|\mathbf{k}_1'\mathbf{k}_2'\rangle$ of the density matrix

$$\rho=e^{-\Omega f}e^{\beta gN}\exp(-\beta H^{(N)}). \tag{8}$$

The momenta of these "reduced" density matrices[13] are fixed, or given, momenta which are not summed over, and we shall call them *external* momenta. We let L_e be the number of external unprimed momenta which are zero, and let L_e' be the number of external primed momenta which are zero. Then the off-diagonal generalization of (6) can easily be written down by referring to the argument given below Eq. (3).

$$W_x{}^{(S)}\begin{pmatrix}\mathbf{k}_1\,\mathbf{k}_2\cdots\mathbf{k}_N\\ \mathbf{k}_1'\mathbf{k}_2'\cdots\mathbf{k}_N'\end{pmatrix}=(x\Omega)^{L+L_e+L_e'}[(L+L_e')!]^{-1}[(L_e+L)(L_e+L-1)\cdots(L+1)]^{-1}W^{(S)}\begin{pmatrix}\mathbf{k}_1\,\mathbf{k}_2\cdots\mathbf{k}_N\\ \mathbf{k}_1'\mathbf{k}_2'\cdots\mathbf{k}_N'\end{pmatrix}, \tag{9}$$

where L, L_e, and L_e' are determined in any application of (9) to the calculation of reduced density matrix elements. For example, the matrix elements $\langle\mathbf{k}_1\mathbf{k}_2|\rho_2|\mathbf{k}_1'\mathbf{k}_2'\rangle$ are given by

$$\langle\mathbf{k}_1\mathbf{k}_2|\rho_2|\mathbf{k}_1'\mathbf{k}_2'\rangle=e^{-\Omega f}e^{-\Omega x}\sum_{N=2}^{\infty}[(N-2)!]^{-1}\exp(\beta gN)\sum_{\mathbf{k}_3\cdots\mathbf{k}_N}\exp(-\beta\sum_{i=1}^{N}\omega_i)W_x{}^{(S)}\begin{pmatrix}\mathbf{k}_1\,\mathbf{k}_2\,\mathbf{k}_3\cdots\mathbf{k}_N\\ \mathbf{k}_1'\mathbf{k}_2'\mathbf{k}_3\cdots\mathbf{k}_N\end{pmatrix}, \tag{10}$$

where there are $N(N-1)$ ways of choosing the positions of $\mathbf{k}_1$ and $\mathbf{k}_2$ in the matrix elements of $W_N(\beta)$, all of which are equivalent. One then chooses the identity permutation in (7) so that $\mathbf{k}_1'$ and $\mathbf{k}_2'$ also occur in the first two columns and observes that the remaining bottom row momenta are internal momenta which are equal to the corresponding top row momenta. We shall return to Eq. (10) in Sec. 8.

We complete this section by writing down expressions for some of the thermodynamic functions when the grand potential is expressed in terms of the independent variables β, g, and x.

Pressure

$$\mathcal{P}=\beta^{-1}(\partial/\partial\Omega)(\Omega f). \tag{11}$$

Particle density

$$n\equiv\langle N\rangle/\Omega=\beta^{-1}(\partial f/\partial g). \tag{12}$$

Energy per particle

$$\langle E\rangle/\langle N\rangle=g-n^{-1}(\partial f/\partial\beta). \tag{13}$$

Entropy

$$S=(\partial/\partial T)(\beta^{-1}\Omega f). \tag{14}$$

One must be very careful to observe that in Eqs. (3), (13), and (14) the thermodynamic potential g is treated as an *independent* variable. It will be seen, however, that

[13] See C. N. Yang, Rev. Mod. Phys. 34, 694 (1962).

our method of analysis is such that an expression for the thermodynamic potential in terms of β and x is explicitly substituted into the formalism. This is equivalent to a transition from the variables β, g, and x to the independent variables β and x. In this case we must write Eqs. (3), (13), and (14) as

$$\partial f/\partial\xi=(\partial f/\partial g)(\partial g/\partial\xi)=n\beta(\partial g/\partial\xi)\,,\quad \text{for}\quad \xi>0\,, \tag{3'}$$

$$\langle E\rangle/\langle N\rangle=g-n^{-1}(\partial f/\partial\beta)+\beta(\partial g/\partial\beta)\,, \tag{13'}$$

$$S=(\partial/\partial T)(\beta^{-1}\Omega f)-n\Omega(\partial g/\partial T)\,, \tag{14'}$$

where we have introduced the parameter

$$\xi\equiv x/n\,, \tag{15}$$

which is the fraction of bosons in the zero-momentum state.

3. LINKED-PAIR EXPANSION OF GRAND POTENTIAL

In a previous paper[14] we have written down an explicit expression for the grand potential for the case $\langle x\rangle=0$ in terms of the elementary two-body interactions of the system. The generalization of this result to a degenerate Bose system, with $\langle x\rangle\neq 0$, is

$$\Omega f(x,\beta,g,\Omega)=\Omega f_0(\beta,g,\Omega)-x\Omega+x\Omega e^{\beta g}+\sum_{Q=1}^{\infty}[\text{all different } Q\text{th order linked-pair (0,0) graphs}]\,, \tag{16}$$

where the free-particle grand potential for the nonzero-momentum particles is given by

$$\Omega f_0(\beta,g,\Omega)=-\textstyle\sum_{\mathbf{p}}\ln[1-\exp\beta(g-\omega_{\mathbf{p}})]\,. \tag{17}$$

We shall henceforth adopt the convention of LY V that whenever a momentum $\mathbf{k}$ *does not* take the value zero it will be represented by $\mathbf{p}$. This convention is quite convenient, and it also emphasizes the special treatment of the zero-momentum particles.

Before proceeding with the proof of Eq. (16), it is necessary to define linked-pair (0,0) graphs. In this connection, it is also useful to define linked-pair (μ,ν) graphs, where μ and ν may take on any integer values (including zero). We shall be interested in (0,0), (1,1), (0,2), (2,0), (1,2), (2,1), and (2,2) graphs.

It is first necessary to define the *pair function* which is the vertex function of the theory.

$$\begin{aligned}{}^{t_1t_2}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0}&\equiv\theta(t_1-t_2)\,{}^{t_2}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0}\theta(t_2-t_0)+\theta(t_2-t_1)\,{}^{t_1}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0}\theta(t_1-t_0)\quad \text{if}\quad t_1\neq t_2\\ &\equiv{}^{t_1}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0}\theta(t_1-t_0)\quad \text{if}\quad t_1=t_2\,,\end{aligned} \tag{18}$$

where $\theta(y)$ is a step function defined to be 1 when $y>0$ and 0 when $y<0$, and where

$${}^{t_1}\begin{bmatrix}\mathbf{k}_1\mathbf{k}_2\\ \mathbf{k}_3\mathbf{k}_4\end{bmatrix}_{t_0}\equiv\langle\mathbf{k}_1\mathbf{k}_2|R(t_1,t_0)|\mathbf{k}_3\mathbf{k}_4\rangle+\langle\mathbf{k}_1\mathbf{k}_2|R(t_1,t_0)|\mathbf{k}_4\mathbf{k}_3\rangle\,, \tag{19}$$

$$R(t_1,t_0)\equiv-\frac{\partial}{\partial t_0}\{\exp(t_1H_0^{(2)})\exp[-(t_1-t_0)H^{(2)}]\exp(-t_0H_0^{(2)})\}\,. \tag{20}$$

An explicit expression for the pair function has been given by the author in terms of the reaction matrices for an arbitrary two-body interaction.[14] A pair function is represented graphically by a *cluster vertex 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 β 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 (μ,ν) Graphs

A Qth-*order, linked-pair* (μ,ν) *graph* 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 μ outgoing external solid lines and ν 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 expression are as follows:

(i) It must not be possible to complete a loop in a linked-pair (μ,ν) 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 bond.

(ii) Associate with each missing (zero-momentum) outgoing line a factor of $(x\Omega)^{1/2}e^{\beta g}$, and with each missing incoming line a factor of $(x\Omega)^{1/2}$. 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.

[14] F. Mohling, Phys. Rev. **122**, 1043 (1961).

(iii) External lines are associated with pregiven momenta $\mathbf{p}$, 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 (μ,ν) graphs are different if their topological structures, including internal line types, line directions, and external lines, are different.

(v) Associate with each internal line a different integer $i(i=1, 2, \cdots, m_w+m_s)$ and a corresponding momentum $\mathbf{p}_i$ or $\mathbf{k}_i$ according to whether the line is solid or wiggly.

(vi) Associate with the entire graph a product of Q pair functions corresponding to the Q cluster vertices and explicitly determined by the temperature variables t_j of the cluster vertices and the momentum variable assignments 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 different (μ,ν) graphs (see Sec. 5).

(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 with respect to the wiggly line labels).

(viii) Assign a factor $\nu(\mathbf{p})$ to each solid internal line, where

$$\nu(\mathbf{p})\equiv\frac{\exp\beta(g-\omega_{\mathbf{p}})}{1-\exp\beta(g-\omega_{\mathbf{p}})}. \tag{21}$$

(ix) Finally, sum over all of the (m_s+m_w) internal momentum coordinates and integrate each of the Q temperature variables from 0 to β.

In Fig. 2 we given some examples of linked-pair (0,0) graphs together with their corresponding symmetry numbers. We observe here that in the limit $x\rightarrow 0$, Eq. (16) readily reduces to the corresponding $\langle x\rangle=0$ expression of Ref. 14. Referring to the discussion of Sec. 1, we also observe that the solid internal lines of linked-pair (μ,ν) graphs arise directly from the particle statistics (i.e., from exchange terms), whereas the wiggly lines are due to the particle interactions.

The proof of Eq. (16) begins with the well-known Ursell method, in which cluster functions $U_{N,x}{}^{(S)}$ are defined in terms of the $W_{N,x}{}^{(S)}$ of Eq. (9) as follows:

$$\begin{aligned}
W_x{}^{(S)}\begin{pmatrix}1\\1'\end{pmatrix}&\equiv U_x{}^{(S)}\begin{pmatrix}1\\1'\end{pmatrix},\\
W_x{}^{(S)}\begin{pmatrix}1\,2\\1'2'\end{pmatrix}&\equiv U_x{}^{(S)}\begin{pmatrix}1\\1'\end{pmatrix}U_x{}^{(S)}\begin{pmatrix}2\\2'\end{pmatrix}+U_x{}^{(S)}\begin{pmatrix}1\,2\\1'2'\end{pmatrix},\\
W_x{}^{(S)}\begin{pmatrix}1\,2\,3\\1'2'3'\end{pmatrix}&\equiv U_x{}^{(S)}\begin{pmatrix}1\\1'\end{pmatrix}U_x{}^{(S)}\begin{pmatrix}2\\2'\end{pmatrix}U_x{}^{(S)}\begin{pmatrix}3\\3'\end{pmatrix}+U_x{}^{(S)}\begin{pmatrix}1\\1'\end{pmatrix}U_x{}^{(S)}\begin{pmatrix}2\,3\\2'3'\end{pmatrix}\\
&\quad+U_x{}^{(S)}\begin{pmatrix}2\\2'\end{pmatrix}U_x{}^{(S)}\begin{pmatrix}3\,1\\3'1'\end{pmatrix}+U_x{}^{(S)}\begin{pmatrix}3\\3'\end{pmatrix}U_x{}^{(S)}\begin{pmatrix}1\,2\\1'2'\end{pmatrix}+U_x{}^{(S)}\begin{pmatrix}1\,2\,3\\1'2'3'\end{pmatrix}.
\end{aligned}\tag{22}$$

These equations are such that the Nth equation connects $W_{N,x}{}^{(S)}$ with all of the $U_{1,x}{}^{(S)}, U_{2,x}{}^{(S)},\cdots U_{N,x}{}^{(S)}$. One then defines cluster integrals $b_N{}^{(S)}$ in terms of the $U_{N,x}{}^{(S)}$ by the equation

$$b_N{}^{(S)}\begin{pmatrix}\mathbf{k}_1\,\mathbf{k}_2\cdots\mathbf{k}_M\\\mathbf{k}_1'\mathbf{k}_2'\cdots\mathbf{k}_M'\end{pmatrix}\equiv\Omega^{-1}[(N-M)!]^{-1}\sum_{\mathbf{k}_{M+1}\cdots\mathbf{k}_N}\exp(\beta gN)\exp(-\beta\sum_{i=1}^{N}\omega_i)U_x{}^{(S)}\begin{pmatrix}\mathbf{k}_1\,\mathbf{k}_2\cdots\mathbf{k}_M\,\mathbf{k}_{M+1}\cdots\mathbf{k}_N\\\mathbf{k}_1'\mathbf{k}_2'\cdots\mathbf{k}_M'\mathbf{k}_{M+1}\cdots\mathbf{k}_N\end{pmatrix}, \tag{23}$$

where the $(k_1\cdots k_M)$ and $(k_1'\cdots k_M')$ are external momenta as defined below Eq. (8). One can then show that the grand potential is given by

$$f(x,\beta,g,\Omega)=\sum_{N=1}^{\infty}b_N{}^{(S)}-x, \tag{24}$$

where only the $b_N{}^{(S)}$ with no external momenta are required in this case. The proof of Eq. (24) is made by substituting Eqs. (22) into Eq. (5) and then combining the identical terms which occur after the sum over all momentum states is performed.

It is important to realize in the derivation of Eq. (24) that the $(L!)^{-1}$ of Eq. (6) serves only to eliminate the zero-momentum exchange terms in Eq. (7) (see also Appendix B of LY V). This fact is of prime importance in the subsequent derivation of Eq. (16) from Eq. (24). In fact, we may immediately conclude that Eq. (16) is correct by making the following simple observation, in connection with the derivation of the linked-pair ex-

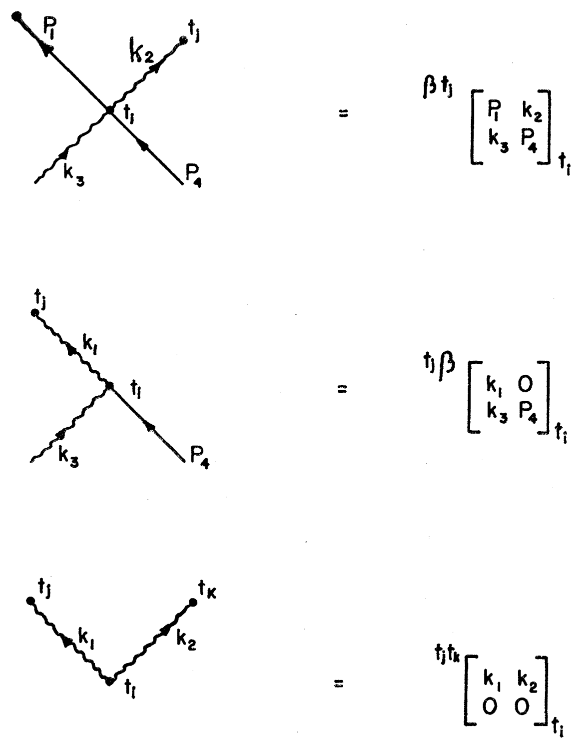

FIG. 1. Three examples of cluster vertices. The upper temperature variables of the corresponding pair functions are determined by the nature of the outgoing lines and the temperature variables at the head ends of the wiggly lines (if any). The explicit expression for a cluster vertex is given by Eqs. (18)–(20).

pansion in Ref. 14 for the case $\langle x\rangle=0$. In particular, the different ways of connecting the solid lines of linked-pair graphs represent the various possible (connected) exchange terms as they arise from Eq. (7). Since such exchanges or permutations among the zero momenta are to be omitted, we do not obtain solid lines for the zero momenta, i.e., the only zero-momentum connections are those due to wiggly lines. Having made this observation, it is then a simple matter to verify that Eq. (16) is correct by proceeding in analogy with the proof given for the $\langle x\rangle=0$ case in Ref. 14. It is noted here that the prescriptions which arise from using either Eqs. (1) or (2) to calculate the grand potential are different precisely because of the treatment of the zero-momentum exchanges as discussed in this paragraph. We also note

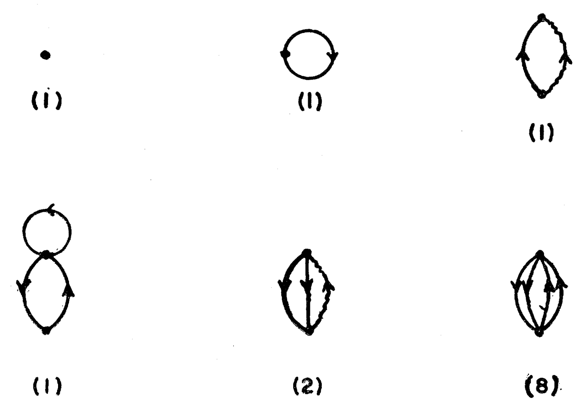

FIG. 2. Some examples of linked-pair (0,0) graphs. Below each graph is included its symmetry number S.

that the term $x\Omega e^{\beta g}$ in Eq. (16) is the zero-momentum counterpart of the free-particle grand potential Ωf_0.

Momentum Distribution

In a similar manner, we may discuss any of the distribution functions for a degenerate Bose system. Thus, the difference between Eqs. (9) and (6) lies only in the treatment of the external momenta which are zero. The extra numerical factors of Eq. (9) serve to eliminate any distinction between "external" zero momenta and the "internal" zero momenta, or missing lines of (0,0) graphs. This is accomplished by eliminating the exchange terms involving these external momenta which arise either in Eq. (7) or in the selection of top row positions, such as in Eqs. (10) or (22). We consider here the special case of the momentum distribution, and in Sec. 8 we shall discuss the pair-distribution function.

From the preceding paragraph it should be clear that the different cases of zero and nonzero external momenta are best discussed separately. The starting point in both cases is the definition of the momentum distribution as a reduced density matrix element, which is, in turn, given by an equation similar to Eq. (10). Then

$$\langle n(\mathbf{k}_1)\rangle=\langle\mathbf{k}_1|\rho_1|\mathbf{k}_1\rangle$$

$$=e^{-\Omega f}e^{-\Omega x}\sum_{N=1}^{\infty}[(N-1)!]^{-1}\exp(\beta gN)\sum_{\mathbf{k}_2\cdots\mathbf{k}_N}\exp(-\beta\sum_{i=1}^{N}\omega_i)W_x{}^{(S)}\begin{pmatrix}\mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N\\ \mathbf{k}_1\mathbf{k}_2\cdots\mathbf{k}_N\end{pmatrix},\qquad(25)$$

where the off-diagonal reduced density matrix elements $\langle\mathbf{k}_1|\rho_1|\mathbf{k}_1'\rangle$ vanish because of momentum conservation. The $W_{N,x}{}^{(S)}$ are again written in terms of the $U_{N,x}{}^{(S)}$ by the Ursell equations (22).

It is at this point that the distinction between zero- and nonzero-momentum cases must be made. Thus, one can show by means of a simple combinatorial analysis, similar to that used in the derivation of Eq. (24), that

$$\langle n(\mathbf{p}_1)\rangle=\Omega\sum_{N=1}^{\infty}b_N{}^{(s)}\begin{pmatrix}\mathbf{p}_1\\ \mathbf{p}_1\end{pmatrix}.\qquad(26)$$

One then shows, in analogy with the derivation of Eq.

(16) from Eq. (24), that

$$\langle n(\mathbf{p})\rangle=\nu(\mathbf{p})+\nu(\mathbf{p})[1+\nu(\mathbf{p})]\times\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order linked-pair (1,1) graphs}]_{\mathbf{p}}, \quad (27)$$

where $\nu(\mathbf{p})$ is given by Eq. (21), and where one can use the identity

$$\nu(\mathbf{p})=\exp\beta(g-\omega_{\mathbf{p}})[1+\nu(\mathbf{p})] \quad (28)$$

in the derivation of (27).

For the average number of zero-momentum particles, one finds that the only difference between the calculation of $\langle n(0)\rangle$ and the calculation of the grand partition function by Eq. (24), is the extra factor of $(x\Omega)$ which occurs in Eq. (9). Then, owing to the normalization factor in Eq. (25) one immediately obtains

$$\langle n(0)\rangle=\langle x\rangle\Omega, \quad (29)$$

where we may replace x by $\langle x\rangle$ because of the theorem associated with Eq. (3). Of course, this last result can also be derived by merely using Eq. (2) to compute $\langle L\rangle$ and then using Eq. (3).

Equations (27) and (29) may be combined to give an expression for the density of the Bose system in the limit of infinite volume.

$$n=\langle x\rangle+(2\pi)^{-3}\int d^3p\langle n(\mathbf{p})\rangle. \quad (30)$$

This expression is equivalent to Eq. (12) for the particle density or, assuming that the density is a given parameter of the system, it is equivalent to Eqs. (3) or (3′) for the determination of $\langle x\rangle$.

4. DUAL GRAPHS

It has been emphasized by Lee and Yang in their analysis of the degenerate Bose system[9] that *as it stands*, the expression (16) for the grand potential is completely useless for any calculation of the thermodynamic properties of a real degenerate Bose gas. The reason for this is associated with the fact that the difference $[\langle n(\mathbf{p})\rangle-\nu(\mathbf{p})]$ as given by Eq. (27) becomes extremely large as the temperature $T\rightarrow 0$. Moreover, the function $\nu(\mathbf{p})$ has an unphysical singularity at $\omega_{\mathbf{p}}=g$, where, for a gas of hard spheres, for example, $g>0$ at very low temperatures. Thus, the solid line weighting factors in integrals are completely unphysical and therefore, so must the associated thermodynamic predictions be unphysical, when in (16) only a few (0,0) graphs are considered.

The solution to the above dilemma is to regroup the terms in the linked-pair expansion (16) 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[9] have taken the first important step in this direction by their analysis of the momentum distribution. In this section we shall give the results of their analysis as adapted to the interaction representation.

The starting point in this analysis is to introduce a function $N_{1,1}(\mathbf{p})$, defined by

$$N_{1,1}(\mathbf{p})\equiv\exp[\beta(g-\omega_{\mathbf{p}})][1+\langle n(\mathbf{p})\rangle]$$
$$=\nu(\mathbf{p})\{1+\nu(\mathbf{p})\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order linked-pair (1,1) graphs}]_{\mathbf{p}}\}, \quad (31)$$

where the second line of this equation follows from (27). Now, the program in this section is to analyze self-energy graphs, where a self-energy graph is any graph with (one or) two external lines. The reason why self-energy graphs are important is because, as is clear from Eq. (31), they are intimately associated with the determination of the momentum distribution, and this is the problem of interest as stated at the beginning of this section. We might also add that the analysis of the momentum distribution can be viewed as a study of the momentum space ordering in a degenerate many-body system. London[15] has given a beautiful discussion of the importance of momentum space ordering to the understanding of the physics of degenerate many-body systems.

When $\langle x\rangle=0$, and there is no macroscopic occupation of a single quantum state, then the analysis of self-energy graphs is completely equivalent to the analysis of $N_{1,1}(\mathbf{p})$, Eq. (31). 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 $N_{0,2}(\mathbf{p})$ and $N_{2,0}(\mathbf{p})$, defined by

$$N_{0,2}(\mathbf{p})\equiv\nu(\mathbf{p})\nu(-\mathbf{p})\times\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order linked-pair (0,2) graphs}]_{\mathbf{p}}=N_{0,2}(-\mathbf{p}), \quad (32)$$

$$N_{2,0}(\mathbf{p})\equiv\nu(\mathbf{p})\nu(-\mathbf{p})\times\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order linked-pair (2,0) graphs}]_{\mathbf{p}}=N_{2,0}(\mathbf{p}). \quad (33)$$

In this section we analyze the self-energy graphs only with respect to their solid lines. Then, in Secs. 5–7, we analyze the remaining wiggly-line self-energy graphs. We next define proper and improper graphs as follows.

Definitions

A linked-pair (μ,ν) graph is called *improper* if by cutting any *one* of its solid internal lines open the entire

[15] F. London, *Superfluids* (John Wiley & Sons, Inc., New York, 1950), Vol. I, pp. 1–9 (see also Ref. 1).

graph can be separated into two disconnected graphs. Otherwise, the (μ,ν) graph is called *proper*.

With these definitions in mind, we next define three functions $K_{1,1}(\mathbf{p})$, $K_{0,2}(\mathbf{p})$, and $K_{2,0}(\mathbf{p})$.

$$K_{1,1}(\mathbf{p})\equiv \sum_{Q=1}^{\infty} [\text{all different } Q\text{th-order proper linked-pair (1,1) graphs}]_{\mathbf{p}},$$

$$K_{0,2}(\mathbf{p})\equiv \sum_{Q=1}^{\infty} [\text{all different } Q\text{th-order proper linked-pair (0,2) graphs}]_{\mathbf{p}} = K_{0,2}(-\mathbf{p}), \tag{34}$$

$$K_{2,0}(\mathbf{p})\equiv \sum_{Q=1}^{\infty} [\text{all different } Q\text{th-order proper linked-pair (2,0) graphs}]_{\mathbf{p}} = K_{2,0}(-\mathbf{p}).$$

In these definitions the momenta associated with the external lines are both $\mathbf{p}$ in the case of the (1,1) graphs, and $\mathbf{p}$ and $-\mathbf{p}$ in the case of the (0,2) and (2,0) graphs.

We next write down a set of algebraic equations which relate the $N_{\mu,\nu}(\mathbf{p})$ and the $K_{\mu,\nu}(\mathbf{p})$. These are

$$\begin{aligned} N_{1,1}(\mathbf{p}) &= \nu(\mathbf{p})[1+K_{1,1}(\mathbf{p})N_{1,1}(\mathbf{p})+K_{0,2}(\mathbf{p})N_{2,0}(\mathbf{p})] \\ &= \nu(\mathbf{p})[1+K_{1,1}(\mathbf{p})N_{1,1}(\mathbf{p})+K_{2,0}(\mathbf{p})N_{0,2}(\mathbf{p})], \end{aligned} \tag{35}$$

$$\begin{aligned} N_{0,2}(\mathbf{p}) &= \nu(\mathbf{p})[K_{1,1}(\mathbf{p})N_{0,2}(\mathbf{p})+K_{0,2}(\mathbf{p})N_{1,1}(-\mathbf{p})] \\ &= \nu(-\mathbf{p})[K_{1,1}(-\mathbf{p})N_{0,2}(\mathbf{p})+K_{0,2}(\mathbf{p})N_{1,1}(\mathbf{p})], \end{aligned} \tag{36}$$

$$\begin{aligned} N_{2,0}(\mathbf{p}) &= \nu(-\mathbf{p})[K_{1,1}(-\mathbf{p})N_{2,0}(\mathbf{p})+K_{2,0}(\mathbf{p})N_{1,1}(\mathbf{p})] \\ &= \nu(\mathbf{p})[K_{1,1}(\mathbf{p})N_{2,0}(\mathbf{p})+K_{2,0}(\mathbf{p})N_{1,1}(-\mathbf{p})]. \end{aligned} \tag{37}$$

These equations are easy to prove diagrammatically, and their diagrammatic representation is given in Fig. 9 of LY V. It is interesting to note that Beliaev[16] 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. Equations (35)–(37) only complete the treatment of self-energy graphs as far as improper graphs are concerned. Thus, the internal structure of the functions $K_{\mu,\nu}(\mathbf{p})$ may include many "improper parts" in the sense that cutting any two solid lines may separate a proper graph into two parts. In order to deal effectively with this internal structure we next introduce dual (μ,ν) graphs.

Dual (μ,ν) Graphs

A Qth-*order, dual* (μ,ν) *graph* 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 μ outgoing external solid lines and ν incoming external solid lines. Each *internal solid* line carries two arrows, one for each end, whereas the external lines each carry only one arrow. Thus, there are three different kinds of internal solid lines depending on whether the two arrows are parallel to each other, point towards each other or point away from each other. The rules for connecting the Q cluster vertices by the (m_s+m_w) internal lines and the procedures for determining the corresponding expression are as follows:

(i)–(iv) Same as rules (i)–(iv) for linked-pair (μ,ν) graphs (Sec. 3), except for the word replacement (linked-pair) → (dual).

(v) Assign to *each arrow* of the m_s solid internal lines a different integer i $(i=1, 2, \cdots, 2m_s)$ and a corresponding momentum $\mathbf{p}_i$. Assign to each internal wiggly line an integer i $(i=2m_s+1, \cdots, 2m_s+m_w)$ and a corresponding momentum $\mathbf{k}_i$.

(vi) Same as rule (vi) for linked-pair (μ,ν) graphs (Sec. 3).

(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 $2m_s$ integers associated with the arrows of the internal solid lines which leave the graph topologically unchanged (including the positions of these integers with respect to the arrows, but not necessarily with respect to the wiggly line labels).

(viii) Assign a factor to each internal solid line with arrows i and j of

$\delta(\mathbf{p}_i,\mathbf{p}_j)N_{1,1}(\mathbf{p}_i)$ when the arrows are pointing parallel to each other,

$\delta(\mathbf{p}_i,-\mathbf{p}_j)N_{0,2}(\mathbf{p}_i)$ when the arrows are pointing towards each other,

$\delta(\mathbf{p}_i,-\mathbf{p}_j)N_{2,0}(\mathbf{p}_i)$ when the arrows are pointing away from each other.

Here, the $\delta(\ ,\ )$ symbols are Kronecker δ's.

(ix) Finally, sum over all of the $(2m_s+m_w)$ internal momentum coordinates and integrate each of the Q temperature variables from 0 to β.

In Fig. 3 we give some examples of dual (μ,ν) graphs together with their corresponding symmetry numbers. It is to be emphasized that in (0,2) and (2,0) graphs, the external $\mathbf{p}$ and $-\mathbf{p}$ lines are distinguishable. Before we can express the $K_{\mu,\nu}(\mathbf{p})$ of (34) in terms of dual (μ,ν) graphs, we must first define reducible and irreducible dual graphs.

Definitions

A dual (μ,ν) graph is called *reducible* if by cutting any two of its internal solid lines open the entire graph can be separated into two (or more) disconnected dual graphs at least one of which is a (1,1), (0,2), or (2,0) graph. A dual (μ,ν) graph which is not reducible is called *irreducible*.

The $K_{\mu,\nu}(\mathbf{p})$ of Eqs. (34) can now be expressed in terms

[16] S. T. Beliaev, Zh. Eksperim. i Teor. Fiz. 34, 417 (1958) [English transl.: Soviet Phys.—JETP 7, 289 (1958)].

of irreducible (μ,ν) graphs as follows:

$$K_{\mu,\nu}(\mathbf{p})=\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order irreducible dual } (\mu,\nu) \text{ graphs}]_{\mathbf{p}}, \quad (38)$$

where $(\mu,\nu)=(1,1)$, (0,2), or (2,0). As with all results of this kind, a formal mathematical proof is difficult to give. The best procedure is to replace the solid line factors of rule (viii) for each dual (μ,ν) graph of (38) by Eqs. (31)–(33), and then to study the resulting expanded forms. The proof is also discussed in Appendix E of LY V. We note that with Eq. (38), the relations (35)–(37) have become integral equations. One can also show using the Hermitian property of the Hamiltonian $H^{(N)}$ (see LY V) that

$$\begin{aligned} K_{2,0}(\mathbf{p})&=\exp[\beta(\omega_{\mathbf{p}}+\omega_{-\mathbf{p}}-2g)]K_{0,2}(\mathbf{p}),\\ N_{2,0}(\mathbf{p})&=\exp[\beta(\omega_{\mathbf{p}}+\omega_{-\mathbf{p}}-2g)]N_{0,2}(\mathbf{p}). \end{aligned} \quad (39)$$

We finally discuss an important theorem which is proved in Appendix H of LY V. This theorem states that if, as $\Omega\to\infty$, the solution to Eq. (3) is $x=\langle x\rangle$ for $\langle x\rangle$ real and positive, then at $x=\langle x\rangle$ the solution to the integral Eqs. (35)–(37) satisfies the identities

$$\begin{aligned} \lim_{\mathbf{p}\to 0}[N_{1,1}^{-1}(\mathbf{p})]&=0,\\ \lim_{\mathbf{p}\to 0}[N_{1,1}^{-1}(\mathbf{p})N_{0,2}(\mathbf{p})e^{-\beta g}]&=-1. \end{aligned} \quad (40)$$

The first of these identities shows that the momentum distribution $\langle n(\mathbf{p})\rangle$, Eq. (31), exhibits a singularity at $\mathbf{p}=0$ when $\langle x\rangle>0$. This consequence is consistent with the interpretation of the x-ensemble formulation (2), as discussed below Eq. (3), in which $\langle x\rangle\neq 0$ corresponds to a macroscopic occupation of the zero-momentum state.

Grand Potential

It was indicated at the outset of this section that one of the objectives in the analysis of the self-energy problem is to be able to simplify the calculation of thermodynamic quantities from the grand potential. Thus, we should like to express the grand potential (16) in terms of irreducible dual (0,0) graphs. In Appendix G of LY V, Lee and Yang have shown how this objective may be achieved. A few minor modifications of their proof yields the result

$$\begin{aligned} \Omega f(x,\beta,g,\Omega)=&\sum_{\mathbf{p}}\ln\{\exp\beta(\omega_{\mathbf{p}}-g)[N_{1,1}(\mathbf{p})N_{1,1}(-\mathbf{p})-N_{0,2}(\mathbf{p})N_{2,0}(\mathbf{p})]^{1/2}\}\\ &+\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order irreducible dual (0,0) graphs}]-\sum_{\mathbf{p}}[\nu^{-1}(\mathbf{p})N_{1,1}(\mathbf{p})-1]-x\Omega+x\Omega e^{\beta g}. \quad (41) \end{aligned}$$

As will be seen in the next three sections, Eq. (41) is only the first step towards obtaining a *useful* expression for the grand potential.

5. ZERO-MOMENTUM FACTORS

In rule (vi), Sec. 3, for either linked-pair or dual (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. Moreover, it is important to realize that such graphical structures cannot be omitted from the formalism, and we shall show in our subsequent papers that the correct analysis of these structures has important consequences even for "lowest order" calculations. We begin this analysis by defining irregular, regular, and zero-regular graphs.

Definitions

An irreducible dual (μ,ν) graph is called *irregular* if, by cutting any *one* of its wiggly internal lines open, the entire graph can be separated into two disconnected graphs. An irreducible dual (μ,ν) graph is *zero regular* if (1) it is not irregular with respect to zero-momentum lines and if (2) a zero-momentum factor $G_{\text{out}}(t)$ or $G_{\text{in}}(t)$ is included for each missing line. A *regular* dual (μ,ν) graph is a zero-regular dual (μ,ν) graph, which is not irregular. Regular graphs will be considered further in the next section. The zero-momentum factors introduced in these definitions are specified more carefully by first writing down pair functions, Eq. (18), for which there are missing lines. Thus, in zero-regular graphs, we must make the replacements

$$\begin{aligned} {}^{t_j\beta}\begin{bmatrix}\mathbf{k}_1 & 0\\ \mathbf{k}_3\mathbf{p}_4\end{bmatrix}_{t_i} &\to \int_0^\beta ds G_{\text{out}}(s)\,{}^{t_js}\begin{bmatrix}\mathbf{k}_1 & 0\\ \mathbf{k}_3\mathbf{p}_4\end{bmatrix}_{t_i},\\ {}^{t_j\beta}\begin{bmatrix}\mathbf{k}_1\mathbf{p}_2\\ \mathbf{k}_3 & 0\end{bmatrix}_{t_i} &\to {}^{t_j\beta}\begin{bmatrix}\mathbf{k}_1\mathbf{p}_2\\ \mathbf{k}_3 & 0\end{bmatrix}_{t_i} G_{\text{in}}(t_i), \end{aligned} \quad (42)$$

where

$$\begin{aligned} G_{\text{out}}(t)&=\delta(\beta-t)+K_{\text{out}}(t),\\ G_{\text{in}}(t)&=1+K_{\text{in}}(t). \end{aligned} \quad (43)$$

It now remains to define $K_{\text{out}}(t)$ and $K_{\text{in}}(t)$.

Consider any given cluster vertex at which there is a missing line. It is clear that $K_{\text{in}}(t)$ or $K_{\text{out}}(t)$ must be the sum over all possible graphical structures which can attach at that point with a zero-momentum wiggly line. These quantities can therefore be defined by simple

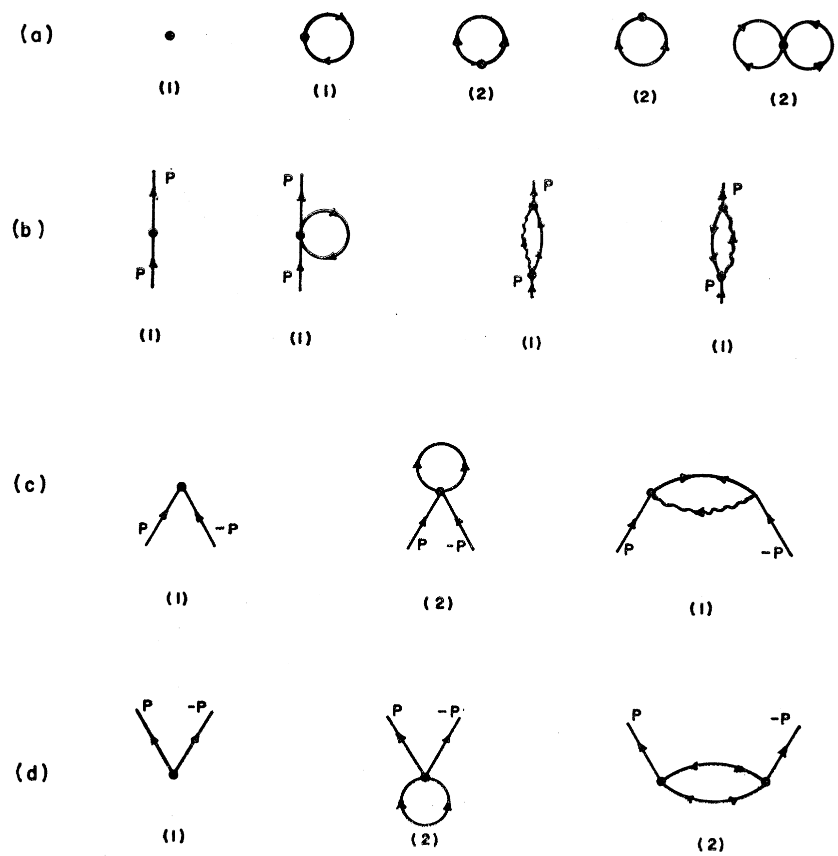

FIG. 3. Some examples of dual (μ,ν) graphs: (a) (0,0) graphs, (b) (1,1) graphs, (c) (0,2) graphs, and (d) (2,0) graphs. Below each graph is included its symmetry number S. Each of the graphs shown is irreducible.

functional differentiations as

$$K_{\rm in}(t)\equiv(x\Omega e^{\beta g})^{-1}\frac{\delta}{\delta G_{\rm out}(t)}\times\Big\{\sum_{Q=1}^{\infty}[\text{all different }Q\text{th-order zero-regular dual (0,0) graphs}]\Big\}_N,\quad(44)$$

in which the functional differentiation includes the elimination of one temperature integration of the type introduced in (42); and

$$K_{\rm out}(t)\equiv(x\Omega e^{\beta g})^{-1}\frac{\delta}{\delta G_{\rm in}(t)}\times\Big\{\sum_{Q=1}^{\infty}[\text{all different }Q\text{th-order zero-regular dual (0,0) graphs}]\Big\}_N,\quad(45)$$

in which no temperature integration is eliminated. Note that the definitions (44) and (45) include the division by both of the factors $(x\Omega)^{1/2}e^{\beta g}$ and $(x\Omega)^{1/2}$ of rule (ii) in Sec. 3. The subscripts N in (44) and (45) indicate that the line factors $N_{\mu,\nu}$ are to be held constant in the functional differentiation.

Equations (42)–(45) provide a completely consistent set of coupled integral equations for the calculation of the zero-momentum factors $K_{\rm out}(t)$ and $K_{\rm in}(t)$. Moreover, it can be verified by the iteration of the zero-momentum factors in (42) that

$$\sum_{Q=1}^{\infty}[\text{all different }Q\text{th-order irreducible dual }(\mu,\nu)\text{ graphs}]=\sum_{Q=1}^{\infty}[\text{all different }Q\text{th-order zero-regular dual }(\mu,\nu)\text{ graphs}]\quad(46)$$

for $(\mu,\nu)\neq(0,0)$. Therefore, we may immediately substitute Eq. (46) into Eq. (38) to obtain

$$K_{\mu,\nu}(\mathbf{p})=\sum_{Q=1}^{\infty}[\text{all different }Q\text{th-order zero-regular dual }(\mu,\nu)\text{ graphs}]_{\mathbf{p}},\quad(47)$$

where $(\mu,\nu)=(1,1)$, (0,2), or (2,0).

Grand Potential

Equation (46) is not valid for (0,0) graphs and therefore we must consider these graphs specially before we can write the grand potential (41) in terms of zero-regular graphs. In Fig. 4 we given an example of an irregular dual (0,0) graph, where we note here that a (0,0) graph cannot be irregular with respect to a nonzero momentum line. There are nine islands in the irregular dual (0,0) graph of Fig. 4, where an *island* is defined to be a not irregular part of an irreducible dual (0,0) graph. We next let

$$n_I \equiv [\text{number of islands in an irreducible dual (0,0) graph}], \quad (48)$$

and observe that

$$\sum_{Q=1}^{\infty} [\text{all different } Q\text{th-order zero-regular dual (0,0) graphs}] = \sum_I n_I S_I^{-1} L_I(\beta), \quad (49)$$

where the sum $\sum_I$ is over all irregular dual (0,0) graphs $S_I^{-1}L_I(\beta)$, each with symmetry number S_I and containing n_I islands. The proof of this result is very similar to that of theorem 4 in Appendix B of Ref. 17, and we shall not repeat it here.

We now see that for (0,0) graphs, the expression (46) becomes

$$\sum_{Q=1}^{\infty} [\text{all different } Q\text{th-order irreducible dual (0,0) graphs}]$$
$$= \sum_{Q=1}^{\infty} [\text{all different } Q\text{th-order zero-regular dual (0,0) graphs}] - \sum_I (n_I - 1) S_I^{-1} L_I(\beta), \quad (50)$$

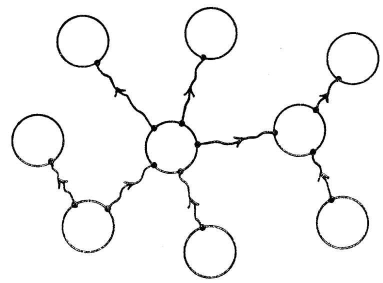

FIG. 4. An irregular dual (0,0) graph with nine islands ($n_I = 9$), where each island is a not irregular part of the graph. For convenience, the temperature variables at the ends of the eight zero-momentum (wiggly) lines have been omitted.

where $(n_I - 1)$ is the number of (identically) zero-momentum (wiggly) lines in $S_I^{-1}L_I(\beta)$. One may now write the second term on the right-hand side of (50) in terms of the functions $K_{\rm in}(t)$ and $K_{\rm out}(t)$ defined by Eqs. (44) and (45). One finds that

$$\sum_I (n_I - 1) S_I^{-1} L_I(\beta) = (x\Omega e^{\beta g}) \int_0^\beta dt K_{\rm out}(t) K_{\rm in}(t), \quad (51)$$

a result which can be easily verified after observing that each of the zero-momentum lines in Fig. 4 can occur between the $K_{\rm out}(t)$ and $K_{\rm in}(t)$ on the right-hand side of (51).

Equations (50) and (51) can now be substituted into Eq. (41) for the grand potential to give

$$\Omega f(x,\beta,g,\Omega) = \sum_{\mathbf{p}} \ln\{\exp\beta(\omega_{\mathbf{p}} - g)[N_{1,1}(\mathbf{p})N_{1,1}(-\mathbf{p}) - N_{0,2}(\mathbf{p})N_{2,0}(\mathbf{p})]^{1/2}\}$$
$$+ \sum_{Q=1}^{\infty} [\text{all different } Q\text{th-order zero-regular dual (0,0) graphs}] - \sum_{\mathbf{p}} [\nu^{-1}(\mathbf{p})N_{1,1}(\mathbf{p}) - 1] - x\Omega$$
$$+ (x\Omega e^{\beta g})\left[G_{\rm in}(\beta) - \int_0^\beta dt G_{\rm out}(t) K_{\rm in}(t)\right]. \quad (52)$$

With this result we have taken the second step in the analysis of self-energy graphs as discussed at the beginning of Sec. 4. We observe here that the analysis of this section could just as well have been presented before the analysis of Sec. 4 without affecting the final results (47) and (52).

6. MASTER GRAPHS

At the beginning of Sec. 4 we have introduced the concept of self-energy graphs merely from a graphical structure point of view. We have also indicated that the analysis of these graphical structures is intimately associated with the momentum space ordering of the degenerate Bose system. The final justification of these assertions can only be made in an *a posteriori* examination of the consequences of our analysis for a real or model degenerate Bose system.

We shall show in the second paper of this series that the final step in the analysis of the self-energy structures is the Λ transformation. The interpretation of the Λ transformation will be that it transforms the theory from a description in terms of free bosons into one in terms of the quantum-mechanical normal modes or quasiparticles. In this quasiparticle description, the basic energy-momentum relation for the quasiparticles will no longer be $\omega_{\mathbf{p}} = \hbar^2 p^2/2M$, but rather some new relation $\epsilon_{\mathbf{p}}$, which results from the Λ transformation. It is this consequence of the analysis which finally justifies the use of the term "self-energy graphs" because it is these graphs which result in a transformed energy-momentum relation.

A prerequisite to the application of the Λ transformation is an analysis of the *irregular* (1,1), (0,2), and (2,0) graphs defined at the beginning of Sec. 5. This analysis is culminated by the introduction of master graphs and the derivation of an expression for the grand potential in terms of master graphs (Sec. 7). We begin the analysis of graphs which are irregular with respect to nonzero-

17 F. Mohling, Phys. Rev. 122, 1062 (1961).

momentum wiggly lines by the introduction of L graphs.

Corresponding to each zero-regular dual (μ,ν) graph, we define a *zero-regular* (μ,ν) L *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

$$L_{\mu,\nu}(t_2,t_1,\mathbf{k})\equiv\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order zero-regular } (\mu,\nu)\ L \text{ graphs}]_{\mathbf{k}}, \quad (53)$$

where $(\mu,\nu)=(1,1)$, $(0,2)$, or $(2,0)$. The definition is such that the external lines of (μ,ν) 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 shall adopt the convention that the temperature variable (in the position) t_2 is always to be associated with the momentum $\mathbf{k}$, so that in the case of (0,2) and (2,0) L graph, the temperature variable t_1 is to be associated with the momentum $-\mathbf{k}$. It should be clear that $L_{\mu,\nu}(t_2,t_1,\mathbf{k})=L_{\mu,\nu}(t_1,t_2,-\mathbf{k})$ when $(\mu,\nu)=(0,2)$ or $(2,0)$ [see also Eqs. (32) and (33)]. 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 δ-function factor $\delta(t_2-t_1)$. Also, the (μ,ν) L graphs with external wiggly lines can have $\mathbf{k}=0$ as well as $\mathbf{k}=\mathbf{p}$. In the particular case where both of the external lines are solid, then $\mathbf{k}=\mathbf{p}$ only and Eq. (47) can be written in terms of the $L_{\mu,\nu}(t_2,t_1,\mathbf{k})$ functions as follows:

$$\begin{aligned} K_{1,1}(\mathbf{p})&=\int_0^\beta dt_1L_{1,1}(\beta,t_1,\mathbf{p}),\\ K_{0,2}(\mathbf{p})&=\int_0^\beta dt_2dt_1L_{0,2}(t_2,t_1,\mathbf{p}),\\ K_{2,0}(\mathbf{p})&=L_{2,0}(\beta,\beta,\mathbf{p}). \end{aligned} \quad (54)$$

We next introduce functions $K_{\mu,\nu}(t_2,t_1,\mathbf{k})$ by the definition

$$K_{\mu,\nu}(t_2,t_1,\mathbf{k})\equiv\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order regular } (\mu,\nu)\ L \text{ graphs}]_{\mathbf{k}}, \quad (55)$$

where a regular (μ,ν) L graph is a zero-regular (μ,ν) L graph which is not irregular (see beginning of Sec. 5). The identity $K_{\mu,\nu}(t_2,t_1,\mathbf{k})=K_{\mu,\nu}(t_1,t_2,-\mathbf{k})$, when $(\mu,\nu)=(0,2)$ or $(2,0)$, holds for this restricted class of L graphs as well as for the functions (53). In analogy with Eqs. (35)–(37) we next write down a set of simple integral equations which relate the functions of (53) and (55).

$$\begin{aligned} L_{1,1}(t_2,t_1,\mathbf{k})&=\int_0^\beta ds[G_{1,1}(t_2,s,\mathbf{k})K_{1,1}(s,t_1,\mathbf{k})+L_{2,0}(t_2,s,\mathbf{k})K_{0,2}(s,t_1,\mathbf{k})]\\ &=\int_0^\beta ds[K_{1,1}(t_2,s,\mathbf{k})G_{1,1}(s,t_1,\mathbf{k})+K_{2,0}(t_2,s,\mathbf{k})L_{0,2}(s,t_1,\mathbf{k})], \end{aligned} \quad (56)$$

$$\begin{aligned} L_{0,2}(t_2,t_1,\mathbf{k})&=\int_0^\beta ds[L_{0,2}(t_2,s,\mathbf{k})K_{1,1}(s,t_1,-\mathbf{k})+G_{1,1}(s,t_2,\mathbf{k})K_{0,2}(s,t_1,\mathbf{k})]-K_{0,2}^{(1)}(t_2,t_1,\mathbf{k})\\ &=\int_0^\beta ds[K_{1,1}(s,t_2,\mathbf{k})L_{0,2}(s,t_1,\mathbf{k})+K_{0,2}(t_2,s,\mathbf{k})G_{1,1}(s,t_1,-\mathbf{k})]-K_{0,2}^{(1)}(t_2,t_1,\mathbf{k}), \end{aligned} \quad (57)$$

$$\begin{aligned} L_{2,0}(t_2,t_1,\mathbf{k})&=\int_0^\beta ds[L_{2,0}(t_2,s,\mathbf{k})K_{1,1}(t_1,s,-\mathbf{k})+G_{1,1}(t_2,s,\mathbf{k})K_{2,0}(s,t_1,\mathbf{k})]-\delta(t_2,t_1)K_{2,0}^{(1)}(t_2,t_1,\mathbf{k})\\ &=\int_0^\beta ds[K_{1,1}(t_2,s,\mathbf{k})L_{2,0}(s,t_1,\mathbf{k})+K_{2,0}(t_2,s,\mathbf{k})G_{1,1}(t_1,s,-\mathbf{k})]-\delta(t_2,t_1)K_{2,0}^{(1)}(t_2,t_1,\mathbf{k}), \end{aligned} \quad (58)$$

where

$$G_{1,1}(t_2,t_1,\mathbf{k})\equiv\delta(t_2-t_1)+L_{1,1}(t_2,t_1,\mathbf{k}). \quad (59)$$

The quantities $K_{0,2}^{(1)}(t_2,t_1,\mathbf{k})$ and $K_{2,0}^{(1)}(t_2,t_1,\mathbf{k})$ are those parts of $K_{0,2}(t_2,t_1,\mathbf{k})$ and $K_{2,0}(t_2,t_1,\mathbf{k})$ in which both external wiggly lines attach at the same vertex, and $\delta(t_2,t_1)$ is a Kronecker δ function. Of course, $K_{0,2}^{(1)}(t_2,t_1,\mathbf{k})$ includes a $\delta(t_2-t_1)$ factor [see discussion below Eq. (53)] and this term is to be subtracted only when both incoming external wiggly lines attach at their *tail* ends to the same vertex [see rule (i) for linked-pair (μ,ν) graphs in Sec. 3]. The graphical representation of Eqs. (56)–(58) is given in Figs. 5–7. Note that the concept of external wiggly lines, as introduced with Eq. (53), is essential to the derivation of these integral equations.

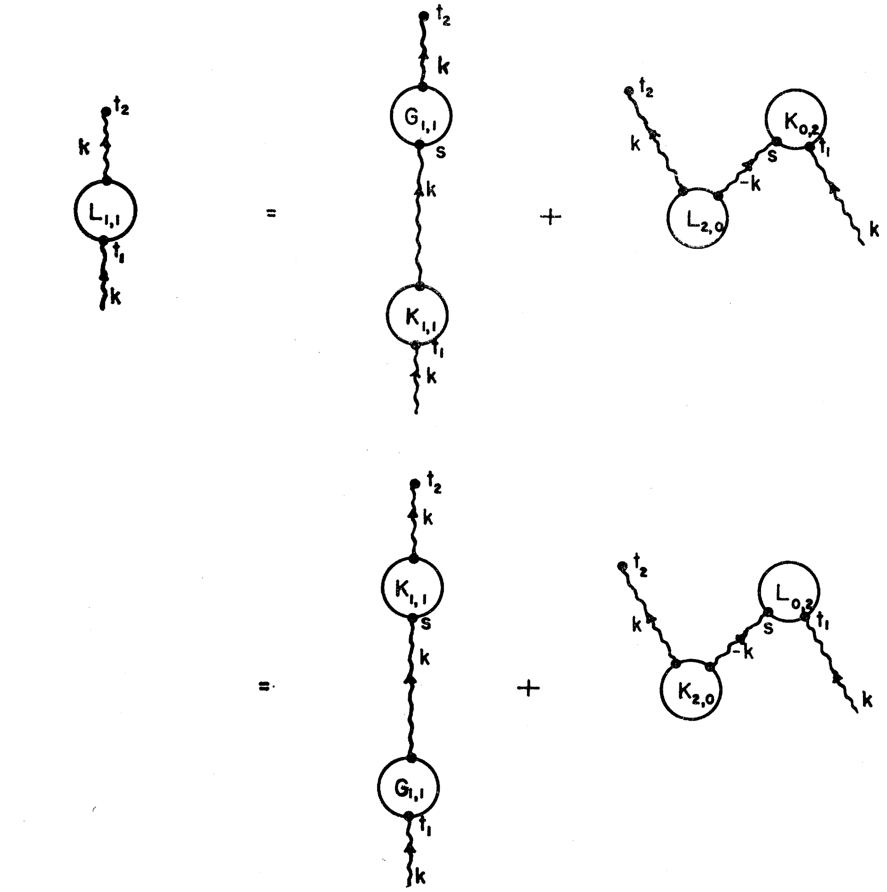

FIG. 5. The graphical representation of the integral equation (56).

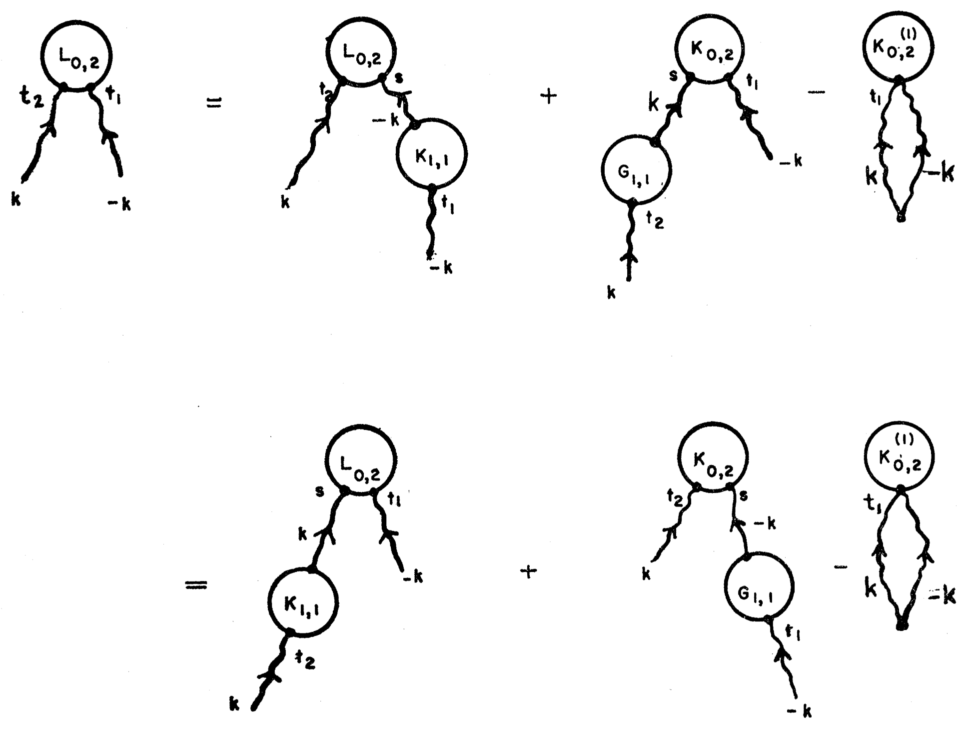

FIG. 6. The graphical representation of the integral equation (57). The function $K_{0,2}^{(1)}(t_2,t_1,\mathbf{k})$ includes a $\delta(t_2-t_1)$ factor, and it is defined below Eq. (59).

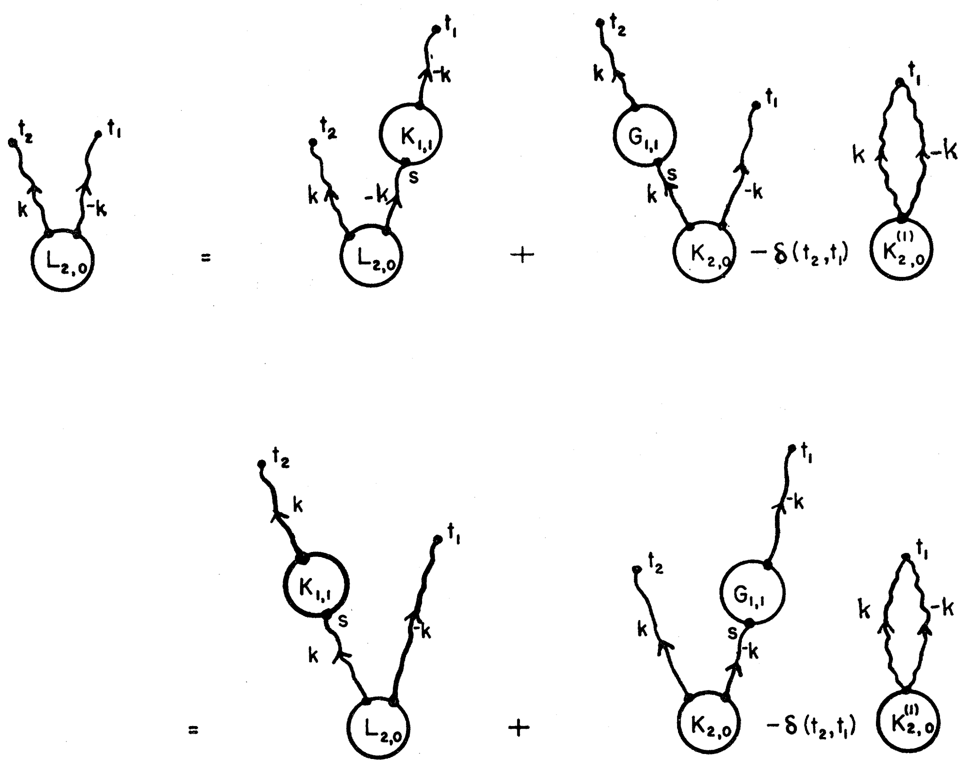

FIG. 7. The graphical representation of the integral equation (58). The function $K_{2,0}^{(1)}(t_2,t_1,\mathbf{k})$ is defined below Eq. (59).

We next write down the equations which one obtains instead of (57)–(59) when $\langle x\rangle=0$. These are

$$L(t_2,t_1,\mathbf{k})\equiv\int_0^\beta dsG(t_2,s,\mathbf{k})K_{1,1}(s,t_1,\mathbf{k})\,, \tag{60}$$

$$G(t_2,t_1,\mathbf{k})\equiv\delta(t_2-t_1)+L(t_2,t_1,\mathbf{k})\,, \tag{61}$$

where we have now introduced two new functions $L(t_2,t_1,\mathbf{k})$ and $G(t_2,t_1,\mathbf{k})$. We also define a function $P(t_2,t_1,\mathbf{k})$ as follows:

$$P(t_2,t_1,\mathbf{k})\equiv K_{1,1}(t_2,t_1,\mathbf{k})+\int_0^\beta ds_1ds_2K_{2,0}(t_2,s_1,\mathbf{k})G(s_2,s_1,\,-\mathbf{k})K_{0,2}(t_1,s_2,\mathbf{k})\,. \tag{62}$$

With the aid of the three functions defined by (60)–(62), one can write down a partial solution to the integral equations (56)–(58).

$$\begin{aligned}L_{1,1}(t_2,t_1,\mathbf{k})&=\int_0^\beta dsG_{1,1}(t_2,s,\mathbf{k})P(s,t_1,\mathbf{k})\\&=\int_0^\beta dsP(t_2,s,\mathbf{k})G_{1,1}(s,t_1,\mathbf{k})\,,\end{aligned} \tag{63}$$

$$\begin{aligned}L_{0,2}(t_2,t_1,\mathbf{k})&=\int_0^\beta ds_2ds_1K_{0,2}(s_2,s_1,\mathbf{k})G_{1,1}(s_2,t_2,\mathbf{k})G(s_1,t_1,\,-\mathbf{k})-K_{0,2}^{(1)}(t_2,t_1,\mathbf{k})\\&=\int_0^\beta ds_2ds_1K_{0,2}(s_2,s_1,\mathbf{k})G(s_2,t_2,\mathbf{k})G_{1,1}(s_1,t_1,\,-\mathbf{k})-K_{0,2}^{(1)}(t_2,t_1,\mathbf{k})\,,\end{aligned} \tag{64}$$

$$\begin{aligned}L_{2,0}(t_2,t_1,\mathbf{k})&=\int_0^\beta ds_2ds_1G_{1,1}(t_2,s_2,\mathbf{k})G(t_1,s_1,\,-\mathbf{k})K_{2,0}(s_2,s_1,\mathbf{k})-\delta(t_2,t_1)K_{2,0}^{(1)}(t_2,t_1,\mathbf{k})\\&=\int_0^\beta ds_2ds_1G(t_2,s_2,\mathbf{k})G_{1,1}(t_1,s_1,\,-\mathbf{k})K_{2,0}(s_2,s_1,\mathbf{k})-\delta(t_2,t_1)K_{2,0}^{(1)}(t_2,t_1,\mathbf{k})\,.\end{aligned} \tag{65}$$

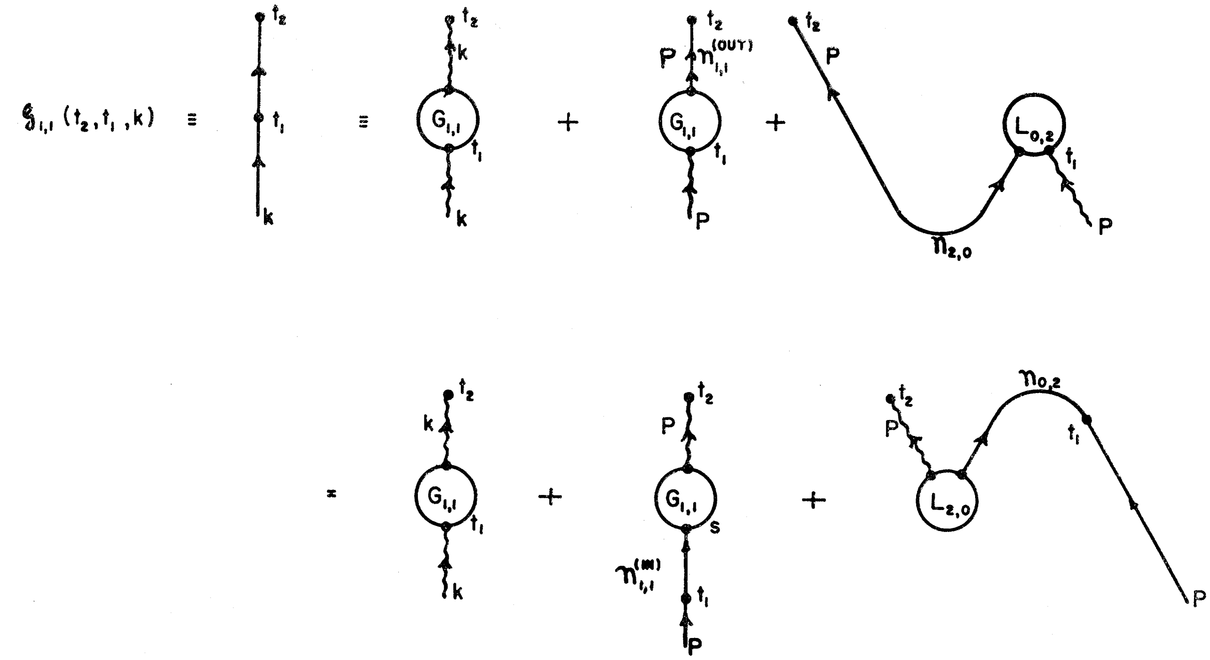

FIG. 8. The diagrammatic representation of Eq. (66). When **k** cannot be zero, then we make the replacement $\mathbf{k}\to\mathbf{p}$. The graphical symbol for $\mathcal{G}_{1,1}(t_2,t_1,\mathbf{k})$ is defined in this figure.

Equations (63)–(65) can be proved diagrammatically by iterating Eqs. (56)–(58) and then regrouping the terms. These last equations are important for the successful application of the Λ transformation in the following paper, but they are not essential to the present development. The functions $K_{0,2}{}^{(1)}(t_2,t_1,\mathbf{k})$ and $K_{2,0}{}^{(1)}(t_2,t_1,\mathbf{k})$ are defined below Eq. (59).

Equations (56)–(59) only complete the treatment of self-energy graphs, as far as irregular graphs are concerned. Thus, the internal structure of the functions $K_{\mu,\nu}(t_2,t_1,\mathbf{k})$ may include many "irregular (μ,ν) parts" in the sense that cutting any two wiggly lines *or* a wiggly line and a solid line may separate a regular graph into two parts. An *irregular* (μ,ν) *part* is then defined to be any such resulting part for which $(\mu+\nu)=2$. In order to deal effectively with this internal structure, we must introduce functions $\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{k})$ which include the sum over all irregular (μ,ν) parts. These functions will then become the "line factors" of master (μ,ν) graphs. Thus, we define (with $\mathbf{k}\to\mathbf{p}$ when **k** cannot be zero)

$$\mathcal{G}_{1,1}(t_2,t_1,\mathbf{k})\equiv G_{1,1}(t_2,t_1,\mathbf{k})+\mathfrak{N}_{1,1}{}^{(\text{out})}(t_2,\mathbf{p})G_{1,1}(\beta,t_1,\mathbf{p})+\mathfrak{N}_{2,0}(t_2,\mathbf{p})\int_0^\beta ds L_{0,2}(t_1,s,\mathbf{p})$$

$$=G_{1,1}(t_2,t_1,\mathbf{k})+\int_0^\beta ds G_{1,1}(t_2,s,\mathbf{p})\mathfrak{N}_{1,1}{}^{(\text{in})}(t_1,\mathbf{p})+L_{2,0}(t_2,\beta,\mathbf{p})\mathfrak{N}_{0,2}(t_1,\mathbf{p})\,, \tag{66}$$

$$\mathcal{G}_{0,2}(t_2,t_1,\mathbf{k})\equiv L_{0,2}(t_2,t_1,\mathbf{k})+\mathfrak{N}_{0,2}(t_2,\mathbf{p})G_{1,1}(\beta,t_1,-\mathbf{p})+\mathfrak{N}_{1,1}{}^{(\text{in})}(t_2,\mathbf{p})\int_0^\beta ds L_{0,2}(s,t_1,\mathbf{p})$$

$$=L_{0,2}(t_2,t_1,\mathbf{k})+G_{1,1}(\beta,t_2,\mathbf{p})\mathfrak{N}_{0,2}(t_1,-\mathbf{p})+\int_0^\beta ds L_{0,2}(t_2,s,\mathbf{p})\mathfrak{N}_{1,1}{}^{(\text{in})}(t_1,-\mathbf{p})\,, \tag{67}$$

$$\mathcal{G}_{2,0}(t_2,t_1,\mathbf{k})\equiv L_{2,0}(t_2,t_1,\mathbf{k})+\mathfrak{N}_{1,1}{}^{(\text{out})}(t_2,\mathbf{p})L_{2,0}(\beta,t_1,\mathbf{p})+\mathfrak{N}_{2,0}(t_2,\mathbf{p})\int_0^\beta ds G_{1,1}(t_1,s,-\mathbf{p})$$

$$=L_{2,0}(t_2,t_1,\mathbf{k})+L_{2,0}(t_2,\beta,\mathbf{p})\mathfrak{N}_{1,1}{}^{(\text{out})}(t_1,-\mathbf{p})+\int_0^\beta ds G_{1,1}(t_2,s,\mathbf{p})\mathfrak{N}_{2,0}(t_1,-\mathbf{p})\,, \tag{68}$$

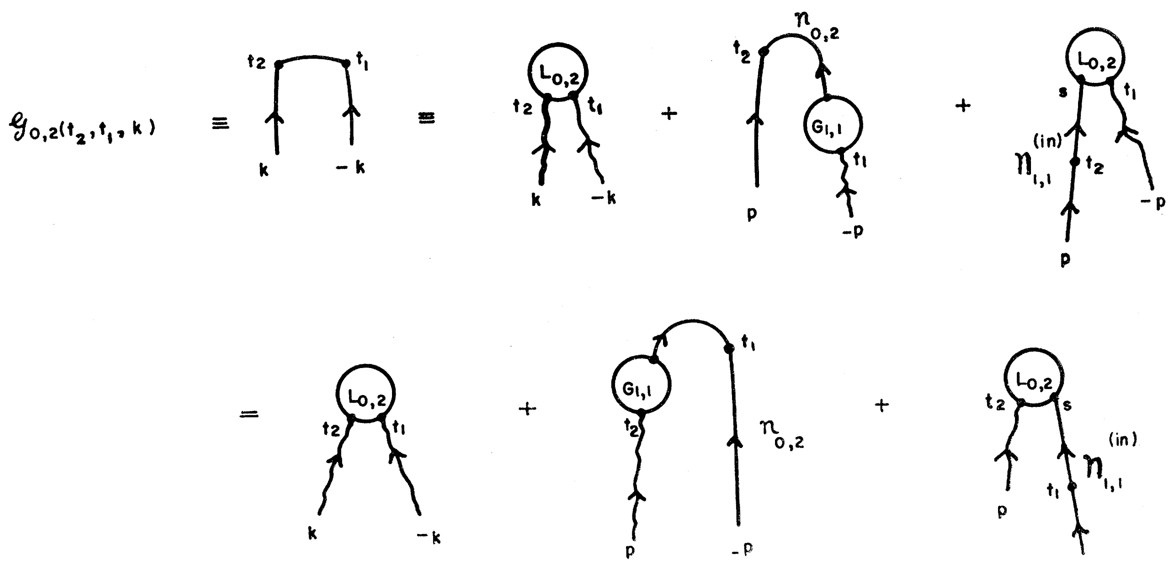

FIG. 9. The diagrammatic representation of Eq. (67). When $\mathbf{k}$ cannot be zero, then we make the replacement $\mathbf{k}\to\mathbf{p}$. The graphical symbol for $\mathcal{G}_{0,2}(t_2,t_1,\mathbf{k})$ is defined in this figure.

where the functions $\mathfrak{N}_{\mu,\nu}(t,\mathbf{p})$ are defined by the equations

$$\mathfrak{N}_{1,1}{}^{(\mathrm{out})}(t,\mathbf{p})\equiv N_{1,1}(\mathbf{p})\int_0^\beta dsG_{1,1}(t,s,\mathbf{p})+N_{0,2}(\mathbf{p})L_{2,0}(t,\beta,\mathbf{p})\underset{t\to\beta}{\longrightarrow}\langle n(\mathbf{p})\rangle=[\exp\beta(\omega_{\mathbf{p}}-g)N_{1,1}(\mathbf{p})-1], \tag{69}$$

$$\mathfrak{N}_{1,1}{}^{(\mathrm{in})}(t,\mathbf{p})\equiv N_{1,1}(\mathbf{p})G_{1,1}(\beta,t,\mathbf{p})+N_{2,0}(\mathbf{p})\int_0^\beta dsL_{0,2}(t,s,\mathbf{p}),\qquad \int_0^\beta dt\mathfrak{N}_{1,1}{}^{(\mathrm{in})}(t,\mathbf{p})=\langle n(\mathbf{p})\rangle, \tag{70}$$

$$\mathfrak{N}_{0,2}(t,\mathbf{p})\equiv N_{0,2}(\mathbf{p})G_{1,1}(\beta,t,\mathbf{p})+N_{1,1}(-\mathbf{p})\int_0^\beta dsL_{0,2}(t,s,\mathbf{p}),\qquad \int_0^\beta dt\mathfrak{N}_{0,2}(t,\mathbf{p})=\exp\beta(\omega_{\mathbf{p}}-g)N_{0,2}(\mathbf{p}), \tag{71}$$

$$\mathfrak{N}_{2,0}(t,\mathbf{p})\equiv N_{2,0}(\mathbf{p})\int_0^\beta dsG_{1,1}(t,s,\mathbf{p})+N_{1,1}(-\mathbf{p})L_{2,0}(t,\beta,\mathbf{p})\underset{t\to\beta}{\longrightarrow}\exp\beta(\omega_{\mathbf{p}}-g)N_{2,0}(\mathbf{p}). \tag{72}$$

The second parts of each of Eqs. (69)–(72) can be verified by combining Eqs. (54), (59), (31), and (35)–(37), The diagrammatic representation of Eqs. (66)–(68) is given in Figs. 8–10, and the graphical symbols for each of the $\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{k})$ are also defined in the figures. The diagrammatic representation of Eqs. (69)–(72) is given in Figs. 11 and 12, and, again, the graphical symbols for each of the $\mathfrak{N}_{\mu,\nu}(t,\mathbf{p})$ are defined in the figures. It is instructive to demonstrate the equivalence of the two forms of each of Eqs. (66)–(68) by substituting Eqs. (69)–(72). It is then fairly easy to demonstrate that the $\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{k})$ represent the sums over all possible irregular (μ,ν) parts as defined below Eq. (65). With this observation we can now introduce master (μ,ν) graphs.

Master (μ,ν) Graphs

A *Qth-order, master (μ,ν) graph* is a collection of Q cluster vertices (Fig. 1) which are entirely interconnected by m solid lines. In addition to these internal lines, there are also μ outgoing external solid lines and ν incoming external solid lines. There are no wiggly lines in master (μ,ν) graphs. Each internal line carries two arrows, one for each end, whereas the external lines each carry only one arrow. Thus, there are three different kinds of internal lines depending on whether the two arrows are parallel to each other, point towards each other, or point away from each other. Master (μ,ν) graphs are irreducible (see Sec. 4). The rules for connecting the Q cluster vertices by the m internal lines and the procedures for determining the corresponding expression are as follows:

(i) Associate with each missing (zero-momentum) outgoing line a factor of $(x\Omega)^{1/2}e^{\beta g}G_{\mathrm{out}}(t)$ and with each missing incoming line a factor of $(x\Omega)^{1/2}G_{\mathrm{in}}(t)$ [see Eqs. (42)]. For each pair of missing incoming (or outgoing) lines which occurs at the same vertex a factor of $\frac{1}{2}$ must

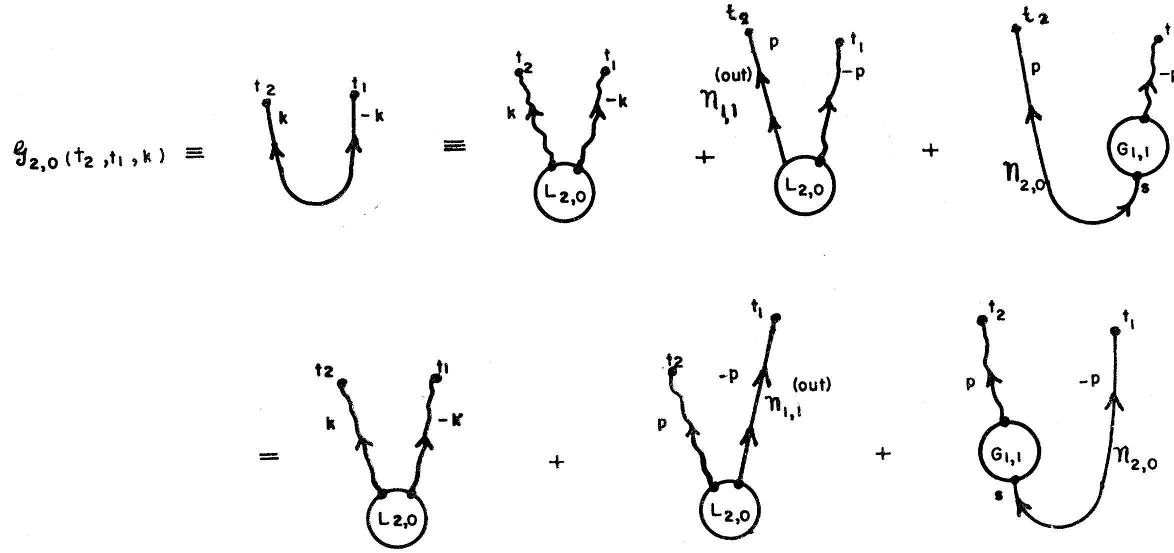

FIG. 10. The diagrammatic representation of Eq. (68). When $\mathbf{k}$ cannot be zero, then we make the replacement $\mathbf{k}\rightarrow\mathbf{p}$. The graphical symbol for $\mathcal{G}_{2,0}(t_2,t_1,\mathbf{k})$ is defined in this figure.

be included in the corresponding expression for the graph.

(ii) External lines are associated with pregiven momenta $\mathbf{p}$, 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.

(iii) Two master (μ,ν) graphs are different if their topological structures, including arrow directions and external line assignments, are different.

(iv) Associate with each arrow of the m internal lines a different integer i $(i=1, 2, \cdots, 2m)$ and a corresponding momentum $\mathbf{k}_i$.

(v) 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 $2m$ integers associated with the arrows of the internal lines, which leave the graph topologically unchanged (including the positions of these integers with respect to the arrows).

(vi) Assign a different temperature variable to each of the Q cluster vertices and to the head end of each (internal) arrow which points away from a cluster vertex. Associate with the entire graph a product of Q pair functions (18) corresponding to the Q cluster vertices and the momentum variable assignments of rules (ii) and (iv).

(vii) Assign a factor to each internal line with arrows i and j of $\delta(\mathbf{k}_i,\mathbf{k}_j)\mathcal{G}_{1,1}(t,s,\mathbf{k}_i)$ when the arrows are pointing parallel to each other, $\delta(\mathbf{k}_i,-\mathbf{k}_j)\mathcal{G}_{0,2}(t,s,\mathbf{k}_i)$ when the

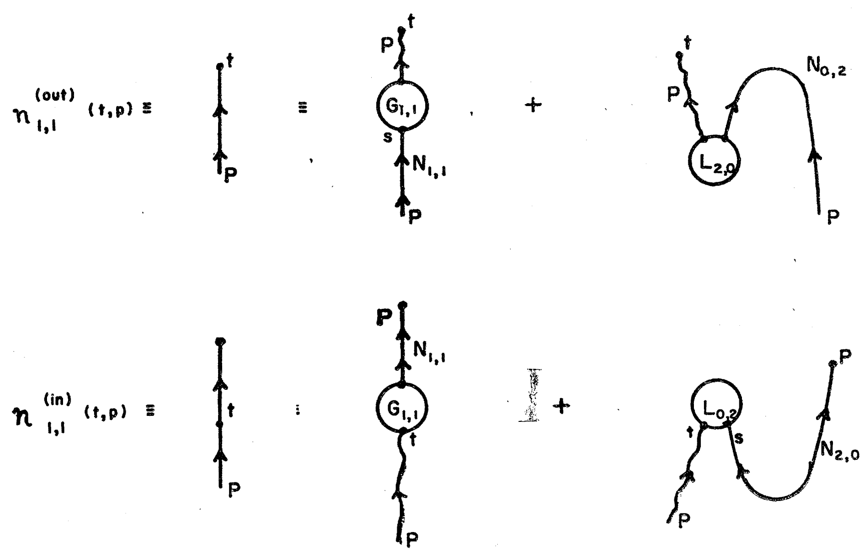

FIG. 11. The diagrammatic representation of Eqs. (69) and (70). The graphical symbols for $\mathfrak{N}_{1,1}{}^{(\text{out})}(t,\mathbf{p})$ and $\mathfrak{N}_{1,1}{}^{(\text{in})}(t,\mathbf{p})$ are defined in this figure.

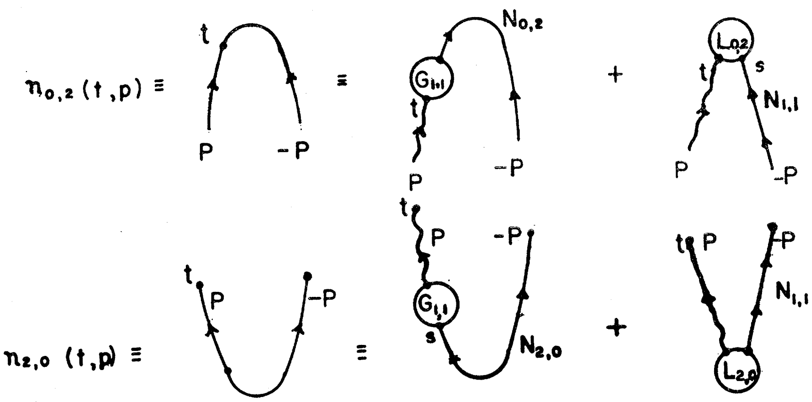

FIG. 12. The diagrammatic representation of Eqs. (71) and (72). The graphical symbols for $\mathfrak{N}_{0,2}(t,\mathbf{p})$ and $\mathfrak{N}_{2,0}(t,\mathbf{p})$ are defined in this figure.

arrows are pointing towards each other, and $\delta(\mathbf{k}_i, -\mathbf{k}_j) \times \mathcal{G}_{2,0}(t,s,\mathbf{k}_i)$ when the arrows are pointing away from each other, where the temperature variables t and s are determined by the assignments of rule (vi) (see also Figs. 8–10). Here, the $\delta(\ ,\ )$ symbols are Kronecker δ's.

(viii) When two internal lines connecting the same two vertices are associated with the product $\mathcal{G}_{1,1}(t_3,t_1,\mathbf{k}_1) \times \mathcal{G}_{1,1}(t_3,t_2,\mathbf{k}_2)$, then the wiggly-line double-bond term $\delta(t_3-t_1)\cdot\delta(t_3-t_2)$ must be subtracted [see rule (i) for linked-pair (μ,ν) graphs in Sec. 3].

(ix) Finally, sum over the $2m$ internal momentum coordinates and integrate from 0 to β over each of the temperature variables as assigned in rule (vi) and to the outgoing zero-momentum factors of rule (i).

In Fig. 13 we give some examples of master (0,0) graphs together with their associated symmetry numbers. In order to distinguish master (μ,ν) graphs from the preceding graphs of Secs. 3 and 4, a circle is placed around each cluster vertex. The circle also makes it easier to distinguish internal-line temperature variables from the

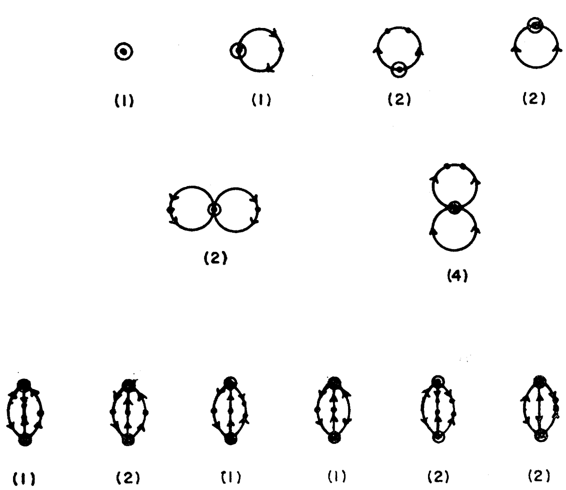

FIG. 13. Some examples of master (0,0) graphs. Below each graph is included its symmetry number S. For convenience, the temperature variables of the cluster vertices (circled) and of the line factors $\mathcal{G}_{\mu,\nu}$ have been omitted.

cluster vertices [see rule (vi)]. When $(\mu,\nu)\neq(0,0)$, it is more convenient to consider master (μ,ν) L graphs instead of the master (μ,ν) graphs just defined.

Master (μ,ν) *L* Graphs

A *master* (μ,ν) *L graph*, where $(\mu,\nu)\neq(0,0)$, is defined to be a master (μ,ν) graph with wiggly external lines and in which (1) each integration over a temperature variable at a vertex to which an incoming external line (if any) attaches is not performed; and (2) the pair-function "upper temperature variable" (see Fig. 1) corresponding to an outgoing external line is a variable $t<\beta$.

We can now write the functions $K_{\mu,\nu}(t_2,t_1,\mathbf{k})$ of Eq. (55) in terms of master (μ,ν) L graphs as follows:

$$K_{\mu,\nu}(t_2,t_1,\mathbf{k})=\sum_{Q=1}^{\infty}\left[\text{all different } Q\text{th-order master } (\mu,\nu)\ L \text{ graphs}\right]_{\mathbf{k}}, \quad (73)$$

where $(\mu,\nu)=(1,1)$, (0,2), or (2,0). Equation (73) can be proved by substituting the $\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{k})$ functions of Eqs. (66)–(68) into the master (μ,ν) L graphs and showing that the expanded form gives Eq. (55). There are no real symmetry number complications in this proof. It is only the cyclic symmetry of (0,0) graphs which produces the difficulties of the next section, where the grand potential is expressed in terms of master (μ,ν) graphs.

7. MASTER GRAPH EXPANSION OF THE GRAND POTENTIAL

The master graph formulation of quantum statistics, outlined at the end of the preceding section, completes the analysis in this paper of self-energy graphs as discussed at the beginning of Secs. 4 and 6. Thus, in Eq. (73), all of the "self-energy structure" is contained in the line factors $\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{k})$ of Eqs. (66)–(68). Unfortunately, the simplicity with which Eq. (73) can be derived does not carry over into the corresponding derivation of a master-graph expansion of the grand potential. It is the purpose of this section to carry through the latter derivation and we begin by examining the third term in the grand potential (52). With the aid of Eq. (35)

this term can be written as

$$\sum_{\mathbf{p}}[\nu^{-1}(\mathbf{p})N_{1,1}(\mathbf{p})-1]$$
$$=\sum_{\mathbf{p}}[N_{1,1}(\mathbf{p})K_{1,1}(\mathbf{p})+\tfrac{1}{2}N_{2,0}(\mathbf{p})K_{0,2}(\mathbf{p})K_{0,2}(\mathbf{p})+\tfrac{1}{2}N_{0,2}(\mathbf{p})K_{2,0}(\mathbf{p})]$$
$$=\sum_{\mathbf{p}}[\sum_{(1,1)}N_{1,1}(\mathbf{p})S_{1,1}^{-1}T_{1,1}(\mathbf{p})+\tfrac{1}{2}\sum_{(0,2)}N_{2,0}(\mathbf{p})S_{0,2}^{-1}T_{0,2}(\mathbf{p})+\tfrac{1}{2}\sum_{(2,0)}N_{0,2}(\mathbf{p})S_{2,0}^{-1}T_{2,0}(\mathbf{p})], \quad (74)$$

where in the second line we have substituted Eq. (47) in the form

$$K_{\mu,\nu}(\mathbf{p})=\sum_{(\mu,\nu)}S_{\mu,\nu}^{-1}T_{\mu,\nu}(\mathbf{p}). \quad (75)$$

In Eq. (75) the sum is over all different zero-regular dual (μ,ν) graphs $S_{\mu,\nu}^{-1}T_{\mu,\nu}(\mathbf{p})$, where $S_{\mu,\nu}$ is the symmetry number of any given graph.

The sum over $\mathbf{p}$ in the second line of Eq. (74) is equivalent to converting each zero-regular dual (μ,ν) graph, multiplied by $N_{\nu,\mu}(\mathbf{p})$, into a (0,0) graph. In fact, by studying the relation between the symmetry number $S_{\mu,\nu}$ of a given zero-regular dual (μ,ν) graph, where $(\mu+\nu)=2$, to the number of ways in which this (μ,ν) graph can be obtained by breaking any line of the corresponding (0,0) graph, one can show that

$$\sum_{\mathbf{p}}[\nu^{-1}(\mathbf{p})N_{1,1}(\mathbf{p})-1]=\sum_{(0,0)}N_{0,0}S_{0,0}^{-1}T_{0,0}. \quad (76)$$

In Eq. (76), the sum on the right-hand side is over all zero-regular dual (0,0) graphs $S_{0,0}^{-1}T_{0,0}$ with $N_{0,0}$ lines and symmetry number $S_{0,0}$. The proof of (76) is made by carefully applying lemma 1 in Appendix G of LY V to the second line of (74). Equation (76) can then be substituted into Eq. (52) for the grand potential to give

$$\Omega f(x,\beta,g,\Omega)=\sum_{\mathbf{p}}\ln\{\exp\beta(\omega_{\mathbf{p}}-g)[N_{1,1}(\mathbf{p})N_{1,1}(-\mathbf{p})-N_{0,2}(\mathbf{p})N_{2,0}(\mathbf{p})]^{1/2}\}$$
$$-\sum_{(0,0)}(N_{0,0}-1)S_{0,0}^{-1}T_{0,0}-x\Omega+(x\Omega e^{\beta g})\left[G_{\text{in}}(\beta)-\int_0^\beta dtG_{\text{out}}(t)K_{\text{in}}(t)\right]. \quad (77)$$

In order to proceed it is now necessary to define open and closed (μ,ν) graphs.

Definitions

An *open* (μ,ν) graph is a zero-regular dual (μ,ν) graph which can be separated into two parts, one of which is a zero-regular (μ,ν) L graph with $\mu+\nu=2$, by cutting one solid line and one wiggly line. A *closed* (μ,ν) graph is a zero-regular dual (μ,ν) graph which is *not open*, and in which the following replacements are made for the solid line factors of rule (viii) in Sec. 4.

$$N_{\mu,\nu}(\mathbf{p})\to[\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{p})-G_{\mu,\nu}(t_2,t_1,\mathbf{p})],$$

where, with $\mu+\nu=2$,

$$G_{\mu,\nu}(t_2,t_1,\mathbf{k})\equiv\delta_{\mu,\nu}\delta(t_2-t_1)+L_{\mu,\nu}(t_2,t_1,\mathbf{k}). \quad (78)$$

With the aid of these definitions, one can prove the following identity:

$$\sum_{(0,0)}(N_{0,0}-1)S_{0,0}^{-1}T_{0,0}=\sum_{(0,0)C}(N_{0,0}-1)S_{0,0}^{-1}T_{0,0}^{(C)}, \quad (79)$$

where the sum of the right-hand side of (79) is over all closed (0,0) graphs. This identity can be proved by generalizing the proof given for the corresponding $\langle x\rangle=0$ case in Appendix A of Ref. 17. We shall not give the generalization here as it does not involve any new difficulties.

Before substituting Eq. (79) into the grand potential (77) we consider the first term on the right-hand side of (79) and carry through, in reverse, the steps leading from Eqs. (74) to (76), as applied to closed graphs. This gives the result

$$\sum_{(0,0)C}N_{0,0}S_{0,0}^{-1}T_{0,0}^{(C)}=\tfrac{1}{2}\sum_{\mathbf{p}}\int_0^\beta dt_2dt_1\sum_{\substack{(\mu,\nu)\\ \mu+\nu=2}}(1+\delta_{\mu,\nu})[\mathcal{G}_{\nu,\mu}(t_1,t_2,\mathbf{p})-G_{\nu,\mu}(t_1,t_2,\mathbf{p})]K_{\mu,\nu}(t_2,t_1,\mathbf{p}), \quad (80)$$

where the sum over (μ,ν) is here over the three possibilities for which $\mu+\nu=2$, and the $K_{\mu,\nu}(t_2,t_1,\mathbf{k})$ are now given by

$$K_{\mu,\nu}(t_2,t_1,\mathbf{k})=\sum_{Q=1}^{\infty}[\text{all different }Q\text{th-order closed }(\mu,\nu)\ L\text{ graphs}]_{\mathbf{k}}, \quad (81)$$

instead of by Eq. (55). Upon substituting Eqs. (79) and (80) into Eq. (77) we obtain for the grand potential

$$\Omega f(x,\beta,g,\Omega)=\sum_{\mathbf{p}}\ln\{\exp\beta(\omega_{\mathbf{p}}-g)[N_{1,1}(\mathbf{p})N_{1,1}(-\mathbf{p})-N_{0,2}(\mathbf{p})N_{2,0}(\mathbf{p})]^{1/2}\}$$

$$+\sum_{(0,0)C}S_{0,0}{}^{-1}T_{0,0}{}^{(C)}-x\Omega+(x\Omega e^{\beta g})\left[G_{\text{in}}(\beta)-\int_0^\beta dtG_{\text{out}}(t)K_{\text{in}}(t)\right]$$

$$-\tfrac{1}{2}\sum_{\mathbf{k}}\int_0^\beta dt_2dt_1\sum_{\substack{(\mu,\nu)\\ \mu+\nu=2}}(1+\delta_{\mu,\nu})[\mathcal{G}_{\nu,\mu}(t_1,t_2,\mathbf{k})-G_{\nu,\mu}(t_1,t_2,\mathbf{k})]K_{\mu,\nu}(t_2,t_1,\mathbf{k}).\quad(82)$$

In Eq. (82) it should be clear, from the quantities being summed over, that the sum $\sum_{(0,0)C}$ is a sum over all different closed (0,0) graphs, whereas the sum $\sum_{(\mu,\nu)}$, with $\mu+\nu=2$, is a sum over only three different terms. This somewhat confusing situation will be alleviated by our subsequent treatment of the former term. In fact, we now observe that all of the terms in (82) except the sum over closed (0,0) graphs can be expressed in terms of master (μ,ν) graphs, using the results of Sec. 6. In particular, Eq. (81) is an unnecessary expression, its usefulness only being for the derivation of Eq. (80), and we may immediately replace it by Eq. (73). We finally observe that there is no $\mathbf{k}=0$ contribution to the last term in Eq. (82) according to Eqs. (66)–(68), and this justifies the replacement of $\mathbf{p}$ by $\mathbf{k}$ in Eq. (80) before it is substituted into (77).

The most difficult step in the analysis of this section is the derivation of an expression for the sum over all closed (0,0) graphs in Eq. (82) in terms of master (μ,ν) graphs. In order to facilitate this analysis, it is necessary to define several new quantities, the first of which is

$$\Omega F(x,\beta,g,\Omega)\equiv\sum_{Q=1}^{\infty}[\text{all different }Q\text{th-order master (0,0) graphs}].\quad(83)$$

The problem is to determine an expression for the difference between this quantity and the sum over all closed (0,0) graphs. This difference can be expressed in terms of the following quantities which are generalizations of the $L_{\mu,\nu}(t_2,t_1,\mathbf{k})$ and $G_{\mu,\nu}(t_2,t_1,\mathbf{k})$, defined by Eqs. (56)–(59) and (78).

$$L_{1,1}{}^{(\tau)}(t_2,t_1,\mathbf{k})\equiv\int_0^\tau ds[G_{1,1}{}^{(\tau)}(t_2,s,\mathbf{k})K_{1,1}(s,t_1,\mathbf{k})+L_{2,0}{}^{(\tau)}(t_2,s,\mathbf{k})K_{0,2}(s,t_1,\mathbf{k})],\quad(84)$$

$$L_{0,2}{}^{(\tau)}(t_2,t_1,\mathbf{k})\equiv\int_0^\tau ds[L_{0,2}{}^{(\tau)}(t_2,s,\mathbf{k})K_{1,1}(s,t_1,-\mathbf{k})+G_{1,1}{}^{(\tau)}(s,t_2,\mathbf{k})K_{0,2}(s,t_1,\mathbf{k})]-K_{0,2}{}^{(1)}(t_2,t_1,\mathbf{k}),\quad(85)$$

$$L_{2,0}{}^{(\tau)}(t_2,t_1,\mathbf{k})\equiv\int_0^\tau ds[L_{2,0}{}^{(\tau)}(t_2,s,\mathbf{k})K_{1,1}(t_1,s,-\mathbf{k})+G_{1,1}{}^{(\tau)}(t_2,s,\mathbf{k})K_{2,0}(s,t_1,\mathbf{k})]-\delta(t_2,t_1)K_{2,0}{}^{(1)}(t_2,t_1,\mathbf{k}),\quad(86)$$

$$G_{\mu,\nu}{}^{(\tau)}(t_2,t_1,\mathbf{k})\equiv\delta(t_2-t_1)\delta_{\mu,\nu}+L_{\mu,\nu}{}^{(\tau)}(t_2,t_1,\mathbf{k}),\quad(87)$$

where $\beta>\tau\geqq(t_2,t_1)$ and the functions $K_{0,2}{}^{(1)}(t_2,t_1,\mathbf{k})$ and $K_{2,0}{}^{(1)}(t_2,t_1,\mathbf{k})$ are defined below Eq. (59). The integral equations (84)–(86) serve to define the functions $L_{\mu,\nu}{}^{(\tau)}(t_2,t_1,\mathbf{k})$ for a general temperature parameter τ. It should be emphasized that these definitions do not entail any modifications of the *internal line factors* $\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{k}')$ of the $K_{\mu,\nu}(t_2,t_1,\mathbf{k})$ and the $L_{\mu,\nu}{}^{(\tau)}(t_2,t_1,\mathbf{k})$.

We now state the result which one obtains for the difference between the sum over all closed (0,0) graphs and ΩF of Eq. (83).

$$\left[\sum_{(0,0)C}S_{0,0}{}^{-1}T_{0,0}{}^{(C)}-\Omega F(x,\beta,g,\Omega)\right]=-\tfrac{1}{2}\sum_{\mathbf{k}}\int_0^\beta dt_2dt_1\sum_{\substack{(\mu,\nu)\\ \mu+\nu=2}}(1+\delta_{\mu,\nu})G_{\nu,\mu}(t_1,t_2,\mathbf{k})K_{\mu,\nu}(t_2,t_1,\mathbf{k})$$

$$+\tfrac{1}{2}\sum_{\mathbf{k}}\int_0^\beta dt_1\int_0^{t_1}dt_2\Big\{\sum_{\substack{(\mu,\nu)\\ \mu+\nu=2}}G_{\nu,\mu}{}^{(t_1)}(t_1,t_2,\mathbf{k})K_{\mu,\nu}(t_2,t_1,\mathbf{k})+G_{1,1}{}^{(t_1)}(t_2,t_1,\mathbf{k})K_{1,1}(t_1,t_2,\mathbf{k})\Big\}.\quad(88)$$

Equation (88) can be derived by first proving a generalization of Eq. (54) in Ref. 17 to the case $\langle x\rangle\neq0$. The proof for the $\langle x\rangle\neq0$ generalization is very similar to that given in Appendix B of Ref. 17 for the $\langle x\rangle=0$ case and we shall not repeat it here. The second step in the derivation of Eq. (88) is made by applying the following theorem: If

$f(t_1,t_2,\cdots,t_m)$ is a cyclic function in the m temperature variables, then

$$m^{-1}\int_0^\beta dt_m\int_0^\beta dt_{m-1}\cdots\int_0^\beta dt_1 f(t_1,t_2,\cdots t_m)=\int_0^\beta dt_m\int_0^{t_m} dt_{m-1}\int_0^{t_m} dt_{m-2}\cdots\int_0^{t_m} dt_1 f(t_1,t_2,\cdots t_m)\,. \tag{89}$$

In the application of Eq. (89) to a cycle of $K_{\mu,\nu}(t_2,t_1,\mathbf{k})$ functions, one must observe that the arrows on the wiggly lines of this cycle, change direction at every $K_{0,2}$ and $K_{2,0}$ function. For this reason one obtains both of the $G_{1,1}K_{1,1}$ terms in the second part of Eq. (88).

We finally note that although the corresponding second lines of Eqs. (56)–(58) have not been repeated in Eqs. (84)–(86), they are nevertheless valid, as one can easily verify by iteration. For example, the corresponding second line of Eq. (84) is

$$\begin{aligned}L_{1,1}^{(\tau)}(t_2,t_1,\mathbf{k})&=\int_0^\tau ds[K_{1,1}(t_2,s,\mathbf{k})G_{1,1}^{(\tau)}(s,t_1,\mathbf{k})+K_{2,0}(t_2,s,\mathbf{k})L_{0,2}^{(\tau)}(s,t_1,\mathbf{k})]\\&=\int_0^\tau ds[K_{1,1}(t_2,s,\mathbf{k})G_{1,1}^{(\tau)}(s,t_1,\mathbf{k})+K_{2,0}(s,t_2,-\mathbf{k})L_{0,2}^{(\tau)}(t_1,s,-\mathbf{k})]\,,\end{aligned} \tag{90}$$

where the second line of Eq. (90) follows from the identity $L_{2,0}^{(\tau)}(t_2,t_1,\mathbf{k})=L_{2,0}^{(\tau)}(t_1,t_2,-\mathbf{k})$ which can be easily proved [see below Eqs. (53) and (55) for the case $\tau=\beta$].

If Eqs. (88) and (90) are now substituted into Eq. (82) one obtains the final result of this section

$$\begin{aligned}\Omega f(x,\beta,g,\Omega)=&\sum_{\mathbf{p}}\ln\{\exp\beta(\omega_{\mathbf{p}}-g)[N_{1,1}(\mathbf{p})N_{1,1}-(\mathbf{p})-N_{0,2}(\mathbf{p})N_{2,0}(\mathbf{p})]^{1/2}\}+(x\Omega e^{\beta g})\left[G_{\text{in}}(\beta)-\int_0^\beta dtG_{\text{out}}(t)K_{\text{in}}(t)\right]-x\Omega\\&-\tfrac{1}{2}\sum_{\mathbf{k}}\int_0^\beta dt_1dt_2\{\sum_{\substack{(\mu,\nu)\\ \mu+\nu=2}}(1+\delta_{\mu,\nu})\mathcal{G}_{\nu,\mu}(t_1,t_2,\mathbf{k})K_{\mu,\nu}(t_2,t_1,\mathbf{k})+K_{2,0}^{(1)}(t_1,t_2,\mathbf{k})K_{0,2}^{(1)}(t_2,t_1,\mathbf{k})\}\\&+\Omega F(x,\beta,g,\Omega)+\sum_{\mathbf{k}}\int_0^\beta dt_1L_{1,1}^{(t_1)}(t_1,t_1,\mathbf{k})\,,\end{aligned} \tag{91}$$

where we have also used Eq. (84) to obtain the last term. The $K_{2,0}^{(1)}(t_1,t_2,\mathbf{k})\times K_{0,2}^{(1)}(t_2,t_1,\mathbf{k})$ term originates in Eq. (88), and the factor $\delta(t_2-t_1)$ in this product makes it possible to change the t_2 integration limits for this term. [Note that the integral of a δ function times a step function of the same argument equals $\frac{1}{2}$.] In Eq. (91), every quantity can be expressed in terms of master (μ,ν) L graphs or master (0,0) graphs. The objective of this section has therefore been achieved. In the application of Eq. (91), however, one requires $L_{1,1}^{\tau}(t_2,t_1,\mathbf{k})$ in a form similar to Eq. (63) for the case $\tau=\beta$. Thus, we write

$$\begin{aligned}L_{1,1}^{(\tau)}(t_2,t_1,\mathbf{k})&=\int_0^\tau dsG_{1,1}^{(\tau)}(t_2,s,\mathbf{k})P^{(\tau)}(s,t_1,\mathbf{k})\,,\\G_{1,1}^{(\tau)}(t_2,t_1,\mathbf{k})&=\delta(t_2-t_1)+L_{1,1}^{(\tau)}(t_2,t_1,\mathbf{k})\,,\\P^{(\tau)}(t_2,t_1,\mathbf{k})&=K_{1,1}(t_2,t_1,\mathbf{k})+\int_0^\tau ds_1ds_2K_{2,0}(t_2,s_1,\mathbf{k})G^{(\tau)}(s_2,s_1,-\mathbf{k})K_{0,2}(t_1,s_2,\mathbf{k})\,,\\G^{(\tau)}(t_2,t_1,\mathbf{k})&=\delta(t_2-t_1)+L^{(\tau)}(t_2,t_1,\mathbf{k})\,,\\L^{(\tau)}(t_2,t_1,\mathbf{k})&=\int_0^\tau dsG^{(\tau)}(t_2,s,\mathbf{k})K_{1,1}(s,t_1,\mathbf{k})\,.\end{aligned} \tag{92}$$

Also, the calculation of the zero-momentum factors $K_{\text{in}}(t)$ and $K_{\text{out}}(t)$ must be stated in the master graph formulation. By referring to the definitions of these factors, (44) and (45), one can verify that the expressions

$$\begin{aligned}K_{\text{in}}(t)&=(x\Omega e^{\beta g})^{-1}[\delta(\Omega F)/\delta G_{\text{out}}(t)]|\mathcal{G}\,,\\K_{\text{out}}(t)&=(x\Omega e^{\beta g})^{-1}[\delta(\Omega F)/\delta G_{\text{in}}(t)]|\mathcal{G}\,,\end{aligned} \tag{93}$$

where $\Omega F(x,\beta,g,\Omega)$ is defined by Eq. (83), are correct. In Eqs. (93), the line factors $\mathcal{G}_{\mu,\nu}(t_2,t_1,\mathbf{k})$ are to be held constant in the functional differentiations. It is somewhat remarkable that the expressions (93) are equivalent to (44) and (45).

8. PAIR-DISTRIBUTION FUNCTION

The pair-distribution function $P_2(\mathbf{r},\mathbf{r}')$ is a quantity of considerable interest in a many-body system because its Fourier transform is directly related to the scattering cross-section measurement when a weakly interacting particle is scattered from the system. Thus, it is a directly measurable quantity. Its microscopic definition for $\langle N\rangle \ggg 1$ is

$$P_2(\mathbf{r},\mathbf{r}') \equiv n^{-2}[\langle n(\mathbf{r})n(\mathbf{r}')\rangle - \langle n(\mathbf{r})\rangle \delta(\mathbf{r},\mathbf{r}')], \quad (94)$$

where $n(\mathbf{r})$ is the number of particles at the position $\mathbf{r}$ and $\delta(\mathbf{r},\mathbf{r}')$ is a Kronecker δ of the positions $\mathbf{r}$ and $\mathbf{r}'$.

The definition (94) is not directly useful for a calculation applied to a degenerate system, characterized by momentum space ordering. However, the pair-distribution function can also be calculated by computing the Fourier transform of the off-diagonal reduced density matrix elements $\langle \mathbf{k}_1\mathbf{k}_2|\rho_2|\mathbf{k}_1'\mathbf{k}_2'\rangle$, Eq. (10). Thus, we may write

$$P_2(\mathbf{r},\mathbf{r}') = (n\Omega)^{-2} \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} e^{i(\mathbf{k}_1-\mathbf{k}_1')\cdot(\mathbf{r}-\mathbf{r}')} \times \langle \mathbf{k}_1\mathbf{k}_2|\rho_2|\mathbf{k}_1'\mathbf{k}_2'\rangle \equiv D(\mathbf{r}-\mathbf{r}'), \quad (94a)$$

where we have used the conservation of momentum of the density matrix elements to simplify the exponential factor and to demonstrate that it is a function of the difference $(\mathbf{r}-\mathbf{r}')$ only.

As with the momentum distribution, discussed at the end of Sec. 3, we must consider the various cases $\mathbf{k}_i=0$ and $\mathbf{k}_i=\mathbf{p}_i$ in Eq. (94a) separately.

An Ursell expansion applied to Eq. (10) yields the following results:

$$\begin{aligned}
\langle 00|\rho_2|00\rangle &= \langle (L^2-L)\rangle = (\langle x\rangle\Omega)^2,\\
\langle \mathbf{p}_1 0|\rho_2|\mathbf{p}_1'0\rangle &= \langle \mathbf{p}_1 0|\rho_2|0\mathbf{p}_1'\rangle = \langle x\rangle\Omega\langle n(\mathbf{p}_1)\rangle\delta(\mathbf{p}_1,\mathbf{p}_1'),\\
\langle 00|\rho_2|\mathbf{p}_1',\mathbf{p}_2'\rangle &= \langle x\rangle\Omega N_{0,2}(\mathbf{p}_1')\exp\beta[\omega(\mathbf{p}_1')+\omega(-\mathbf{p}_1')]\delta(\mathbf{p}_1',-\mathbf{p}_2'),\\
\langle \mathbf{p}_1\mathbf{p}_2|\rho_2|00\rangle &= \langle x\rangle\Omega N_{2,0}(\mathbf{p}_1)\delta(\mathbf{p}_1,-\mathbf{p}_2),\\
\langle \mathbf{p}_1 0|\rho_2|\mathbf{p}_1'\mathbf{p}_2'\rangle &= \langle x\rangle\Omega\nu(\mathbf{p}_1)[1+\nu(\mathbf{p}_1')][1+\nu(\mathbf{p}_2')]P_{1,2}\begin{pmatrix}\mathbf{p}_1\,0\\ \mathbf{p}_1'\mathbf{p}_2'\end{pmatrix},\\
\langle \mathbf{p}_1\mathbf{p}_2|\rho_2|\mathbf{p}_1'0\rangle &= \langle x\rangle\Omega\nu(\mathbf{p}_1)\nu(\mathbf{p}_2)[1+\nu(\mathbf{p}_1')]P_{2,1}\begin{pmatrix}\mathbf{p}_1\mathbf{p}_2\\ \mathbf{p}_1'0\end{pmatrix},\\
\langle \mathbf{p}_1\mathbf{p}_2|\rho_2|\mathbf{p}_1'\mathbf{p}_2'\rangle &= \langle n(\mathbf{p}_1)\rangle\langle n(\mathbf{p}_2)\rangle[\delta(\mathbf{p}_1,\mathbf{p}_1')\delta(\mathbf{p}_2,\mathbf{p}_2')+\delta(\mathbf{p}_1,\mathbf{p}_2')\delta(\mathbf{p}_2,\mathbf{p}_1')]\\
&\quad + N_{2,0}(\mathbf{p}_1)N_{0,2}(\mathbf{p}_1')\exp\beta[\omega(\mathbf{p}_1')+\omega(-\mathbf{p}_1')]\delta(\mathbf{p}_1,-\mathbf{p}_2)\delta(\mathbf{p}_1',-\mathbf{p}_2')\\
&\quad + \nu(\mathbf{p}_1)\nu(\mathbf{p}_2)[1+\nu(\mathbf{p}_1')][1+\nu(\mathbf{p}_2')]P_{2,2}\begin{pmatrix}\mathbf{p}_1\,\mathbf{p}_2\\ \mathbf{p}_1'\mathbf{p}_2'\end{pmatrix},
\end{aligned} \quad (95)$$

where

$$\begin{aligned}
P_{1,2}\begin{pmatrix}\mathbf{p}_1\,0\\ \mathbf{p}_1'\mathbf{p}_2'\end{pmatrix} &\equiv (x\Omega)^{-1/2}\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order linked-pair (1,2) graphs}],\\
P_{1,2}\begin{pmatrix}\mathbf{p}_1\mathbf{p}_2\\ \mathbf{p}_1'0\end{pmatrix} &\equiv (x\Omega)^{-1/2}\sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order linked-pair (2,1) graphs}],\\
P_{2,2}\begin{pmatrix}\mathbf{p}_1\,\mathbf{p}_2\\ \mathbf{p}_1'\mathbf{p}_2'\end{pmatrix} &\equiv \sum_{Q=1}^{\infty}[\text{all different } Q\text{th-order linked-pair (2,2) graphs}],
\end{aligned} \quad (96)$$

and the linked-pair (μ,ν) graphs are defined in Sec. 3. In Eqs. (96) we must set $x=\langle x\rangle$ at the end of any calculation, as in Eq. (29). We observe that we can use the first of Eqs. (95) and Eq. (29) to verify that the fluctuation in the average number of zero-momentum bosons in a system with $\langle x\rangle > 0$ is $\langle(\Delta L)^2\rangle = \langle x\rangle\Omega$ [see below Eq. (3)].

When Eqs. (95) are substituted into Eq. (94a), one obtains for the pair-distribution function $D(\mathbf{r})$

$$D(\mathbf{r}) = 1+\xi[F_{1,1}(\mathbf{r})+F_{1,1}(-\mathbf{r})+F_{0,2}(\mathbf{r})+F_{0,2}(-\mathbf{r})+F_{1,2}(\mathbf{r})+F_{1,2}(-\mathbf{r})] + F_{2,2}(\mathbf{r})+F_{1,1}(\mathbf{r})F_{1,1}(-\mathbf{r})+F_{0,2}(\mathbf{r})F_{0,2}(-\mathbf{r}), \quad (97)$$

where ξ is defined by Eq. (15), setting $x=\langle x\rangle$. The various functions on the right-hand side of Eq. (97) are defined as follows:

$$F_{1,1}(\mathbf{r})\equiv(n\Omega)^{-1}\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}\langle n(\mathbf{p})\rangle\,,$$

$$F_{0,2}(\mathbf{r})\equiv(n\Omega)^{-1}\sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}}N_{0,2}(\mathbf{p})\exp\beta(\omega_{\mathbf{p}}+\omega_{-\mathbf{p}}-2g)\,,$$

$$F_{1,2}(\mathbf{r})\equiv(n\Omega)^{-1}\sum_{\mathbf{p}_1\mathbf{p}_1'\mathbf{p}_2'}[e^{i\mathbf{p}_1'\cdot\mathbf{r}}+e^{i\mathbf{p}_2'\cdot\mathbf{r}}]\nu(\mathbf{p}_1)[1+\nu(\mathbf{p}_1')][1+\nu(\mathbf{p}_2')]P_{1,2}\begin{pmatrix}\mathbf{p}_1\,0\\ \mathbf{p}_1'\mathbf{p}_2'\end{pmatrix}, \quad (98)$$

$$F_{2,2}(\mathbf{r})\equiv(n\Omega)^{-2}\sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_1'\mathbf{p}_2'} e^{i(\mathbf{p}_1-\mathbf{p}_1')\cdot\mathbf{r}}\nu(\mathbf{p}_1)\nu(\mathbf{p}_2)[1+\nu(\mathbf{p}_1')][1+\nu(\mathbf{p}_2')]P_{2,2}\begin{pmatrix}\mathbf{p}_1\,\mathbf{p}_2\\ \mathbf{p}_1'\mathbf{p}_2'\end{pmatrix}.$$

In deriving Eq. (97), one must make use of the second of Eqs. (39) and the relation

$$\langle\mathbf{p}_1 0|\rho_2|\mathbf{p}_1'\mathbf{p}_2'\rangle=\langle\mathbf{p}_1'\mathbf{p}_2'|\rho_2|\mathbf{p}_1 0\rangle\,, \quad (99)$$

which also follows from the Hermitian property of the Hamiltonian $H^{(N)}$. We observe that the functions of Eqs. (96) each contain an Ω^{-1} dependence, which, together with the conservation of momentum, makes the corresponding functions in (98) well defined in the limit $\Omega\rightarrow\infty$.

In order to bring the expression (97) to a form which is suitable for calculation, one must express $F_{1,2}(\mathbf{r})$ and $F_{2,2}(\mathbf{r})$ in terms of master (μ,ν) L graphs. Of course, the remaining terms of (97) can all be readily expressed in terms of master (μ,ν) L graphs by using Eqs. (31), (35), (36), (54), and (73). We observe, in analogy with Eq. (35), that when $F_{1,2}(\mathbf{r})$ or $F_{2,2}(\mathbf{r})$ is expressed in terms of the dual (μ,ν) graphs of Sec. 4, each of the outgoing lines can be either $N_{1,1}(\mathbf{p})$ or $N_{2,0}(\mathbf{p})$, whereas each of the incoming lines can be $N_{1,1}(\mathbf{p})$ or $N_{0,2}(\mathbf{p})$. Therefore, $F_{1,2}(\mathbf{r})$ will be expressed in terms of all dual (μ,ν) graphs for which $(\mu+\nu)=3$ and $F_{2,2}(\mathbf{r})$ will be expressed in terms of all dual (μ,ν) graphs for which $(\mu+\nu)=4$. A similar situation occurs when each of the dual (μ,ν) graphs is expressed in terms of the master (μ,ν) L graphs of Sec. 6. There are no essential difficulties in this analysis, but since it is lengthy we shall not give it in this paper.

We conclude our discussion of the pair-distribution function by observing that for an isotropic system at rest, the various $F_{\mu,\nu}(\mathbf{r})$ must be independent of direction. In this case, Eq. (97) can be simplified to the form

$$D(r)=1+2\xi[F_{1,1}(r)+F_{0,2}(r)+F_{1,2}(r)]+\mathrm{F}_{2,2}(r)+[F_{1,1}(r)]^2+[F_{0,2}(r)]^2. \quad (100)$$