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Many-Body Problem in Quantum Statistical Mechanics. V. Degenerate Phase in Bose-Einstein Condensation*

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The formulation of the previous paper (paper IV) is extended so that it becomes applicable in an interacting system in the presence of a Bose-Einstein degeneracy. This extension is carried out by the introduction of an x-ensemble, which enables one to utilize an Ursell-type expansion even in the presence of a Bose-Einstein degeneracy. The variational principle of the previous paper is also extended. It is proved that in the presence of a Bose-Einstein degeneracy, the average occupation number of a single particle state with momentum $\mathbf{p}$ approaches infinity as $\mathbf{p} \to 0$. The method is applied to a dilute system of Bose hard spheres.

1. INTRODUCTION

IN the previous paper[1] (paper IV) it was shown that the logarithm of the grand partition function $\mathcal{Q}_\Omega^s$ for a system of Bose particles can be expressed in terms of the average occupation number $\langle n_\mathbf{k}\rangle$ in the momentum space. Furthermore, both $\mathcal{Q}_\Omega^s$ and the integral equation satisfied by $\langle n_\mathbf{k}\rangle$ can be obtained from a variational principle. It was pointed out that for an infinite system, the average occupation number $\langle n_\mathbf{k}\rangle$ may be singular at $\mathbf{k}=0$ as the fugacity z increases to a certain critical value z_c. For $z>z_c$ while $\langle n_\mathbf{k}\rangle$ is still well defined, its integral equation as derived in the previous paper becomes quite useless.

The purpose of this paper is to show that by introducing the concept of an x-ensemble, the method developed in the previous paper can be generalized and extended to the region where $\langle n_\mathbf{k}\rangle$ is singular at $\mathbf{k}=0$. Physically, the occurrence of such a singularity in $\langle n_\mathbf{k}\rangle$ corresponds to a particular type of phase transition which is a consequence of the symmetric statistics. A special example is the well-known phenomenon of Bose-Einstein condensation for a system of free Bose particles. The formalism presented in this paper, therefore, gives a general discussion of such condensation for a system of interacting Bosons. It will be shown that in the condensed phase as well as the gaseous phase it is possible to express the thermodynamical functions in terms of the average occupation number. Furthermore, a variational principle is developed which enables one to compute the thermodynamical functions and $\langle n_\mathbf{k}\rangle$ in both phases.

As an example, the method is applied to a dilute system of Bose hard spheres.

2. x-ENSEMBLE

In the grand canonical ensemble the relative probability of finding N Bose particles in the configuration $\mathbf{k}_1, \cdots \mathbf{k}_N$ is given by

$$(N!)^{-1}z^N\langle \mathbf{k}_1,\cdots \mathbf{k}_N | W_N{}^s | \mathbf{k}_1,\cdots \mathbf{k}_N\rangle, \tag{V.1}$$

where $W_N{}^s$ is related to the Boltzmann W_N function by [see Eq. (I.23)]

$$\langle \mathbf{k}_1',\cdots \mathbf{k}_N' | W_N{}^s | \mathbf{k}_1,\cdots \mathbf{k}_N\rangle = \sum_{P'} P'\langle \mathbf{k}_1',\cdots \mathbf{k}_N' | W_N | \mathbf{k}_1,\cdots \mathbf{k}_N\rangle. \tag{V.2}$$

Let L be a function of $\mathbf{k}_1'\cdots \mathbf{k}_N'$ which is defined by

$$L(\mathbf{k}_1'\cdots \mathbf{k}_N') = \text{number of } \mathbf{k}_i' \text{ that are zero.} \tag{V.3}$$

As remarked in paper IV, when the fugacity z exceeds a certain critical value z_c the most probable value of L for a large system is comparable to the total number of particles.[2] Thus, in the sum (V.2) the permutations between particles of zero momenta give an exceedingly large number of identical terms. Indeed, it is easy to show that the main reason that the previous explicit expression of $\ln \mathcal{Q}_\Omega^s$ in terms of $\langle n_\mathbf{k}\rangle$ [e.g., Eqs. (IV.33) and (IV.34)] becomes useless for $z \geqq z_c$ is precisely due to such permutations between particles of zero momenta. Therefore, it is desirable to sum over the $L!$ identical terms in (V.2) arising from permutations between particles of zero momenta *before* the Ursell expansions.

The difficulty in this procedure lies in the fact that after the partial summation it becomes almost impossible to evaluate the logarithm of the partition function via the usual Ursell expansion of $W_N{}^s$ in terms of the $U_l{}^s$ functions. To overcome this difficulty we introduce the concept of an x-ensemble.

We define a $W_N{}^x$ function to be

$$\langle \mathbf{k}_1',\cdots \mathbf{k}_N' | W_N{}^x | \mathbf{k}_1,\cdots \mathbf{k}_N\rangle \equiv (L!)^{-1}(x\Omega)^L\langle \mathbf{k}_1',\cdots \mathbf{k}_N' | W_N{}^s | \mathbf{k}_1,\cdots \mathbf{k}_N\rangle \tag{V.4}$$

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[1] T. D. Lee and C. N. Yang, Phys. Rev. 117, 22 (1960), hereafter referred to as IV. We adopt the same notations as used in IV.

[2] For simplicity, throughout this paper we shall restrict ourselves to systems with total momentum equal to zero. Otherwise, because of Galilean invariance it is necessary to consider systems which have macroscopic average occupation number $\langle n_\mathbf{k}\rangle$ for $\mathbf{k}\neq 0$. It is, however, easy to see that the presence of these states with total momentum not equal to zero does not affect the form of any thermodynamic functions obtained in this paper.

where L is defined in (V.3). The corresponding x-partition function $\mathcal{Q}_\Omega{}^x$ is defined to be

$$\mathcal{Q}_\Omega{}^x \equiv [\exp(-x\Omega)] \sum_{N=0}^{\infty} (N!)^{-1} z^N \times \sum_{\mathbf{k}_1\cdots\mathbf{k}_N} \langle \mathbf{k}_1,\cdots\mathbf{k}_N | W_N{}^x | \mathbf{k}_1,\cdots\mathbf{k}_N\rangle. \quad \text{(V.5)}$$

An x-ensemble, then, represents a collection of systems, each of which is described by the number of particles N, and by their momenta $\mathbf{k}_1$, $\mathbf{k}_2$, $\cdots\mathbf{k}_N$. The relative probability of occurrence of a system is given by

$$(N!)^{-1} z^N \langle \mathbf{k}_1,\cdots\mathbf{k}_N | W_N{}^x | \mathbf{k}_1,\cdots\mathbf{k}_N\rangle. \quad \text{(V.6)}$$

In (V.6), as in (V.1), $\mathbf{k}_1$, $\mathbf{k}_2$, $\cdots$ and $\mathbf{k}_N$ are each independently and freely variable over the whole momentum space.

The following theorem establishes the connection between a grand canonical ensemble and an x-ensemble.

Theorem 1 (proved in Appendix A).—If

$$\Omega^{-1}(\partial/\partial x) \ln \mathcal{Q}_\Omega{}^x = 0 \quad \text{at} \quad x = \bar{x} \quad \text{(V.7)}$$

where $\bar{x}$ is real and positive, then

$$\Omega^{-1} \ln \mathcal{Q}_\Omega{}^x(x=\bar{x}) = \Omega^{-1} \ln \mathcal{Q}_\Omega{}^g \quad \text{as} \quad \Omega \to \infty. \quad \text{(V.8)}$$

If (V.7) has no real and positive solution for x, then (V.8) is still true provided we set

$$\bar{x} = 0. \quad \text{(V.9)}$$

To evaluate $\ln \mathcal{Q}_\Omega{}^x$ it is possible to take advantage of the usual Ursell expansion method. We define the $U_l{}^x$ functions by

$$\begin{aligned}
&\langle \mathbf{k}_1' | W_1{}^x | \mathbf{k}_1\rangle \\
&\quad \equiv \langle \mathbf{k}_1' | U_1{}^x | \mathbf{k}_1\rangle, \\
&\langle \mathbf{k}_1',\mathbf{k}_2' | W_2{}^x | \mathbf{k}_1,\mathbf{k}_2\rangle \\
&\quad \equiv \langle \mathbf{k}_1' | U_1{}^x | \mathbf{k}_1\rangle\langle \mathbf{k}_2' | U_1{}^x | \mathbf{k}_2\rangle + \langle \mathbf{k}_1',\mathbf{k}_2' | U_2{}^x | \mathbf{k}_1,\mathbf{k}_2\rangle, \\
&\langle \mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3' | W_3{}^x | \mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle \\
&\quad \equiv \langle \mathbf{k}_1' | U_1{}^x | \mathbf{k}_1\rangle\langle \mathbf{k}_2' | U_1{}^x | \mathbf{k}_2\rangle\langle \mathbf{k}_3' | U_1{}^x | \mathbf{k}_3\rangle \qquad \text{(V.10)} \\
&\qquad + \langle \mathbf{k}_1' | U_1{}^x | \mathbf{k}_1\rangle\langle \mathbf{k}_2',\mathbf{k}_3' | U_2{}^x | \mathbf{k}_2,\mathbf{k}_3\rangle \\
&\qquad + \langle \mathbf{k}_2' | U_1{}^x | \mathbf{k}_2\rangle\langle \mathbf{k}_1',\mathbf{k}_3' | U_2{}^x | \mathbf{k}_1,\mathbf{k}_3\rangle \\
&\qquad + \langle \mathbf{k}_3' | U_1{}^x | \mathbf{k}_3\rangle\langle \mathbf{k}_1',\mathbf{k}_2' | U_2{}^x | \mathbf{k}_1,\mathbf{k}_2\rangle \\
&\qquad\qquad + \langle \mathbf{k}_1',\mathbf{k}_2',\mathbf{k}_3' | U_3{}^x | \mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle,
\end{aligned}$$

etc.

The relationship between W^x and U^x is the same as that between W and U. Using the result[3] of Appendix A of I, one thus obtains

$$\Omega^{-1} \ln \mathcal{Q}_\Omega{}^x = \sum_n b_n{}^x(\Omega) z^n - x, \quad \text{(V.11)}$$

where

$$b_n{}^x(\Omega) = (n!\Omega)^{-1} \sum_{\mathbf{k}_1\cdots\mathbf{k}_n} \langle \mathbf{k}_1,\cdots\mathbf{k}_n | U_n{}^x | \mathbf{k}_1,\cdots\mathbf{k}_n\rangle. \quad \text{(V.12)}$$

[3] T. D. Lee and C. N. Yang, Phys. Rev. **113**, 1165 (1959), hereafter referred to as I.

By using (V.10), (V.4) and Rule A of paper I, these $U_n{}^x$ can be expressed in terms of sums of products of the Boltzmann U_n functions. In the following we state the general rule of such sums:

Rule C (proved in Appendix B).—Let us consider first

$$\langle \mathbf{k}_1',\cdots\mathbf{k}_n' | U_n{}^x | \mathbf{k}_1,\cdots\mathbf{k}_n\rangle,$$

in which, say, l of the n final momenta $\mathbf{k}_1'$, $\mathbf{k}_2'\cdots\mathbf{k}_n'$ are zero. For definiteness we denote the particles with zero final momenta as A_1, A_2, $\cdots A_l$ and particles with nonzero final momenta as B_1, B_2, $\cdots B_{n-l}$; i.e.,

$$\mathbf{k}_{A_1}' = \mathbf{k}_{A_2}' = \cdots = \mathbf{k}_{A_l}' = 0, \quad \text{(V.13)}$$

while the rest, $\mathbf{k}_{B_1}'$, $\mathbf{k}_{B_2}'\cdots$ etc., are all not zero. To compute $U_n{}^x$ we first distribute the n integers 1, 2, $\cdots n$ into m_α groups each containing α integers, with $\sum_\alpha m_\alpha \alpha = n$. Such a grouping may be represented as follows:

$$\{(a)(b)\cdots\}\{(cd)(ef)\cdots\}\{(ghi)\cdots\}\cdots, \quad \text{(V.14)}$$

where a, b, c, $d\cdots$ are the integers 1, 2, $\cdots n$. Similar to Rule A, in the first curely bracket there are m_1 round brackets with one integer in each, ($m_1 = 0, 1, 2, \cdots$) and in the second curly bracket there are m_2 round brackets with two integers in each, ($m_2 = 0, 1, 2, \cdots$), etc. Within each round bracket the integers are arranged in ascending order. Within each curly bracket the round brackets are arranged such that their first integers follow an ascending sequence.

Next, corresponding to each such grouping (V.14) we form a sum

$$\textstyle\sum_P S_P, \quad \text{(V.15)}$$

where

$$\begin{aligned}
S_P \equiv (x\Omega)^l &\{\langle \mathbf{k}_\alpha' | U_1 | \mathbf{k}_a\rangle\langle \mathbf{k}_\beta' | U_1 | \mathbf{k}_b\rangle\cdots\} \\
&\times\{\langle \mathbf{k}_\gamma',\mathbf{k}_\delta' | U_2 | \mathbf{k}_c,\mathbf{k}_d\rangle \\
&\qquad\times\langle \mathbf{k}_\epsilon',\mathbf{k}_\phi' | U_2 | \mathbf{k}_e,\mathbf{k}_f\rangle\cdots\}\cdots, \quad \text{(V.16)}
\end{aligned}$$

in which α, β, $\cdots\gamma$, δ, ϵ, ϕ, $\cdots$ is a permutation of the integers 1, 2, $\cdots n$. Therefore, it is also a permutation of A_1, $\cdots A_l$, B_1, $\cdots B_{(n-l)}$.

$$(\alpha,\beta,\cdots\gamma,\delta,\epsilon,\cdots) = P(A_1,\cdots A_l,B_1,\cdots B_{(n-l)}). \quad \text{(V.17)}$$

In (V.15), we sum only over those permutations P which satisfy the following two conditions:

(a) Among the set of $l!$ permutations which differ from each other *only* in the *final positions of* $A_1\cdots A_l$, only one is included in the sum (V.15). Because of (V.13) it is immaterial which one among the $l!$ permutations is included.

(b) If we set in (V.16)

$$\begin{aligned}
\mathbf{k}_{B_i}' &= \mathbf{k}_{B_i} \quad [i = 1, 2, \cdots (n-l)], \\
\mathbf{k}_{A_j}' &= 0 \quad [j = 1, 2, \cdots l],
\end{aligned}$$

and regard the resulting product on the right-hand side as a function of $\mathbf{k}_1$, $\cdots\mathbf{k}_n$, this function must not be of

the form of a product of two factors one of which depends only on some, but not all, of the variables $\mathbf{k}_1, \cdots \mathbf{k}_n$ while the other depends only on the rest of these variables.

We then sum up all expressions (V.15) over the different groupings (V.14). This total sum is equal to

$$\langle \mathbf{k}_1' \cdots \mathbf{k}_n' | U_n^x | \mathbf{k}_1 \cdots \mathbf{k}_n \rangle.$$

Similar to the simplification from rule A (of paper I) to rule A′ (of paper IV) many terms in the sum (V.15) can be further combined by introducing [see Eq. (I.30)]

$$\langle \mathbf{k}_1' \cdots \mathbf{k}_n' | \Upsilon_n^s | \mathbf{k}_1 \cdots \mathbf{k}_n \rangle \equiv \sum_{P'} P' \langle \mathbf{k}_1' \cdots \mathbf{k}_n' | U_n | \mathbf{k}_1 \cdots \mathbf{k}_n \rangle, \quad \text{(V.18)}$$

where the sum extends over all permutations P' of $\mathbf{k}_1' \cdots \mathbf{k}_n'$.

In the following we give some examples to illustrate rule C. It is convenient to introduce the notation $\mathbf{p}$ (or $\mathbf{p}_i$, $\mathbf{p}'$, $\mathbf{p}_i'$) which is identical with $\mathbf{k}$ (or $\mathbf{k}_i$, $\mathbf{k}'$, $\mathbf{k}_i'$) except that

$$\mathbf{p} \neq 0 \quad \text{(V.19)}$$

(and similarly for $\mathbf{p}_i$, $\mathbf{p}'$ and $\mathbf{p}_i'$) while $\mathbf{k}$ (or $\mathbf{k}_i$, $\mathbf{k}'$, $\mathbf{k}_i'$) may or may not be zero. This convention will be used throughout this paper.

Example 1.

$$\langle \mathbf{p}' | U_1^x | \mathbf{p} \rangle = \langle \mathbf{p}' | U_1 | \mathbf{p} \rangle = \delta_{\mathbf{p}\mathbf{p}'} \exp(-\beta p^2),$$

and

$$\langle 0 | U_1^x | 0 \rangle = x\Omega. \quad \text{(V.20)}$$

Example 2.

$$\begin{aligned} \langle \mathbf{p}_1', \mathbf{p}_2' | U_2^x | \mathbf{k}_1, \mathbf{k}_2 \rangle &= \langle \mathbf{p}_1', \mathbf{p}_2' | U_2^s | \mathbf{k}_1, \mathbf{k}_2 \rangle \\ &= \langle \mathbf{p}_2' | U_1 | \mathbf{k}_1 \rangle \langle \mathbf{p}_1' | U_1 | \mathbf{k}_2 \rangle \\ &\quad + \langle \mathbf{p}_1', \mathbf{p}_2' | \Upsilon_2^s | \mathbf{k}_1, \mathbf{k}_2 \rangle, \end{aligned}$$

$$\langle \mathbf{p}_1', 0 | U_2^x | \mathbf{k}_1, \mathbf{k}_2 \rangle = x\Omega \langle \mathbf{p}_1', 0 | U_2^s | \mathbf{k}_1, \mathbf{k}_2 \rangle,$$

and

$$\langle 0,0 | U_2^x | \mathbf{k}_1, \mathbf{k}_2 \rangle = (2!)^{-1} (x\Omega)^2 \langle 0,0 | \Upsilon_2^s | \mathbf{k}_1, \mathbf{k}_2 \rangle. \quad \text{(V.21)}$$

Example 3.

$$\langle \mathbf{p}_1', \cdots \mathbf{p}_n' | U_n^x | \mathbf{k}_1, \cdots \mathbf{k}_n \rangle = \langle \mathbf{p}_1', \cdots \mathbf{p}_n' | U_n^s | \mathbf{k}_1, \cdots \mathbf{k}_n \rangle \quad \text{(V.22)}$$

for all n.

Example 4. If

$$\mathbf{p} \neq \mathbf{p}' \neq -\mathbf{p},$$

then using momentum conservation one obtains

$$\langle 0, 0, \mathbf{p} | U_3^x | \mathbf{p}', -\mathbf{p}', \mathbf{p} \rangle = (2!)^{-1} (x\Omega)^2 \langle 0, 0, \mathbf{p} | \Upsilon_3^s | \mathbf{p}', -\mathbf{p}', \mathbf{p} \rangle, \quad \text{(V.23)}$$

and

$$\begin{aligned} \langle 0, 0, \mathbf{p} | U_3^x | \mathbf{p}, \mathbf{p}', -\mathbf{p}' \rangle &= (2!)^{-1} (x\Omega)^2 \langle 0, 0, \mathbf{p} | \Upsilon_3^s | \mathbf{p}, \mathbf{p}', -\mathbf{p}' \rangle \\ &\quad + (2!)^{-1} (x\Omega)^2 \langle \mathbf{p} | U_1 | \mathbf{p} \rangle \langle 0, 0 | \Upsilon_2^s | \mathbf{p}', -\mathbf{p}' \rangle. \quad \text{(V.24)} \end{aligned}$$

Example 5.

$$\begin{aligned} \Omega b_2^x = \tfrac{1}{2} \sum_{\mathbf{p}_1 \mathbf{p}_2} & [\langle \mathbf{p}_2 | U_1 | \mathbf{p}_1 \rangle \langle \mathbf{p}_1 | U_1 | \mathbf{p}_2 \rangle + \langle \mathbf{p}_1, \mathbf{p}_2 | \Upsilon_2^s | \mathbf{p}_1, \mathbf{p}_2 \rangle] \\ & + \sum_{\mathbf{p}} (x\Omega) [\langle \mathbf{p} | U_1 | 0 \rangle \langle 0 | U_1 | \mathbf{p} \rangle + \langle \mathbf{p}, 0 | \Upsilon_2^s | \mathbf{p}, 0 \rangle] \\ & + (\tfrac{1}{2})^2 (x\Omega)^2 \langle 0,0 | \Upsilon_2^s | 0,0 \rangle, \quad \text{(V.25)} \end{aligned}$$

in which the sums[4] extend over all $\mathbf{p}_i$ compatible with (V.19).

It will be shown in Appendix C that in the sum (V.11), Υ_n^s always occurs in the combination

$$\begin{aligned} \langle \mathbf{p}_1', \mathbf{p}_2' \cdots \mathbf{p}_s' | \Upsilon_{s,t}^x | \mathbf{p}_1, \mathbf{p}_2, \cdots \mathbf{p}_t \rangle &\equiv \sum_{n \geq s,\, n \geq t} [(n-s)!(n-t)!]^{-1} (xz\Omega)^{n-\frac{1}{2}s-\frac{1}{2}t} \\ & \times \langle \mathbf{p}_1', \mathbf{p}_2' \cdots \mathbf{p}_s', 0, \cdots 0 | \Upsilon_n^s | \mathbf{p}_1, \mathbf{p}_2, \cdots \mathbf{p}_t, 0, \cdots 0 \rangle. \quad \text{(V.26)} \end{aligned}$$

In (V.26) n varies from the larger of s and t to infinity. For example,

$$\langle \mathbf{p}' | \Upsilon_{1,1}^x | \mathbf{p} \rangle = \sum_{n=1}^{\infty} [(n-1)!]^{-2} (xz\Omega)^{n-1} \times \langle \mathbf{p}', 0, \cdots 0 | \Upsilon_n^s | \mathbf{p}, 0, \cdots 0 \rangle, \quad \text{(V.27)}$$

and

$$\langle \, | \Upsilon_{0,2}^x | \mathbf{p}_1, \mathbf{p}_2 \rangle = \sum_{n=2}^{\infty} [n!(n-2)!]^{-1} (xz\Omega)^{n-1} \times \langle 0, \cdots 0 | \Upsilon_n^s | \mathbf{p}_1, \mathbf{p}_2, 0, \cdots 0 \rangle. \quad \text{(V.28)}$$

It is of interest to notice that while in U_n^x only the zero momenta in the final state carry factors $(x\Omega)$, in the sum (V.26) the zero momenta in the initial and final states are treated in a symmetrical way.

3. PRIMARY GRAPHS AND CONTRACTED GRAPHS

A convenient way to express $\ln \mathfrak{Q}_\Omega^x$ as a sum over products of $\Upsilon_{s,t}^x$ is to use the graphical method. Similar to the discussions presented in paper IV, we introduce the general definition of a primary graph.

A primary graph is a single (i.e., all parts are connected) graphical structure containing at least one vertex. The lines are connected with each other at various vertices. Each line has a direction indicated by an arrow. Each vertex is characterized by two numbers s and t where s and t can be any positive integers 0, 1, 2, $\cdots$ provided

$$(s+t) \geq 2. \quad \text{(V.29)}$$

An (s,t)-vertex connects t incoming (i.e., with their arrows pointing towards the vertex) lines and s outgoing (i.e., with their arrows pointing away from the vertex)

[4] Throughout this paper we adopt the convention that for a cube of volume Ω, a vector $\mathbf{k}$ (or $\mathbf{k}_i$, $\mathbf{k}'$, $\mathbf{k}_i'$) refers to momentum whose components are $2\pi\Omega^{-\frac{1}{3}}(m_1,m_2,m_3)$, where $m_i = 0, \pm 1, \pm 2, \cdots$. A vector $\mathbf{p}$ (or $\mathbf{p}_i$, $\mathbf{p}'$, $\mathbf{p}_i'$) always refers to a similar momentum $2\pi\Omega^{-\frac{1}{3}}(m_1,m_2,m_3)$ except that m_1, m_2, m_3 cannot be all equal to zero. All sums with respect to $\mathbf{p}$ (or $\mathbf{p}_i$, $\mathbf{p}'$, $\mathbf{p}_i'$) therefore extend over all integral values of m_i except $m_1 = m_2 = m_3 = 0$.

lines. A line which has vertices at both of its ends is called an internal line; otherwise, it is called an external line.

A *primary* (μ,ν)-*graph* is a primary graph which has ν external incoming lines and μ external outgoing lines.[5]

To every external line we assign a nonzero momentum $\mathbf{q}_i$, where

$$i=1,\,2,\,\cdots(\mu+\nu).$$

These external momenta are always considered to be distinguishable. Two primary graphs are different only if their topological structures, which include the positions of these distinguishable external momenta, are different.

To each primary (μ,ν)-graph we assign a term determined by the following procedures:

(i) Associate with each internal line a different integer i $(i=1,\,2,\,\cdots l)$ and a corresponding (nonzero) momentum $\mathbf{p}_i$.

(ii) To each (s,t)-vertex, assign a factor

$$\langle \mathbf{p}_{B1}',\cdots \mathbf{p}_{Bs}'|\Upsilon_{s,t}^x|\mathbf{p}_{A1},\cdots \mathbf{p}_{At}\rangle, \qquad \text{(V.30)}$$

where $\mathbf{p}_{A1},\,\cdots \mathbf{p}_{At}$ are the momenta associated with its incoming (internal or external) lines and $\mathbf{p}_{B1}',\,\cdots \mathbf{p}_{Bs}'$ are the momenta associated with its outgoing (internal or external) lines.

(iii) Assign a factor z to each *internal* line.

(iv) Assign a factor

$$(\text{symmetry number})^{-1}$$

to the entire graph where the symmetry number is defined as follows:

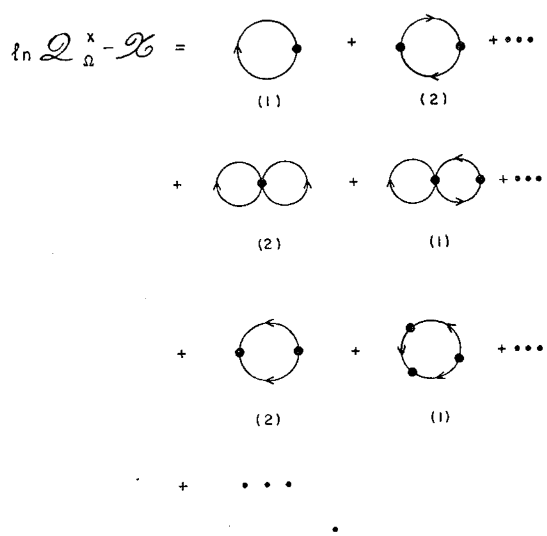

FIG. 1. $(\ln \mathcal{Q}^x\Omega-\mathfrak{X})$ as a sum of primary (0,0)-graphs. The numbers under these graphs are their symmetry numbers.

Consider the $l!$ permutations of the positions of the integers associated with the internal lines. The total number of permutations that leave the topological structure of the graph [which includes the positions of these numbers $1,\,2,\,\cdots l$] unchanged [from the situation after step (i) above] is defined to be the symmetry number of the graph.

The term that corresponds to each primary (μ,ν)-graph is given by[4]

$$\sum_{\mathbf{p}_1\cdots\mathbf{p}_l}[\text{product of all factors in (ii)–(iv)}]. \qquad \text{(V.31)}$$

In terms of these primary graphs we can write the sum (V.11) as (proved in Appendix C)

$$\ln \mathcal{Q}_\Omega{}^x = \mathfrak{X} + \sum [\text{all different primary (0,0)-graphs}], \qquad \text{(V.32)}$$

where

$$\mathfrak{X} = -x\Omega + \sum_{n=1}^{\infty}(n!)^{-2}(xz\Omega)^n\langle 0,\cdots 0|\Upsilon_n{}^e|0,\cdots 0\rangle. \qquad \text{(V.33)}$$

In explicit form we can write (V.32) as[4]

$$\begin{aligned}(\ln \mathcal{Q}_\Omega{}^x-\mathfrak{X}) &= \sum_{\mathbf{p}}[z\langle \mathbf{p}|\Upsilon_{1,1}{}^x|\mathbf{p}\rangle+\tfrac{1}{2}z^2\langle \mathbf{p}|\Upsilon_{1,1}{}^x|\mathbf{p}\rangle^2+\cdots]\\ &+\sum_{\mathbf{p}_1\mathbf{p}_2}\langle \mathbf{p}_1,\mathbf{p}_2|\Upsilon_{2,2}{}^x|\mathbf{p}_1,\mathbf{p}_2\rangle[\tfrac{1}{2}z^2+z^3\langle \mathbf{p}_1|\Upsilon_{1,1}{}^x|\mathbf{p}_1\rangle+\cdots]\\ &+\sum_{\mathbf{p}}\langle\ |\Upsilon_{0,2}{}^x|\mathbf{p},-\mathbf{p}\rangle\langle \mathbf{p},-\mathbf{p}|\Upsilon_{2,0}{}^x|\ \rangle\\ &\qquad\times[\tfrac{1}{2}z^2+z^3\langle \mathbf{p}|\Upsilon_{1,1}{}^x|\mathbf{p}\rangle+\cdots]+\cdots. \qquad \text{(V.34)}\end{aligned}$$

The sum (V.34) is illustrated in Fig. 1.

By a procedure similar to that used in the previous paper,[1] we may eliminate[6] the (1,1)-vertices in these graphs by defining

$$m^x(\mathbf{p}) \equiv z[1-z\langle \mathbf{p}|\Upsilon_{1,1}{}^x|\mathbf{p}\rangle]^{-1}. \qquad \text{(V.35)}$$

We, then, define a *contracted* (μ,ν)-*graph* to be of the same topological structure as that of a primary (μ,ν)-graph except that it *does not have any* (1,1)-*vertex*. To each contracted (μ,ν)-graph we assign a term which is determined by the same rules (i)–(iv) used to obtain (V.31) except that (iii) is replaced by

(iii)′ Assign a factor

$$m^x(\mathbf{p}_i)$$

to the ith internal line $(i=1,\,2,\,\cdots l)$.

The term that corresponds to a contracted (μ,ν)-graph is then given by

$$\sum_{\mathbf{p}_1\cdots\mathbf{p}_l}[\text{products of all factors in (ii), (iii)}',\text{ and (iv)}]. \qquad \text{(V.36)}$$

[5] In paper IV, the α-vertex corresponds to the present (α,α)-vertex. Similarly the ζ-graph corresponds to the present (ζ,ζ)-graph.

[6] The elimination of the (1,1)-vertex is merely a matter of convenience. It is not a necessary step for the later introduction of irreducible graphs. See Appendix F for a more detailed discussion.

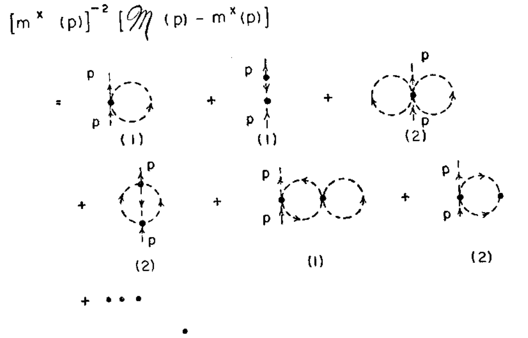

FIG. 2. $[m^x(\mathbf{p})]^{-2}[\mathfrak{M}(\mathbf{p})-m^x(\mathbf{p})]$as a sum of contracted (1,1)-graphs. The numbers under these graphs are their symmetry numbers.

In terms of these contracted graphs, (V.32) becomes

$$\ln \mathcal{Q}_\Omega{}^x = \mathfrak{X} + \sum_{\mathbf{p}} \ln[z^{-1}m^x(\mathbf{p})] + \sum \text{[all different contracted (0,0)-graphs]}. \quad (\text{V.37})$$

4. AVERAGE OCCUPATION NUMBER IN MOMENTUM SPACE AND $\mathfrak{M}(p)$

As in the discussions given in IV, it is useful to introduce $\langle \mathfrak{n}_{\mathbf{k}} \rangle$ which is defined to be the statistical values of the occupation number in momentum space averaged over an x-ensemble. These average numbers can be expressed in terms of $U_l{}^x$ by (proved in Appendix D)[4]

$$\langle \mathfrak{n}_{\mathbf{p}} \rangle = \sum_{l=1}^{\infty} [(l-1)!]^{-1} z^l \times \sum_{\mathbf{k}_1 \cdots \mathbf{k}_{l-1}} \langle \mathbf{k}_1, \cdots \mathbf{k}_{l-1}, \mathbf{p} | U_l{}^x | \mathbf{k}_1, \cdots \mathbf{k}_{l-1}, \mathbf{p} \rangle, \quad (\text{V.38})$$

and

$$\langle \mathfrak{n}_0 \rangle = x(\partial/\partial x)[(\ln \mathcal{Q}_\Omega{}^x) + x\Omega]. \quad (\text{V.39})$$

At $x=\bar{x}$, where $\bar{x}$ is given either by (V.7) or (V.9), (V.39) becomes

$$\Omega^{-1}\langle \mathfrak{n}_0 \rangle = \bar{x}. \quad (\text{V.40})$$

It is convenient to define $\mathfrak{M}(\mathbf{p})$ as

$$\mathfrak{M}(\mathbf{p}) \equiv [\langle \mathfrak{n}_{\mathbf{p}} \rangle + 1]. \quad (\text{V.41})$$

By using Rule C, it is straightforward to express $\mathfrak{M}(\mathbf{p})$ explicitly as sums over expressions (V.15). These sums can be further simplified in terms of either primary or contracted graphs. We write (proved in Appendix C)

$$\mathfrak{M}(\mathbf{p}) = z + z^2 \times \sum \text{[all different primary (1,1)-graphs]}, \quad (\text{V.42})$$

and

$$\mathfrak{M}(\mathbf{p}) = m^x(\mathbf{p}) + [m^x(\mathbf{p})]^2 \times \sum \text{[all different contracted (1,1)-graphs]}. \quad (\text{V.43})$$

Each of the external lines in these graphs carries a momentum $\mathbf{p}$. In the sums (V.42) and (V.43), each graph contributes a term given by (V.31) and (V.36), respectively. More explicitly, we can write, e.g., (V.43) as

$$\begin{aligned}
[m^x(\mathbf{p})]^{-2}[\mathfrak{M}(\mathbf{p}) - m^x(\mathbf{p})] &= \sum_{\mathbf{p}_1} \langle \mathbf{p}, \mathbf{p}_1 | \Upsilon_{2,2}{}^x | \mathbf{p}, \mathbf{p}_1 \rangle m^x(\mathbf{p}_1) \\
&+ \langle \, | \Upsilon_{0,2}{}^x | \mathbf{p}, -\mathbf{p} \rangle \langle \mathbf{p}, -\mathbf{p} | \Upsilon_{2,0}{}^x | \, \rangle m^x(-\mathbf{p}) \\
&+ \tfrac{1}{2} \sum_{\mathbf{p}_1 \mathbf{p}_2} \langle \mathbf{p}, \mathbf{p}_1, \mathbf{p}_2 | \Upsilon_{3,3}{}^x | \mathbf{p}, \mathbf{p}_1, \mathbf{p}_2 \rangle m^x(\mathbf{p}_1) m^x(\mathbf{p}_2) \\
&+ \cdots. \quad (\text{V.44})
\end{aligned}$$

This sum is illustrated in Fig. 2. For clarity we use dotted lines for all contracted graphs. The first three terms on the right-hand side of (V.44) correspond, respectively, to the first three graphs in Fig. 2.

5. IRREDUCIBLE GRAPHS

In the previous paper (IV) the contracted graphs were simplified by the introduction of the irredicible graphs. As was explained in Sec. 6 of paper IV such reduction is not only mathematically advantageous but also physically necessary. The same reasoning also applies directly to the present case.

However, the actual technique of reducing the sum of these contracted (μ,ν)-graphs into a sum of the appropriate irreducible graphs is much more complicated in the present case. To see the difficulty let us consider as an example a subset of all contracted (1,1)-graphs that contain at least one (2,0)-vertex and one (0,2)-vertex. Furthermore, in each of these graphs the external incoming line must terminate at a (0,2)-vertex. Such a set of contracted (1,1)-graphs is illustrated in Fig. 3. It is easy to see that

$$[m^x(\mathbf{p})]^2 \sum \text{[contracted (1,1)-graphs in Fig. 3]} \neq m^x(\mathbf{p})\mathfrak{M}(-\mathbf{p})\mathfrak{M}(\mathbf{p}) \times \langle \, | \Upsilon_{0,2}{}^x | \mathbf{p}, -\mathbf{p} \rangle \langle \mathbf{p}, -\mathbf{p} | \Upsilon_{2,0}{}^x | \, \rangle. \quad (\text{V.45})$$

In particular, e.g., if we substitute (V.43) into (V.45), the coefficient of

$$[m^x(\mathbf{p})]^3[m^x(-\mathbf{p})]^2[\langle \, | \Upsilon_{0,2}{}^x | \mathbf{p}, -\mathbf{p} \rangle \langle \mathbf{p}, -\mathbf{p} | \Upsilon_{2,0}{}^x | \, \rangle]^2$$

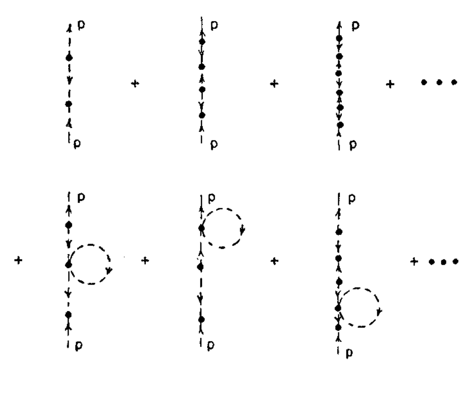

FIG. 3. A subset of all contracted (1,1)-graphs that contain at least one (0,2)-vertex and one (2,0)-vertex. In each graph the external incoming line must terminate at a (0,2)-vertex.

on the right-hand side of (V.45) is 2 while that on the left-hand side, which corresponds to the second graph in Fig. 3, is 1.

To overcome this difficulty it is necessary to define two new functions $\mathfrak{M}_{\text{in}}(\mathbf{p})$ and $\mathfrak{M}_{\text{out}}(\mathbf{p})$.

$$\mathfrak{M}_{\text{in}}(\mathbf{p}) \equiv z^2 \sum [\text{all different primary }(0,2)\text{-graphs}],$$

and

$$\mathfrak{M}_{\text{out}}(\mathbf{p}) \equiv z^2 \times \sum [\text{all different primary }(2,0)\text{-graphs}], \quad \text{(V.46)}$$

where the momenta associated with the two external lines in each of these graphs are $\mathbf{p}$ and $-\mathbf{p}$. In terms of the contracted graphs, (V.46) becomes

$$\mathfrak{M}_{\text{in}}(\mathbf{p}) = [m^x(\mathbf{p})m^x(-\mathbf{p})] \times \sum [\text{all different contracted}(0,2)\text{-graphs}],$$

and

$$\mathfrak{M}_{\text{out}}(\mathbf{p}) = [m^x(\mathbf{p})m^x(-\mathbf{p})] \times \sum [\text{all different contracted }(2,0)\text{-graphs}]. \quad \text{(V.47)}$$

From their definitions it is clear that

$$\mathfrak{M}_\alpha(\mathbf{p}) = \mathfrak{M}_\alpha(-\mathbf{p}), \quad \text{(V.48)}$$

where $\alpha = \text{in}$ or out.

Next we introduce a completely new type of graphs called *dual graphs*. In the following for expediency we shall not discuss the gradual evolution of these new graphical methods but only present the final rules. [See Appendix E for the detailed steps.]

A dual (μ,ν)-graph is defined in exactly the same way as a contracted (μ,ν)-graph except that every internal line carries two arrows, one for each end. Thus, there are three different kinds of internal lines depending on whether these two arrows are parallel to each other, point towards each other, or point away from each other. The external lines, however, carry only one arrow each. Each external line is associated with a nonzero momentum. These external momenta are, again, considered to be distinguishable from each other. Two dual graphs are different only if they have different topological structures which include the positions of these distinguishable external momenta.

Throughout this paper we are only interested in the special cases of $(\mu,\nu) = (0,0)$ and

$$(\mu,\nu) = (1,1), \quad \text{or} \quad (0,2), \quad \text{or} \quad (2,0). \quad \text{(V.49)}$$

If $(\mu,\nu) = (1,1)$, then the momenta of the two external lines are both $\mathbf{p}$. If $(\mu,\nu) = (0,2)$ or $(2,0)$, the momenta of the two external lines are $\mathbf{p}$ and $-\mathbf{p}$.

Similar to the discussions given in Sec. 6 of paper IV, we shall discuss the question of the reducibility of these dual graphs. Let us imagine that any one of the internal lines in such a dual (μ,ν)-graph is cut open. The two ends of this particular internal line would then be separated into two external lines each retaining the original direction of its arrows.

A dual (μ,ν)-graph is called *reducible* if by cutting two of its internal lines open the entire graph can be separated into two (or more) disconnected dual (μ_α,ν_α)-graphs with at least one of the disconnected graphs satisfying (V.49). Otherwise, it is called *irreducible* [or, irreducible dual (μ,ν)-graph].

To each irreducible dual graph we assign a corresponding term which is determined by the following procedures:

(i)″ Assign to each arrow of the internal lines an integer i and a corresponding momentum $\mathbf{p}_i$, [$i = 1, 2, \cdots 2m$, where m is the total number of internal lines].

(ii)″ Assign a factor

$$\langle \mathbf{p}_{B1}', \mathbf{p}_{B2}', \cdots \mathbf{p}_{Bs}' | \Upsilon_{s,t}^x | \mathbf{p}_{A1}, \mathbf{p}_{A2}, \cdots \mathbf{p}_{At} \rangle$$

to each (s,t)-vertex which connects the incoming arrows (i.e., pointing towards the vertex) of momenta $\mathbf{p}_{A1}$, $\mathbf{p}_{A2} \cdots \mathbf{p}_{At}$ with the outgoing arrows (i.e., pointing away from the vertex) of momenta $\mathbf{p}_{B1}'$, $\mathbf{p}_{B2}' \cdots \mathbf{p}_{Bs}'$. These arrows can be associated with either internal or external lines.

(iii)″ Assign, respectively, a factor

$$\delta(\mathbf{p}_i - \mathbf{p}_j)\mathfrak{M}(\mathbf{p}_i), \quad \delta(\mathbf{p}_i + \mathbf{p}_j)\mathfrak{M}_{\text{in}}(\mathbf{p}_i)$$

or

$$\delta(\mathbf{p}_i + \mathbf{p}_j)\mathfrak{M}_{\text{out}}(\mathbf{p}_i)$$

to each internal line which carries two arrows, i and j that are pointing parallel to each other, towards each other or away from each other. The $\delta(\mathbf{p})$ function is defined here for discrete $\mathbf{p}$ by

$$\delta(\mathbf{p}) = 1 \quad \text{for} \quad \mathbf{p} = 0,$$
$$\delta(\mathbf{p}) = 0 \quad \text{otherwise.}$$

(iv)″ Assign a factor

$$(\text{symmetry number})^{-1}$$

to the entire graph. We consider the $(2m)!$ permutations of the positions of the integers $1, 2, \cdots 2m$ that are assigned to the arrows of the internal lines in step (i). The symmetry number of the irreducible dual graph is defined to be the total number of such permutations that leave the topological structure of the graph [which includes the positions of these numbers] unchanged [from the situation after step (i)].

The term corresponding to an irreducible dual graph is then given by[4]

$$\sum_{\mathbf{p}_1 \cdots \mathbf{p}_{2m}} [\text{products of all factors in (ii)}'', \text{(iii)}'', \text{and (iv)}'']. \quad \text{(V.50)}$$

We now define

$$\mathcal{K}(\mathbf{p}) \equiv \sum [\text{all different irreducible dual }(1,1)\text{-graphs}],$$
$$\mathcal{K}_{\text{in}}(\mathbf{p}) \equiv \sum [\text{all different irreducible dual }(0,2)\text{-graphs}],$$

and

$$\mathcal{K}_{\text{out}}(\mathbf{p}) \equiv \sum [\text{all different irreducible dual }(2,0)\text{-graphs}]. \quad \text{(V.51)}$$

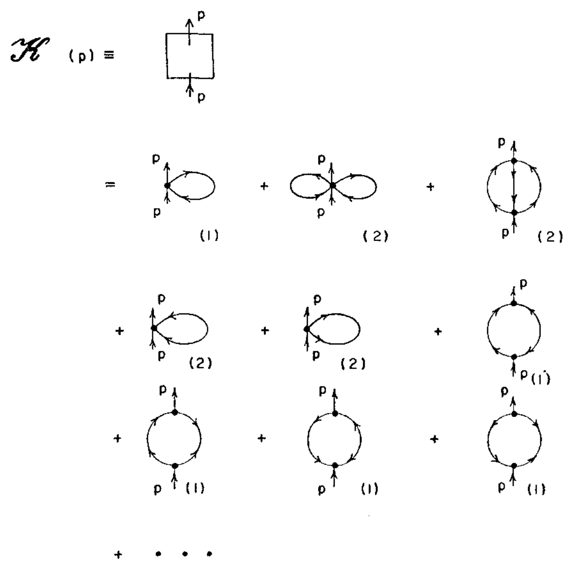

FIG. 4. $\mathcal{K}(\mathbf{p})$ as a sum of irreducible dual (1,1)-graphs. The numbers under these graphs are their symmetry numbers.

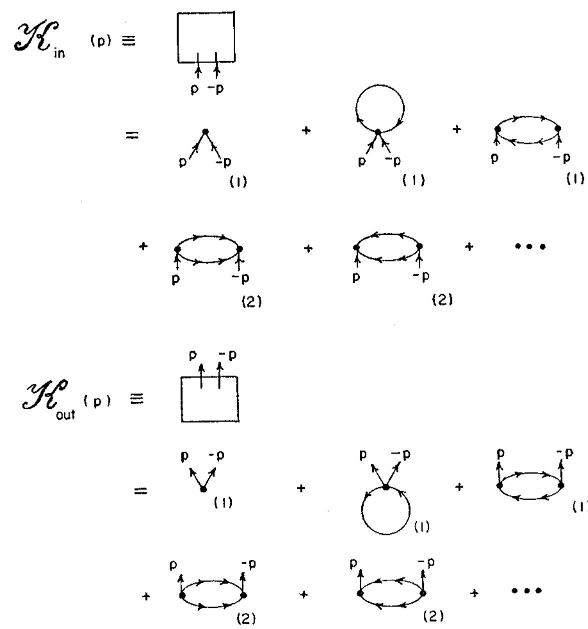

FIG. 5. $\mathcal{K}_{\text{in}}(\mathbf{p})$ and $\mathcal{K}_{\text{out}}(\mathbf{p})$ as sums of irreducible dual (0,2)-graphs and (2,0)-graphs. The numbers under these graphs are their symmetry numbers.

These sums are illustrated in Fig. 4 and Fig. 5. In terms of these graphs, (V.51) becomes

$$\begin{aligned}
\mathcal{K}(\mathbf{p})=&\sum_{\mathbf{p}_1}\langle\mathbf{p},\mathbf{p}_1|\Upsilon_{2,2}{}^x|\mathbf{p},\mathbf{p}_1\rangle\mathcal{M}(\mathbf{p}_1)\\
&+\sum_{\mathbf{p}_1\mathbf{p}_2}\tfrac{1}{2}\langle\mathbf{p},\mathbf{p}_1,\mathbf{p}_2|\Upsilon_{3,3}{}^x|\mathbf{p},\mathbf{p}_1,\mathbf{p}_2\rangle\prod_{i=1}^{2}\mathcal{M}(\mathbf{p}_i)\\
&+\sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_3}\tfrac{1}{2}[\langle\mathbf{p},\mathbf{p}_1|\Upsilon_{2,2}{}^x|\mathbf{p}_2,\mathbf{p}_3\rangle]\\
&\qquad\times[\langle\mathbf{p}_2,\mathbf{p}_3|\Upsilon_{2,2}{}^x|\mathbf{p},\mathbf{p}_1\rangle\prod_{i=1}^{3}\mathcal{M}(\mathbf{p}_i)\\
&+\sum_{\mathbf{p}_1}\tfrac{1}{2}\langle\mathbf{p}|\Upsilon_{1,3}{}^x|\mathbf{p},\,\mathbf{p}_1,\,-\mathbf{p}_1\rangle\mathcal{M}_{\text{out}}(\mathbf{p}_1)\\
&\qquad+\sum_{\mathbf{p}_1}\tfrac{1}{2}\langle\mathbf{p},\,\mathbf{p}_1,\,-\mathbf{p}_1|\Upsilon_{3,1}{}^x|\mathbf{p}\rangle\mathcal{M}_{\text{in}}(\mathbf{p})+\cdots,
\end{aligned}$$

$$\begin{aligned}
\mathcal{K}_{\text{in}}(\mathbf{p})=&\langle\ |\Upsilon_{0,2}{}^x|\mathbf{p},\,-\mathbf{p}\rangle+\sum_{\mathbf{p}_1}\langle\mathbf{p}_1|\Upsilon_{1,3}{}^x|\mathbf{p}_1,\,\mathbf{p},\,-\mathbf{p}\rangle\mathcal{M}(\mathbf{p}_1)\\
&+\sum_{\mathbf{p}_1\mathbf{p}_2}\langle\mathbf{p}_2|\Upsilon_{1,2}{}^x|\mathbf{p},\mathbf{p}_1\rangle\langle\mathbf{p}_1|\Upsilon_{1,2}{}^x|-\mathbf{p},\,\mathbf{p}_2\rangle\prod_{i=1}^{2}\mathcal{M}(\mathbf{p}_i)\\
&+\sum_{\mathbf{p}_1\mathbf{p}_2}\tfrac{1}{2}\langle\mathbf{p}_1,\mathbf{p}_2|\Upsilon_{2,1}{}^x|\mathbf{p}\rangle\\
&\qquad\times\langle\ |\Upsilon_{0,3}{}^x|-\mathbf{p},\,\mathbf{p}_1,\,\mathbf{p}_2\rangle\prod_{i=1}^{2}\mathcal{M}(\mathbf{p}_i)+\cdots,
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{K}_{\text{out}}(\mathbf{p})=&\langle\mathbf{p},\,-\mathbf{p}|\Upsilon_{2,0}{}^x|\ \rangle+\sum_{\mathbf{p}_1}\langle\mathbf{p}_1,\,\mathbf{p},\,-\mathbf{p}|\Upsilon_{3,1}{}^x|\mathbf{p}_1\rangle\mathcal{M}(\mathbf{p}_1)\\
&+\sum_{\mathbf{p}_1\mathbf{p}_2}\langle\mathbf{p},\mathbf{p}_1|\Upsilon_{2,1}{}^x|\mathbf{p}_2\rangle\langle-\mathbf{p},\,\mathbf{p}_2|\Upsilon_{2,1}{}^x|\mathbf{p}_1\rangle\prod_{i=1}^{2}\mathcal{M}(\mathbf{p}_i)\\
&+\sum_{\mathbf{p}_1\mathbf{p}_2}\tfrac{1}{2}\langle-\mathbf{p}|\Upsilon_{1,2}{}^x|\mathbf{p}_1,\,\mathbf{p}_2\rangle\langle\mathbf{p},\mathbf{p}_1,\mathbf{p}_2|\Upsilon_{3,0}{}^x|\ \rangle\prod_{i=1}^{2}\mathcal{M}(\mathbf{p}_i)\\
&+\cdots.
\end{aligned}$$

In the above, the terms are so arranged that they represent, respectively, the various graphs listed in the same order in Fig. 4 and Fig. 5.

In terms of these graphs it is easy to see that if we interchange $\mathbf{p}$ and $-\mathbf{p}$, $\mathcal{K}_{\text{in}}(\mathbf{p})$ and $\mathcal{K}_{\text{out}}(\mathbf{p})$ must remain the same. Thus we have, in addition to (V.48),

$$\mathcal{K}_\alpha(\mathbf{p})=\mathcal{K}_\alpha(-\mathbf{p}),\tag{V.52}$$

where $\alpha=$ out or in.

The following theorem now establishes the relations between $\mathcal{M}(\mathbf{p})$, $\mathcal{M}_{\text{in}}(\mathbf{p})$, $\mathcal{M}_{\text{out}}(\mathbf{p})$ and these irreducible graphs:

Theorem 2 (proved in Appendix E).—

$$\boldsymbol{\mathfrak{K}}(\mathbf{p})=[\mathbf{m}^x(\mathbf{p})]^{-1}-\boldsymbol{\mathfrak{M}}^{-1}(\mathbf{p}),\tag{V.53}$$

where

$$\boldsymbol{\mathfrak{K}}(\mathbf{p})=\begin{pmatrix}\mathcal{K}(\mathbf{p}) & \mathcal{K}_{\text{in}}(\mathbf{p})\\ \mathcal{K}_{\text{out}}(\mathbf{p}) & \mathcal{K}(-\mathbf{p})\end{pmatrix},$$

$$\boldsymbol{\mathfrak{M}}(\mathbf{p})=\begin{pmatrix}\mathcal{M}(\mathbf{p}) & \mathcal{M}_{\text{in}}(\mathbf{p})\\ \mathcal{M}_{\text{out}}(\mathbf{p}) & \mathcal{M}(-\mathbf{p})\end{pmatrix}\tag{V.54}$$

and

$$\mathbf{m}^x(\mathbf{p})=\begin{pmatrix}m^x(\mathbf{p}) & 0\\ 0 & m^x(-\mathbf{p})\end{pmatrix}.$$

Furthermore, from the definitions (V.46) and (V.51) it can be shown directly that by using the Hermitian property of the Hamiltonian we have

$$\mathcal{M}_{\text{in}}(\mathbf{p})=\mathcal{M}_{\text{out}}(\mathbf{p})\equiv\mathcal{M}'(\mathbf{p}),$$

and

$$\mathcal{K}_{\text{in}}(\mathbf{p})=\mathcal{K}_{\text{out}}(\mathbf{p})\equiv\mathcal{K}'(\mathbf{p}).\tag{V.55}$$

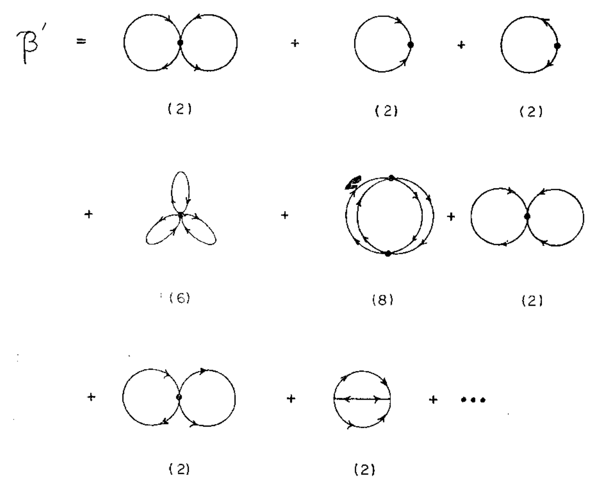

FIG. 6. $\mathfrak{P}'$ as a sum of irreducible dual (0,0)-graphs. The numbers under these graphs are their symmetry numbers.

If the interactions between particles are isotropic, then

$$m^x(\mathbf{p})=m^x(-\mathbf{p}),\quad \mathfrak{M}(\mathbf{p})=\mathfrak{M}(-\mathbf{p}),$$

and

$$\mathcal{K}(\mathbf{p})=\mathcal{K}(-\mathbf{p}). \tag{V.56}$$

Some additional properties of these functions are given in Appendix F.

Next, we proceed to express $\ln \mathcal{Q}_\Omega{}^x$ in terms of sums over irreducible dual graphs. Similar to the notations used in paper IV, we define [see Eq. (IV.34)]

$$\mathfrak{P}'(xz,\mathfrak{M},\mathfrak{M}_{\text{in}},\mathfrak{M}_{\text{out}}) \equiv \sum \text{[all different irreducible dual (0,0)-graphs]}. \tag{V.57}$$

By using (V.55), it can be shown that (proved in Appendix G)

$$\ln \mathcal{Q}_\Omega{}^x=\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}'), \tag{V.58}$$

where

$$\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')=\sum_{\mathbf{p}} \ln\{z^{-1}[\mathfrak{M}^2(\mathbf{p})-\mathfrak{M}'^2(\mathbf{p})]^{\frac{1}{2}}\} -\sum_{\mathbf{p}} [m^x(\mathbf{p})]^{-1}[\mathfrak{M}(\mathbf{p})-m^x(\mathbf{p})]+\mathfrak{P}'+\mathfrak{X}. \tag{V.59}$$

$\mathfrak{X}$ and $\mathfrak{P}'$ are given by (V.33) and (V.57), respectively. The sum (V.57) is illustrated in Fig. 6. In terms of these graphs we find

$$\begin{aligned}\mathfrak{P}'=&\tfrac{1}{2}\sum_{\mathbf{p}_1\mathbf{p}_2}\langle \mathbf{p}_1,\mathbf{p}_2|\Upsilon_{2,2}{}^x|\mathbf{p}_1,\mathbf{p}_2\rangle\mathfrak{M}(\mathbf{p}_1)\mathfrak{M}(\mathbf{p}_2)\\ &+\tfrac{1}{2}\sum_{\mathbf{p}}\langle\ |\Upsilon_{0,2}{}^x|\mathbf{p},-\mathbf{p}\rangle\mathfrak{M}_{\text{out}}(\mathbf{p})\\ &+\tfrac{1}{2}\sum_{\mathbf{p}}\langle\mathbf{p},-\mathbf{p}|\Upsilon_{2,0}{}^x|\ \rangle\mathfrak{M}_{\text{in}}(\mathbf{p})\\ &+\tfrac{1}{6}\sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_3}\langle\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3|\Upsilon_{3,3}{}^x|\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3\rangle\prod_{i=1}^{3}\mathfrak{M}(\mathbf{p}_i)\\ &+\tfrac{1}{8}\sum_{\mathbf{p}_1\cdots\mathbf{p}_4}[\langle\mathbf{p}_1,\mathbf{p}_2|\Upsilon_{2,2}{}^x|\mathbf{p}_3,\mathbf{p}_4\rangle\\ &\qquad\times\langle\mathbf{p}_3,\mathbf{p}_4|\Upsilon_{2,2}{}^x|\mathbf{p}_1,\mathbf{p}_2\rangle]\prod_{i=1}^{4}\mathfrak{M}(\mathbf{p}_i)+\cdots.\end{aligned} \tag{V.60}$$

In (V.60) the first five terms correspond to, respectively, the first five irreducible dual graphs in Fig. 6.

The above formula (V.58) is valid for any x-ensemble of arbitrary x values. However, in order to obtain the thermodynamical functions for the original system in a grand canonical ensemble it is necessary that x should assume a particular value determined by (V.7) or (V.9).

6. VARIATIONAL PRINCIPLE

Equations (V.51) and (V.53) may be regarded as integral equations for $\mathfrak{M}$, from which one may compute $\mathfrak{M}$ and consequently the average occupation number $\langle \mathfrak{n}_{\mathbf{k}}\rangle$. Furthermore, the determination of $\mathfrak{M}$ enables one, through (V.58), to compute the partition function $\mathcal{Q}_\Omega{}^x$. We shall demonstrate in this section that these procedures can be formulated in terms of a single variational principle.

1. In (V.59) we can regard $\mathfrak{P}$ as an explicit functional of x, z, $\mathfrak{M}(\mathbf{p})$, $\mathfrak{M}'(\mathbf{p})$. It is shown in Appendix G that the equations for determining $\mathfrak{M}(\mathbf{p})$, $\mathfrak{M}'(\mathbf{p})$ and x can be obtained by setting the variation of $\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')$ with respect to x, $\mathfrak{M}$ and $\mathfrak{M}'$ separately to zero. Thus if

$$\left[\frac{\delta}{\delta\mathfrak{M}(\mathbf{p})}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\right]_{x,z,\mathfrak{M}'}=0, \tag{V.61}$$

$$\left[\frac{\delta}{\delta\mathfrak{M}'(\mathbf{p})}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\right]_{x,z,\mathfrak{M}}=0, \tag{V.62}$$

and

$$\left[x\frac{\partial}{\partial x}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\right]_{z,\mathfrak{M},\mathfrak{M}'}=0, \tag{V.63}$$

then (V.53) holds and[7]

$$x=\bar{x},$$

where $\bar{x}$ is given by (V.7) or (V.9) according to the rules stated in Theorem 1. Thus by using Theorem 1, the pressure p of a system in the original grand canonical ensemble is given by

$$(\kappa T)^{-1}p=\text{stationary value of } [\Omega^{-1}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')] \tag{V.64}$$

at constant z as $\Omega\to\infty$.

The partial derivative of $\mathfrak{P}$ with respect to z is

[7] It is important to notice that

$$\left[\frac{\partial}{\partial x}\ln\mathcal{Q}_\Omega{}^x\right]_z=\left[\frac{\partial}{\partial x}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\right]_{z,\mathfrak{M},\mathfrak{M}'} =\left[\frac{\partial}{\partial x}\mathfrak{F}(x,\rho,\mathfrak{M},\mathfrak{M}')\right]_{\rho,\mathfrak{M},\mathfrak{M}}$$

provided (V.61) and (V.62) holds. Thus, if (V.63), or

$$\left[x\frac{\partial}{\partial x}\mathfrak{F}(x,\rho,\mathfrak{M},\mathfrak{M}')\right]_{\rho,\mathfrak{M},\mathfrak{M}'}=0$$

has two solutions $x=0$ and $x=\bar{x}>0$, then according to Theorem 1 it is always the nonzero solution that prevails.

related to the particle density ρ by

$$\Omega^{-1}\left[z\frac{\partial}{\partial x}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\right]_{x,\mathfrak{M},\mathfrak{M}'}=\rho \qquad \text{(V.65)}$$

provided (V.61) and (V.62) are satisfied.

2. An alternative variational principle can be formulated in terms of a Legendre transformation. We define

$$\mathfrak{F}(x,\rho,\mathfrak{M},\mathfrak{M}')\equiv\Omega\rho\ln z-\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}'), \qquad \text{(V.66)}$$

in which we use (V.65) and regard

$$z=z(x,\rho,\mathfrak{M},\mathfrak{M}'). \qquad \text{(V.67)}$$

Thus we have

$$\begin{aligned}
&\left[\frac{\delta}{\delta\mathfrak{M}(\mathbf{p})}\mathfrak{F}(x,\rho,\mathfrak{M},\mathfrak{M}')\right]_{x,\rho,\mathfrak{M}'} =-\left[\frac{\delta}{\delta\mathfrak{M}(\mathbf{p})}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\right]_{x,z,\mathfrak{M}'},\\
&\left[\frac{\delta}{\delta\mathfrak{M}'(\mathbf{p})}\mathfrak{F}(x,\rho,\mathfrak{M},\mathfrak{M}')\right]_{x,\rho,\mathfrak{M}} =-\left[\frac{\delta}{\delta\mathfrak{M}'(\mathbf{p})}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\right]_{x,z,\mathfrak{M}} \qquad \text{(V.68)}\\
&\left[x\frac{\partial}{\partial x}\mathfrak{F}(x,\rho,\mathfrak{M},\mathfrak{M}')\right]_{\rho,\mathfrak{M},\mathfrak{M}'} =-\left[x\frac{\partial}{\partial x}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\right]_{z,\mathfrak{M},\mathfrak{M}'}.
\end{aligned}$$

By using (V.64) we find that the Helmholtz free energy F of a system in the original grand canonical ensemble is given by

$$(\Omega\kappa T)^{-1}F=\text{stationary value of }[\Omega^{-1}\mathfrak{F}(x,\rho,\mathfrak{M},\mathfrak{M}')] \qquad \text{(V.69)}$$

at constant ρ as $\Omega\to\infty$.

7. LIMIT OF INFINITE VOLUME

To study the forms of the functions $\mathfrak{P}$ and $\mathfrak{F}$ as $\Omega\to\infty$ it is useful to introduce

$$\begin{aligned}
&\langle\mathbf{p}_1',\cdots\mathbf{p}_s'|v_{s,t}^x|\mathbf{p}_1,\cdots\mathbf{p}_t\rangle\\
&\quad=\textstyle\sum_n[(n-s)!(n-t)!]^{-1}(8\pi^3xz)^{n-\frac{1}{2}s-\frac{1}{2}t}\\
&\qquad\times\langle\mathbf{p}_1',\cdots\mathbf{p}_s',0,\cdots0|v_n^s|\mathbf{p}_1,\cdots\mathbf{p}_t,0,\cdots0\rangle, \qquad \text{(V.70)}
\end{aligned}$$

where v_n^s is defined in (IV.54) and is related in a simple way to the Boltzmann u_n functions introduced in (I.54) for $\Omega=\infty$. In (V.70) the running index n varies from the larger one among the two integers s and t to infinity. By using (IV.126) in paper IV and (V.26) it follows that as $\Omega\to\infty$,

$$\begin{aligned}
&(\Omega/8\pi^3)^{\frac{1}{2}(s+t)-1}\langle\mathbf{p}_1',\cdots\mathbf{p}_s'|\Upsilon_{s,t}^x|\mathbf{p}_1,\cdots\mathbf{p}_t\rangle\to\delta_{\mathbf{P},\mathbf{P}'}\\
&\qquad\times\langle\mathbf{p}_1',\cdots\mathbf{p}_s'|v_{s,t}^x|\mathbf{p}_1,\cdots\mathbf{p}_t\rangle, \qquad \text{(V.71)}
\end{aligned}$$

where

$$\mathbf{P}=\sum_{i=1}^{t}\mathbf{p}_i,\quad \mathbf{P}'=\sum_{j=1}^{s}p_j',$$

and $\delta_{\mathbf{P},\mathbf{P}'}$ is a Kronecker δ-symbol. Thus, for example, as $\Omega\to\infty$

$$m^x(\mathbf{p})=z[1-z\langle\mathbf{p}|v_{1,1}^x|\mathbf{p}\rangle]^{-1}. \qquad \text{(V.72)}$$

The $v_{s,t}^x$ functions are, by definition, independent of the volume.

As $\Omega\to\infty$, (V.59) becomes

$$\begin{aligned}
&\Omega^{-1}\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\\
&\quad=(8\pi^3)^{-1}\int d^3p\,\ln\{z^{-1}[\mathfrak{M}^2(\mathbf{p})-\mathfrak{M}'^2(\mathbf{p})]^{\frac{1}{2}}\}\\
&\qquad-(8\pi^3)^{-1}\int d^3p[m^x(\mathbf{p})]^{-1}[\mathfrak{M}(\mathbf{p})-m^x(\mathbf{p})]\\
&\qquad\qquad+\Omega^{-1}\mathfrak{X}+\Omega^{-1}\mathfrak{P}', \qquad \text{(V.73)}
\end{aligned}$$

where

$$\begin{aligned}
\Omega^{-1}\mathfrak{X}=-x+\sum_{n=1}^{\infty}(n!)^{-2}(xz)^n(8\pi^3)^{n-1}&\\
\times\langle0,\cdots0|v_n^s|0,\cdots0\rangle,& \qquad \text{(V.74)}
\end{aligned}$$

and

$$\begin{aligned}
(8\pi^3)\Omega^{-1}\mathfrak{P}'=&\frac{1}{2}\int\langle\mathbf{p}_1,\mathbf{p}_2|v_{2,2}^x|\mathbf{p}_1,\mathbf{p}_2\rangle\prod_{i=1}^{2}\mathfrak{M}(\mathbf{p}_i)d^3p_i\\
&+\frac{1}{2}\int[\langle\ |v_{0,2}^x|\mathbf{p},-\mathbf{p}\rangle+\langle\mathbf{p},-\mathbf{p}|v_{2,0}^x|\ \rangle]\mathfrak{M}'(\mathbf{p})d^3p\\
&+\frac{1}{6}\int\langle\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3|v_{3,3}^x|\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3\rangle\prod_{i=1}^{3}\mathfrak{M}(\mathbf{p}_i)d^3p_i\\
&+\frac{1}{8}\int[\langle\mathbf{p}_1,\mathbf{p}_2|v_{2,2}^x|\mathbf{p}_3,\mathbf{p}_4\rangle]^2\delta^3(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4)\\
&\times\prod_{i=1}^{4}\mathfrak{M}(\mathbf{p}_i)d^3p_i+\frac{1}{2}\int[\langle\mathbf{p}_1|v_{1,3}^x|\mathbf{p}_1,\mathbf{p}_2,-\mathbf{p}_2\rangle\\
&+\langle\mathbf{p}_1,\mathbf{p}_2,-\mathbf{p}_2|v_{3,1}^x|\mathbf{p}_1\rangle]\mathfrak{M}'(\mathbf{p}_2)\mathfrak{M}(\mathbf{p}_1)d^3p_1d^3p_2\\
&+\cdots. \qquad \text{(V.75)}
\end{aligned}$$

Regarding $\mathfrak{P}$ as a functional of x, z, $\mathfrak{M}$, and $\mathfrak{M}'$ and demanding that it be stationary with respect to independent variations of x and $\mathfrak{M}$ and $\mathfrak{M}'$ at fixed z, one obtains the equilibrium values of x, $\mathfrak{M}$, and $\mathfrak{M}$. The particle density is then given by

$$\rho=x+(8\pi^3)^{-1}\int[z^{-1}\mathfrak{M}(\mathbf{p})-1]d^3p, \qquad \text{(V.76)}$$

which follows from (V.65), (V.63) and the fact that all the $v_{s,t}^x$ depend on x and z only through the combination xz.

To write down the explicit integral equations determining $\mathfrak{M}$ and $\mathfrak{M}'$, one takes the functional derivatives of $\mathfrak{P}$. (V.61) and (V.62) become two coupled integral equations:

$$\mathfrak{M}(\mathbf{p})=m^x(\mathbf{p})+m^x(\mathbf{p})\mathfrak{M}(\mathbf{p})\mathcal{K}(\mathbf{p})+m^x(\mathbf{p})\mathfrak{M}'(\mathbf{p})\mathcal{K}'(\mathbf{p}), \quad \text{(V.77)}$$

$$\mathfrak{M}'(\mathbf{p})=m^x(\mathbf{p})\mathfrak{M}'(\mathbf{p})\mathcal{K}(\mathbf{p})+m^x(\mathbf{p})\mathfrak{M}(\mathbf{p})\mathcal{K}'(\mathbf{p}),$$

where $\mathcal{K}$ and $\mathcal{K}'$ are, according to (V.75),

$$\mathcal{K}(\mathbf{p})=\int\langle\mathbf{p},\mathbf{p}_1|v_{2,2}^x|\mathbf{p},\mathbf{p}_1\rangle\mathfrak{M}(\mathbf{p}_1)d^3p_1+\frac{1}{2}\int\langle\mathbf{p},\mathbf{p}_1,\mathbf{p}_2|v_{3,3}^x|\mathbf{p},\mathbf{p}_1,\mathbf{p}_2\rangle\prod_{i=1}^{2}\mathfrak{M}(\mathbf{p}_i)d^3p_i$$
$$+\frac{1}{2}\int[\langle\mathbf{p},\mathbf{p}_1|v_{2,2}^x|\mathbf{p}_2,\mathbf{p}_3\rangle]^2\delta^3(\mathbf{p}+\mathbf{p}_1-\mathbf{p}_2-\mathbf{p}_3)\times\prod_{i=1}^{3}\mathfrak{M}(\mathbf{p}_i)d^3p_i+\frac{1}{2}\int[\langle\mathbf{p}|v_{1,3}^x|\mathbf{p},\,\mathbf{p}_1,\,-\mathbf{p}_1\rangle$$
$$+\langle\mathbf{p},\,\mathbf{p}_1,\,-\mathbf{p}_1|v_{3,1}^x|\mathbf{p}\rangle]\mathfrak{M}'(\mathbf{p}_1)d^3p_1+\cdots, \quad \text{(V.78)}$$

and

$$\mathcal{K}'(p)=\tfrac{1}{2}[\langle\ |v_{0,2}^x|\mathbf{p},\,-\mathbf{p}\rangle+\langle\mathbf{p},\,-\mathbf{p}|v_{2,0}^x|\ \rangle]+\frac{1}{2}\int[\langle\mathbf{p}_1|v_{1,3}^x|\mathbf{p}_1,\,\mathbf{p},\,-\mathbf{p}\rangle$$
$$+\langle\mathbf{p}_1,\,\mathbf{p},\,-\mathbf{p}|v_{3,1}^x|\mathbf{p}_1\rangle]\mathfrak{M}(\mathbf{p}_1)d^3p_1+\cdots. \quad \text{(V.79)}$$

(V.78) and (V.79) are, of course, identical with the limiting form of (V.51) as the volume becomes infinite.

In the integral equations (V.77), $\mathbf{p}$ is regarded as a continuous variable. It is of interest to know whether the solutions $\mathfrak{M}(\mathbf{p})$ of these equations may become singular as $\mathbf{p}\rightarrow 0$. It can be shown that the occurrence of such a singularity is closely related to $x>0$ where x is determined by (V.7).

Theorem 3 (proved in Appendix H).—If as $\Omega\rightarrow\infty$ the solution for

$$\left[\Omega^{-1}\frac{\partial}{\partial x}\ln\mathfrak{Q}_\Omega^x\right]_z=0 \quad \text{(V.7)}$$

is $x=\bar{x}$ where $\bar{x}$ is real and positive, then at $x=\bar{x}$ the solution for the integral equations (V.77) satisfies

$$\mathfrak{M}^{-1}(\mathbf{p})=0 \quad \text{at} \quad \mathbf{p}=0. \quad \text{(V.80)}$$

Furthermore, at $x=\bar{x}$

$$[\mathfrak{M}'(\mathbf{p})/\mathfrak{M}(\mathbf{p})]=-1 \quad \text{at} \quad \mathbf{p}=0. \quad \text{(V.81)}$$

Consequently, the determination of x is closely related to the study of the behavior $\mathfrak{M}^{-1}(\mathbf{p}\rightarrow 0)$. As will be discussed in the following sections, this theorem together with Theorem 1 give a clear classification of the possible existence of two different phases in a Bose system; one corresponds to

$$x=0 \quad \text{and} \quad \mathfrak{M}^{-1}(\mathbf{p}=0)\geq 0, \quad \text{(V.82)}$$

while the other corresponds to

$$x\geq 0 \quad \text{and} \quad \mathfrak{M}^{-1}(\mathbf{p}=0)=0, \quad \text{(V.83)}$$

where x is the solution of (V.63).

It is easy to see that in the phase $x=0$ all the equations derived in the present paper reduce to the corresponding equations obtained in paper IV.

8. DILUTE SYSTEM OF BOSE HARD SPHERES

In this section the above results will be applied to a dilute Bose system of hard spheres. We shall show that at a given particle density ρ and temperature T it is possible to evaluate the thermodynamical functions of such a system in successive powers of a, provided

$$a\rho\lambda^2\ll 1,$$

and

$$(a/\lambda)\ll 1, \quad \text{(V.84)}$$

where a is the diameter of the hard sphere and λ is the thermal wavelength,

$$\lambda=(4\pi\beta)^{\frac{1}{2}}. \quad \text{(V.85)}$$

We recall that for a small diameter a the explicit forms of v_n^s can be computed by using the binary kernal B. The details of such calculations have been discussed in previous papers. Here we list some useful formulas for $v_{s,t}^x$, $\mathfrak{X}$, $m^x(\mathbf{p})$, etc. for the case of hard-sphere interactions [see e.g., (IV.48) and (IV.61)].

$$\langle\mathbf{p}_1',\cdots\mathbf{p}_n'|v_n^s|\mathbf{p}_1,\cdots\mathbf{p}_n\rangle\sim O[(a\lambda^2)^{n-1}], \quad \text{(V.86)}$$

$$\langle\mathbf{p}_1,\mathbf{p}_2|v_{2,2}^x|\mathbf{p}_1,\mathbf{p}_2\rangle=-(2\pi^3)^{-1}a\lambda^2\times\exp[-\beta(p_1^2+p_2^2)]+O(a^2), \quad \text{(V.87)}$$

$$\langle\ |v_{0,2}^x|\mathbf{p},\,-\mathbf{p}\rangle=\langle\mathbf{p},\,-\mathbf{p}|v_{2,0}^x|\ \rangle=4\pi axzp^{-2}[\exp(-2\beta p^2)-1]+O(a^2), \quad \text{(V.88)}$$

$$[m^x(\mathbf{p})]^{-1}=z^{-1}-\langle\mathbf{p}|v_{1,1}^x|\mathbf{p}\rangle=z^{-1}-\exp(-\beta p^2)\times[1-4a\lambda^2xz+O(a^2)], \quad \text{(V.89)}$$

and

$$\Omega^{-1}\mathfrak{X}=-x+xz-a\lambda^2(xz)^2+O(a^2). \quad \text{(V.90)}$$

In the following we shall use the variational principle (V.69) to evaluate the free energy F in successive powers of a. Throughout the computation we shall consider ρ and T as fixed.

Zeroth Approximation

We shall calculate x, z, $\mathfrak{M}$, $\mathfrak{M}'$, $\mathfrak{F}$ etc. as functions of ρ, T accurate to the zeroth power in a. All the zeroth order quantities are denoted by subscripts 0. From

(V.75) and (V.86) we find

$$\Omega^{-1}\mathfrak{P}_0'=0.$$

Thus, by using (V.89) and (V.90), the zeroth order expression of $\mathfrak{F}$, [Eq. (V.66)], becomes

$$\Omega^{-1}\mathfrak{F}_0(x_0,\rho,\mathfrak{M}_0,\mathfrak{M}_0')=\rho\ln z_0 - (8\pi^3)^{-1}\int d^3p\,\ln(z_0^{-1}[\mathfrak{M}_0^2(\mathbf{p})-\mathfrak{M}_0'^2(\mathbf{p})]^{\frac{1}{2}}) + (8\pi^3)^{-1}\int d^3p\{[z_0^{-1}-\exp(-\beta p^2)]\mathfrak{M}_0(\mathbf{p})-1\} + x_0(1-z_0), \quad (V.91)$$

where z_0 is regarded as a function of $(x_0,\rho,\mathfrak{M}_0,\mathfrak{M}_0')$ determined by (V.76),

$$\rho=x_0+(8\pi^3)^{-1}\int[z_0^{-1}\mathfrak{M}_0(\mathbf{p})-1]d^3p. \quad (V.92)$$

By setting the variational derivatives of $\mathfrak{F}_0$ with respect to $\mathfrak{M}_0$ and $\mathfrak{M}_0'$ to zero, we obtain

$$\mathfrak{M}_0(\mathbf{p})=z_0[1-z_0\exp(-\beta p^2)]^{-1}, \quad (V.93)$$

and

$$\mathfrak{M}_0'(\mathbf{p})=0. \quad (V.94)$$

Substituting these results into (V.91) and (V.92), we find

$$\Omega^{-1}\mathfrak{F}_0(x_0,\rho)=\rho\ln z_0-\lambda^{-3}g_{5/2}(z_0)+x_0(1-z_0), \quad (V.95)$$

and

$$\rho=x_0+\lambda^{-3}g_{3/2}(z_0), \quad (V.96)$$

where

$$g_l(y)=\sum_{n=1}^{\infty} y^n n^{-l}. \quad (V.97)$$

Next we set

$$\left(x_0\frac{\partial}{\partial x_0}\mathfrak{F}_0\right)_\rho=x_0(1-z_0)=0, \quad (V.98)$$

which, according to Theorem 1, determines[7] the functional form of $x_0(\rho,T)$. Solving (V.96) and (V.98) for $x_0\geqq 0$ and z_0, we find that the system exists in two phases:

(a) The gaseous phase in which

$$x_0=0, \quad \lambda^{-3}g_{3/2}(z_0)=\rho. \quad (V.99)$$

This solution obtains for the case $\rho<\rho_c$, where

$$\rho_c=\lambda^{-3}g_{3/2}(1)=\lambda^{-3}(2.612). \quad (V.100)$$

(b) The degenerate phase in which

$$x_0=\rho-\rho_c, \quad z_0=1, \quad \rho>\rho_c. \quad (V.101)$$

Thus, the zeroth order expressions for the free energy F_g and F_d in the two phases are given by

$$\Omega^{-1}F_g=\rho\kappa T\ln z_0-\lambda^{-3}\kappa T g_{5/2}(z_0)+O[a\rho^2] \quad \text{if} \quad \rho<\rho_c, \quad (V.102)$$

and

$$\Omega^{-1}F_d=-(1.342)\lambda^{-3}\kappa T+O[a\rho^2] \quad \text{if} \quad \rho>\rho_c. \quad (V.103)$$

These results are, of course, identical with that of a free Bose gas.

First Order Expression of Free Energy

Next, taking advantage of the variational property of $\mathfrak{F}$ we can substitute the zeroth order solutions x_0, z_0, $\mathfrak{M}_0$, $\mathfrak{M}_0'$, directly into (V.66) and (V.73). By using the explicit forms of $m^x(\mathbf{p})$, $\mathfrak{X}$ and $v_{s,t}{}^x$ given by (V.86)–(V.90), we find the first order expression for $\mathfrak{F}$ to be [neglecting terms proportional to $O(a^n)$ where $n>1$]

$$\Omega^{-1}\mathfrak{F}_1=\rho\ln z_0-\lambda^{-3}g_{5/2}(z_0)+4a\lambda^2(x_0z_0)[\lambda^{-3}g_{3/2}(z_0)] + a\lambda^2(x_0z_0)^2+2a\lambda^2[\lambda^{-3}g_{3/2}(z_0)]^2, \quad (V.104)$$

where $x_0(\rho,T)$ and $z_0(\rho,T)$ are given by (V.99) and (V.101). Thus, we obtain the following results:

(a) In the gaseous phase $(\rho<\rho_c)$ the free energy F_g is given by

$$\Omega^{-1}F_g=\rho\kappa T\ln z_0-\lambda^{-3}(\kappa T)g_{5/2}(z_0) + 8\pi a\rho^2+O[a^2\lambda^{-7}], \quad (V.105)$$

where

$$\rho=\lambda^{-3}g_{3/2}(z_0).$$

(b) In the degenerate phase $(\rho>\rho_c)$,

$$\Omega^{-1}F_d=-\rho_c\kappa T+4\pi a[\rho^2+2\rho\rho_c-\rho_c^2] + O[a^{\frac{3}{2}}\rho^{\frac{5}{2}}\lambda^{-2}]. \quad (V.106)$$

The zeroth order expression of ρ_c is given by (V.100). These results have been previously obtained by using the pseudopotential method.[8] That the next order terms are proportional to $O(a^2)$ and $O(a^{\frac{3}{2}})$ in these two phases will become clear after we evaluate the first order solutions for x, z, $\mathfrak{M}$, and $\mathfrak{M}'$.

First Order Solutions of $\mathfrak{M}$ and $\mathfrak{M}'$

In order to calculate $\mathfrak{M}'$ accurate to $O(a)$ it is necessary to include in (V.75) the first two terms in the sum for $\mathfrak{P}'$. We define[9]

$$\Omega^{-1}\mathfrak{P}_1'=\frac{1}{2}\int\langle\mathbf{p}_1,\mathbf{p}_2|v_{2,2}{}^x|\mathbf{p}_1,\mathbf{p}_2\rangle\prod_{i=1}^{2}\mathfrak{M}_1(\mathbf{p}_i)d^3p_i + \frac{1}{2}\int[\langle\,|v_{0,2}{}^x|\mathbf{p},-\mathbf{p}\rangle+\langle\mathbf{p},-\mathbf{p}|v_{2,0}{}^x|\,\rangle] \times\mathfrak{M}_1'(\mathbf{p})d^3p. \quad (V.107)$$

[8] T. D. Lee and C. N. Yang, Phys. Rev. **112**, 1419 (1958).

[9] We use subscripts 1 for all first order solutions. These first order solutions include both the zeroth order solutions and their corrections.

Correspondingly, the integral equations (V.77) become

$$\mathfrak{M}_1(\mathbf{p})=m^x(\mathbf{p})[1+\mathfrak{M}_1(\mathbf{p})\mathcal{K}_1(\mathbf{p})+\mathfrak{M}_1'(\mathbf{p})\mathcal{K}_1'(\mathbf{p})],$$

and

$$\mathfrak{M}_1'(\mathbf{p})=m^x(\mathbf{p})[\mathfrak{M}_1'(\mathbf{p})\mathcal{K}_1(\mathbf{p})+\mathfrak{M}_1(\mathbf{p})\mathcal{K}_1'(\mathbf{p})],\quad (\text{V.108})$$

where

$$\mathcal{K}_1(\mathbf{p})=\int\langle\mathbf{p},\mathbf{p}'|v_{2,2}{}^x|\mathbf{p},\mathbf{p}'\rangle\mathfrak{M}_1(\mathbf{p}')d^3p',$$

and

$$\mathcal{K}_1'(\mathbf{p})=\tfrac{1}{2}[\langle\ |v_{0,2}{}^x|\mathbf{p},-\mathbf{p}\rangle+\langle\mathbf{p},-\mathbf{p}|v_{2,0}{}^x|\ \rangle].\quad (\text{V.109})$$

By using (V.87)–(V.89) and neglecting terms $O(a^2)$ in these equations, we find the solutions of (V.108) to be

$$\mathfrak{M}_1(\mathbf{p})=z[1-\zeta\exp(-\beta p^2)]^{-1}[1-f^2(\mathbf{p})]^{-1},\quad (\text{V.110})$$

and

$$\mathfrak{M}_1'(\mathbf{p})=f(\mathbf{p})\mathfrak{M}_1(\mathbf{p})\quad (\text{V.111})$$

where

$$f(\mathbf{p})=-4\pi a x_1 z_1{}^2 p^{-2}[1-\exp(-2\beta p^2)]\times[1-\zeta\exp(-\beta p^2)]^{-1},\quad (\text{V.112})$$

and

$$\zeta=z_1\left[1-4a\lambda^2x_1z_1-4a\lambda^2\times\int(8\pi^3)^{-1}\mathfrak{M}_1(\mathbf{p})\exp(-\beta p^2)d^3p\right].\quad (\text{V.113})$$

Correspondingly, (V.76) becomes

$$\rho=x_1+(8\pi^3)^{-1}\int[z_1{}^{-1}\mathfrak{M}_1(\mathbf{p})-1]d^3p.\quad (\text{V.114})$$

The functional form of x_1 can, then, be determined by applying the variational principle (V.69) with respect to x. The detailed forms of these functions are rather complicated. In the following we shall discuss only some simple *partial* results.

(a) In the gaseous region ($\rho<\rho_c$)

$$x_1=0,\quad \mathfrak{M}_1'(\mathbf{p})=0,$$
$$\mathfrak{M}_1(\mathbf{p})=z_1[1-\zeta\exp(-\beta p^2)],\quad (\text{V.115})$$

where

$$\rho=\lambda^{-3}g_{3/2}(\zeta),\quad \zeta=z_1[1-4a\rho\lambda^2].$$

These results are identical with the results obtained in paper IV [see, e.g., (IV.66)]. To $O(a^0)$, ρ_c is given by (V.100).

(b) In the degenerate region ($\rho>\rho_c$), we find

$$x_1=\rho-\rho_c+O[a^{\frac{1}{2}}\rho^{\frac{1}{2}}\lambda^{-2}],$$
$$z_1=1+2a\lambda^2(\rho+\rho_c)+O[(\rho a^3)^{\frac{1}{2}}],$$

and

$$\zeta=1-2a\lambda^2(\rho-\rho_c)+O[(\rho a^3)^{\frac{1}{2}}].\quad (\text{V.116})$$

To study the order of magnitude of $\mathfrak{M}_1(\mathbf{p})$ and $\mathfrak{M}_1'(\mathbf{p})$ it is necessary to separate two different regions of momentum.

(b.i) At $p^2\gg(a\rho)$, we find[10]

$$\mathfrak{M}_1(\mathbf{p})=z_1[1-\zeta\exp(-\beta p^2)]+O[a^2\rho^2p^{-4}],$$

and

$$\mathfrak{M}_1'(\mathbf{p})=-4\pi a x_1 z_1{}^3p^{-2}[1-\exp(-2\beta p^2)]\times[1-\zeta\exp(-\beta p^2)]^{-2}+O[a^3\rho^3p^{-4}].\quad (\text{V.117})$$

(b.ii) At $p^2\simeq O[a\rho]$, we find[10]

$$\mathfrak{M}_1(\mathbf{p})=(2a\lambda^2x_1)^{-1}(q^2+1)[q^2(q^2+2)]^{-1}+O[a^{-\frac{1}{2}}],$$

and

$$\mathfrak{M}_1'(\mathbf{p})=-(2a\lambda^2x_1)^{-1}[q^2(q^2+2)]^{-1}+O[a^{-\frac{1}{2}}],\quad (\text{V.118})$$

where

$$q^2=p^2(8\pi a x_1)^{-1}.\quad (\text{V.119})$$

It is important to notice that the magnitudes of $\mathfrak{M}_1$ and $\mathfrak{M}_1'$ at small p are quite different from that at large p.

Substituting the first order solutions of $\mathfrak{M}_1$, $\mathfrak{M}_1'$, x_1, and z_1 back into (V.66) and (V.73) we can evaluate the next order term for the free energy. In the calculation for $\mathfrak{P}'$, the integration over $p\sim(a\rho)^{\frac{1}{2}}$ yields a term $O[a^{\frac{3}{2}}]$ while the integration over large momentum gives a term proportional to a^2. These results together with a more complete discussion of the first order solutions of x and z will be given in a later publication.

9. DISCUSSIONS

In this section we make some general remarks about the present method.

1. Throughout the present series of papers the effects of statistics are treated separately from the effects of interactions. For a system of interacting particles we characterize their interactions by the various Boltzmann U_l functions (or their symmetrized and antisymmetrized forms, $\Upsilon_l{}^s$ and $\Upsilon_l{}^A$ functions) which are, in principle computable from the corresponding two-body problem through an expansion in terms of the binary kernel.

The effect of statistics enters when we express the $U_N{}^s$ and $U_N{}^A$ functions in the case of symmetrical or antisymmetrical statistics in terms of the corresponding Boltzmann U_l functions by using Rules A and B in paper I. Without using the explicit forms of these Boltzmann U_l functions we can express these two rules in terms of graphs which ultimately lead to a set of

[10] It is important to notice that $\mathfrak{M}(\mathbf{p})$ is related to $\langle \mathfrak{m}_\mathbf{p}\rangle$ by (V.41) where $\langle \mathfrak{m}_\mathbf{p}\rangle$ is the number of particles with momentum $\mathbf{p}$ and not the number of phonons. The transformation between phonons and particles for a system of Bose hard spheres at a finite temperature has been studied by means of the pseudopotential method [T. D. Lee and C. N. Yang, Phys. Rev. **112**, 1419 (1958)]. Using these results, identical expressions for $\mathfrak{M}(\mathbf{p})$ such as those given by (V.117) and (V.118) can also be obtained. It is interesting to notice that from (V.118) for small $\mathbf{p}$, $\langle \mathfrak{m}_\mathbf{p}\rangle\propto p^{-2}$ while the [average number of phonons with momentum $\mathbf{p}$] $\propto p^{-1}$.

integral equations for the average occupation numbers in momentum space.

This approach is especially useful in the case of Bose particles since the appearance of a Bose-Einstein condensation is the consequence only of the symmetrical statistics. While the quantitative properties are of course influenced by the actual forms of the Boltzmann U_l functions, the qualitative features of such a phase transition can be studied by analyzing only the effects of statistics. This is explicitly demonstrated, for example, by the general character of the coupled integral equation (V.77). A Bose-Einstein condensation is simply a transition from a phase, called the nondegenerate phase,

$$x \equiv \lim_{\Omega\to\infty} \Omega^{-1}\langle n_0\rangle = 0 \qquad \text{(V.120)}$$

to a degenerate phase,

$$x>0 \quad \text{and} \quad \mathfrak{M}^{-1}(p=0)=0, \qquad \text{(V.121)}$$

where $\mathfrak{M}(\mathbf{p})$ is the solution of the integral equations (V.77).

Two different kinds of phase transitions, therefore, are possible.

(a) In the nondegenerate phase, at the point of transition,

$$x=0 \quad \text{and} \quad \mathfrak{M}^{-1}(\mathbf{p}=0)>0. \qquad \text{(V.122)}$$

(b) In the nondegenerate phase, at the point of transition,

$$x=0 \quad \text{but} \quad \mathfrak{M}^{-1}(\mathbf{p}=0)=0. \qquad \text{(V.123)}$$

In general, we expect in the former, case (a), a phase transition of the first order while in the latter, case (b), a phase transition of higher order. An example of case (b) is the condensation of a free Bose gas. Another example of case (b) is the approximate solution we obtained for the case of dilute hard spheres.

2. We can apply these results to liquid He. The phase transition between He I and He II is of second order. Therefore, we expect the λ transition to be of the type (b) discussed above. Since at the point of transition $\mathfrak{M}(\mathbf{p})$ has a singularity even in the nondegenerate phase and since all thermodynamical functions can be expressed as sums of integrals of products of the $\mathfrak{M}$ function it is quite possible that some of the thermodynamical functions may become singular in the *nondegenerate* phase at the point of transition. This may have a direct bearing on the observed form[11] of the specific heat near the λ point.

At very low pressures and temperatures there is a phase transition of first order between helium gas and He II. This transition is an example of type (a) discussed above.

In Fig. 7 we plot a schematic p-T diagram of helium. The above results can be summarized as follows:

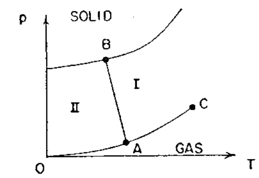

FIG. 7. Schematic p-T diagram of He.

(i) Along the λ line AB, $\mathfrak{M}^{-1}(\mathbf{p}=0)=0$ on both sides.

(ii) Along OA, $\mathfrak{M}^{-1}(\mathbf{p}=0)=0$ on the liquid side but $\mathfrak{M}^{-1}(\mathbf{p}=0)>0$ on the gaseous side.

(iii) Along AC (excluding the triple point A), $\mathfrak{M}^{-1}(\mathbf{p}=0)>0$ (but has a discontinuity) on both sides.

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APPENDIX A[12]

To prove Theorem 1, let us first consider a grand canonical ensemble of systems, each of which satisfies the periodic boundary condition in a cube of volume Ω. We define $\mathcal{P}_\Omega(L)$ to be

$$\mathcal{P}_\Omega(L) \equiv \sum_{N=L}^{\infty} (N!)^{-1} z^N \times \sum_{\mathbf{k}_1\cdots\mathbf{k}_N}^{L} \langle \mathbf{k}_1,\cdots \mathbf{k}_N | W_N{}^s | \mathbf{k}_1,\cdots \mathbf{k}_N\rangle, \qquad \text{(V.124)}$$

where the sum $\sum^L$ extends over all $\mathbf{k}_1\cdots\mathbf{k}_N$ in which L of the momenta $\mathbf{k}_1, \mathbf{k}_2, \cdots \mathbf{k}_N$ are zero. We also define

$$\mathcal{R}_\Omega(x,L) \equiv (L!)^{-1}(x\Omega)^L \mathcal{P}_\Omega(L) \exp(-x\Omega). \qquad \text{(V.125)}$$

Then

$$\mathcal{Q}_\Omega{}^x = \sum_L \mathcal{R}_\Omega(x,L). \qquad \text{(V.126)}$$

For volume $\Omega \to \infty$, we have

$$\Omega^{-1}\ln\mathcal{R}_\Omega = \Omega^{-1}[-x\Omega + L\ln(x\Omega) - L\ln L + L + \ln\mathcal{P}_\Omega], \qquad \text{(V.127)}$$

$$\Omega^{-1}\ln\mathcal{Q}_\Omega{}^s = \Omega^{-1}\ln[\text{max of } \mathcal{P}_\Omega(L)], \qquad \text{(V.128)}$$

and

$$\Omega^{-1}\ln\mathcal{Q}_\Omega{}^x = \Omega^{-1}\ln[\text{max of } \mathcal{R}_\Omega(x,L)], \qquad \text{(V.129)}$$

in which "max of" stands for "maximum of, among various values of L."

To prove Theorem 1, we observe that

$$\frac{\partial}{\partial L}\ln\mathcal{R}_\Omega = \frac{\partial}{\partial L}\ln\mathcal{P}_\Omega(L) + \ln(x\Omega/L) = 0 \qquad \text{(V.130)}$$

[11] Fairbank, Buckingham, and Kellers, Bull. Am. Phys. Soc. 2, 183 (1957).

[12] Throughout this Appendix we will discuss various limits of infinite volume and also consider effects of dividing a large system into two smaller but macroscopic systems. These discussions and, in particular, the proof of the lemma are based essentially on physical arguments. While these statements can be substantiated by considering specific systems such as that of dilute Bose hard spheres, a completely rigorous mathematical treatment of these arguments has not been found.

at the value of L at which $\ln\mathcal{R}_\Omega$ assumes its maximum value. Substituting (V.129) into (V.7) and using (V.130), one obtains

$$\bar{x}=L/\Omega,$$

and

$$\frac{\partial}{\partial L}\ln\mathcal{P}_\Omega(L)=0. \tag{V.131}$$

Substitution of (V.131) into (V.127)–(V.130) leads to Theorem 1 for the case $\bar{x}\neq 0$. For the case that (V.131) cannot be satisfied, $\mathcal{P}_\Omega(L)$ assumes its maximum at $L=0$. (V.8) then follows from the definition of $\mathcal{Q}_\Omega{}^x$.

To render the above arguments more rigorous we must first sharpen the definition (V.124). We impose an additional condition on the range of the summation over $\mathbf{k}_1, \cdots \mathbf{k}_N$: For all nonzero $\mathbf{k}$

$$(\text{number of } \mathbf{k}_i=\mathbf{k})\leqq A\Omega^\alpha,$$

where α and A are constants provided $\frac{2}{3}<\alpha<1$. This condition is introduced so that we need not consider configurations which have a *macroscopic* [i.e., $O(\Omega)$] occupation number for $\mathbf{k}\neq 0$. While such configurations are essential for the study of dynamical properties, they can be neglected in any computation of the thermodynamical functions for a system which is at rest. [See, e.g., reference 2.] Thus, (V.128) still holds. Furthermore, for a large system the value of $\mathcal{P}_\Omega(L)$ gives the relative probability in the grand canonical ensemble of having L particles with zero momentum. We now prove the following lemma.

Lemma.—

$$\left[\Omega\frac{\partial^2}{\partial L^2}\ln\mathcal{P}_\Omega(L)\right]_{z,\Omega}\leqq 0, \tag{V.132}$$

as $\Omega\rightarrow\infty$, but keeping $L/\Omega=$finite.

Proof.—We consider a partition of the volume Ω into two smaller volumes and impose separately the periodic boundary conditions on these two volumes Ω_1 and Ω_2, where

$$\Omega_1=\eta\Omega \quad\text{and}\quad \Omega_2=(1-\eta)\Omega.$$

Correspondingly, we consider a partition of L,

$$L=L_1+L_2,$$

where L_1 and L_2 are, respectively, the number of particles with zero momentum in Ω_1 and Ω_2. Utilizing the property that a configuration of L_1 particles with zero momentum in Ω_1 and L_2 particles with zero momentum in Ω_2 corresponds to a configuration of L particles with zero momentum in Ω but not vice versa, we find, after neglecting the surface effects due to the partition,

$$\mathcal{P}_\Omega(L)\geqq\mathcal{P}_{\Omega_1}(L_1)\mathcal{P}_{\Omega_2}(L_2).$$

Now for every partition,

$$(L/\Omega)=\eta(L_1/\Omega_1)+(1-\eta)(L_2/\Omega_2).$$

Hence as $\Omega\rightarrow\infty$,

$$\Omega^{-1}\ln\mathcal{P}_\Omega(L)\geqq\eta[\Omega_1^{-1}\ln\mathcal{P}_{\Omega_1}(L_1)] +(1-\eta)[\Omega_2^{-1}\ln\mathcal{P}_{\Omega_2}(L_2)]$$

where η is any positive number between 0 and 1. Consequently, if we plot $\lim_{\Omega\rightarrow\infty}[\Omega^{-1}\ln\mathcal{P}_\Omega(L)]$ against (L/Ω) at a fixed fugacity z, the resulting curve must be a convex one, which proves Lemma 1.

Suppose the maximum value of $\Omega^{-1}\ln\mathcal{P}_\Omega(L)$ occurs at $(\bar{L}/\Omega)$, where

$$\text{maximum}[\Omega^{-1}\ln\mathcal{P}_\Omega(L)]=\Omega^{-1}\ln\mathcal{P}_\Omega(\bar{L}). \tag{V.133}$$

(V.129) becomes

$$\Omega^{-1}\ln\mathcal{Q}_\Omega{}^s=\Omega^{-1}\ln\mathcal{P}_\Omega(\bar{L}), \tag{V.134}$$

as $\Omega\rightarrow\infty$.

We now study the curves $\Omega^{-1}\ln\mathcal{R}_\Omega(x,L)$ *vs* L/Ω. The first and second derivatives are given by

$$\frac{\partial}{\partial L}\ln\mathcal{R}_\Omega(x,L)=\frac{\partial}{\partial L}\ln\mathcal{P}_\Omega(L)+\ln[(x\Omega)/L],$$

and

$$\Omega\frac{\partial^2}{\partial L^2}\ln\mathcal{R}_\Omega(x,L)=\Omega\frac{\partial^2}{\partial L^2}\ln\mathcal{P}_\Omega(L)-(\Omega/L). \tag{V.135}$$

Therefore for sufficiently large volume Ω, if we plot $\Omega^{-1}\ln\mathcal{R}_\Omega(x,L)$ against (L/Ω), the resulting curve must be convex just as the curve $\Omega^{-1}\ln\mathcal{P}_\Omega$ *vs* L/Ω is. Furthermore, at any fixed real and positive value of x,

$$\Omega^{-1}\ln\mathcal{R}_\Omega(x,L)\leqq\Omega^{-1}\ln\mathcal{P}_\Omega(L), \tag{V.136}$$

where the equality occurs at (and only at)

$$(L/\Omega)=x.$$

Combining (V.129), (V.135), (V.136), and the lemma we find that for sufficiently large volume $\Omega^{-1}\ln\mathcal{Q}_\Omega{}^x$ varies convexly when plotted against x; i.e.,

$$(\partial^2/\partial x^2)\Omega^{-1}\ln\mathcal{Q}_\Omega{}^x\leqq 0 \tag{V.137}$$

for $x\geqq 0$. Furthermore, as $\Omega\rightarrow\infty$, at any

$$x\geqq 0, \tag{V.138}$$

$$\Omega^{-1}\ln\mathcal{Q}_\Omega{}^x\leqq\Omega^{-1}\ln\mathcal{Q}_\Omega{}^s, \tag{V.139}$$

and the equality occurs at

$$x=\bar{x}=(\bar{L}/\Omega). \tag{V.140}$$

Theorem 1 is a direct consequence of (V.139) and (V.140).

APPENDIX B

To prove Rule C, let us consider a matrix element

$$\langle\mathbf{k}_1',\cdots\mathbf{k}_N'|W_N{}^x|\mathbf{k}_1,\cdots\mathbf{k}_N\rangle, \tag{V.141}$$

in which, say, L of the N final momenta are zero. We denote by $A_1A_2\cdots A_L$ the L particles with zero final momenta and by $B_1B_2\cdots B_{N-L}$ the $(N-L)$ particles

with nonzero final momenta.

$$\mathbf{k}_{A_i}'=0 \quad [i=1,2,\cdots L],$$

and

$$\mathbf{k}_{B_j}'\neq 0 \quad [j=1,2,\cdots(N-L)]. \qquad (\text{V}.142)$$

From (V.2) and (V.4) we find

$$\langle \mathbf{k}_1',\cdots\mathbf{k}_N'|W_N^x|\mathbf{k}_1,\cdots\mathbf{k}_N\rangle=(x\Omega)^L\sum_{P_N'(L)}P_N'(L)$$
$$\times\langle \mathbf{k}_1',\cdots\mathbf{k}_N'|W_N|\mathbf{k}_1,\cdots\mathbf{k}_N\rangle, \qquad (\text{V}.143)$$

where $P_N'(L)$ is any permutation of the N numbers $(A_1,\cdots A_L,B_1,\cdots B_{N-L})$ provided it does not alter the relative order among $A_1, A_2\cdots A_L$; i.e.,

$$P_N'(L)[A_1,A_2,\cdots A_L,B_1,\cdots B_{N-L}]$$
$$=[\cdots A_1,\cdots A_2,\cdots A_{L-1},\cdots A_L,\cdots]. \qquad (\text{V}.144)$$

In (V.143) the sum extends over all $(N!/L!)$ permutations $P_N'(L)$ which apply on the final momenta $\mathbf{k}_1'\cdots\mathbf{k}_N'$ only.

Next, we consider the Ursell expansion of the Boltzmann functions W_n:

$$\langle\mathbf{k}'|W_1|\mathbf{k}\rangle=\langle\mathbf{k}'|U_1|\mathbf{k}\rangle,$$
$$\langle\mathbf{k}_1',\mathbf{k}_2'|W_2|\mathbf{k}_1,\mathbf{k}_2\rangle=\langle\mathbf{k}_1'|U_1|\mathbf{k}_1\rangle\langle\mathbf{k}_2'|U_1|\mathbf{k}_2\rangle$$
$$+\langle\mathbf{k}_1',\mathbf{k}_2'|U_2|\mathbf{k}_1,\mathbf{k}_2\rangle, \quad \text{etc.} \qquad (\text{V}.145)$$

By substituting the appropriate expressions (V.145) for W_N into (V.143), we can express W_N^x as a sum of terms (V.15) over all different groupings (V.14), but without the condition (b) used in (V.15). Combining these results with (V.10), it is straightforward to solve for U_1^x, U_2^x, U_3^x, $\cdots$ in terms of sums of the form (V.15) and (V.16). The result is Rule C.

APPENDIX C

In this Appendix we shall give the steps leading from (V.11) and (V.12) and Rule C to (V.32), and from (V.38), (V.41) to (V.42). Similarly to the introduction of Rule A′ in paper IV, we first combine Rule C and (V.18) into Rule C′.

Rule C′.—Rule C′ is exactly the same as Rule C except for the following two changes:

1. In (V.16) replace every factor

$$\langle\mathbf{k}_{D_1}',\cdots\mathbf{k}_{D_m}'|U_m|\mathbf{k}_{C_1},\cdots\mathbf{k}_{C_m}\rangle$$

by a corresponding factor

$$(l_0!)^{-1}\langle\mathbf{k}_{D_1}',\cdots\mathbf{k}_{D_m}'|\Upsilon_m^s|\mathbf{k}_{C_1},\cdots\mathbf{k}_{C_m}\rangle,$$

where l_0=number of zero momentum among $\mathbf{k}_{D_1}'\cdots\mathbf{k}_{D_m}'$. The resulting expression is called

$$S_p'. \qquad (\text{V}.16)'$$

2. In (V.15) we sum over those permutations P which satisfy, in addition to the two conditions (a) and (b) stated in Rule C, a further condition (c):

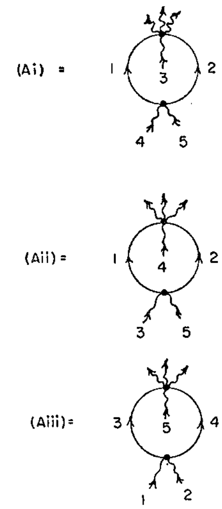

FIG. 8. Examples of numbered $(0,0)_x$-graphs.

(c) Among all the permutations

$$(\alpha,\beta,\cdots\gamma,\delta,\epsilon,\zeta,\cdots)=P(A_1,\cdots A_l,B_1,\cdots B_{(n-l)}), \quad (\text{V}.17)$$

which differ from each other *only* in the relative positions of numbers *within the same bra* [e.g., $\langle\mathbf{k}_\gamma',\mathbf{k}_\delta'|$ and $\langle\mathbf{k}_\delta',\mathbf{k}_\gamma'|$] in (V.16), only one is included in (V.15).

From (V.11) and (V.12) we can write $\Omega^{-1}\ln\mathcal{Q}_\Omega^x$ as

$$\Omega^{-1}\ln\mathcal{Q}_\Omega^x=-x+\sum_{n=1}^{\infty}\sum_{l=0}^{n}z^n(n!\Omega)^{-1}$$
$$\times\sum_{\mathbf{k}_1\cdots\mathbf{k}_n}^{l}\langle\mathbf{k}_1,\cdots\mathbf{k}_n|U_n^x|\mathbf{k}_1,\cdots\mathbf{k}_n\rangle, \qquad (\text{V}.146)$$

where the sum $\sum^l$ extends over all $\mathbf{k}_1\cdots\mathbf{k}_n$ provided

$$(\text{number of zero momenta among } \mathbf{k}_1\cdots\mathbf{k}_n)=l. \qquad (\text{V}.147)$$

By using Rule C′, these sums can be expressed as a sum over expressions (V.16)′ with

$$\mathbf{k}_i'=\mathbf{k}_i, \quad (i=1\cdots n). \qquad (\text{V}.148)$$

For example, in the sum

$$\sum_{\mathbf{k}_1\cdots\mathbf{k}_5}^{l=3}\langle\mathbf{k}_1,\cdots\mathbf{k}_5|U_5^x|\mathbf{k}_1,\cdots\mathbf{k}_5\rangle, \qquad (\text{V}.149)$$

let us consider a definite term (V.16)′:

$$(Ai)=(x\Omega)^3[(3!)^{-1}\langle 0,0,0|\Upsilon_3^s|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3\rangle]$$
$$\times[\langle\mathbf{k}_1,\mathbf{k}_2|\Upsilon_2^s|\mathbf{k}_4,\mathbf{k}_5\rangle], \qquad (\text{V}.150)$$

where $\mathbf{k}_1\neq 0\neq\mathbf{k}_2$ and $\mathbf{k}_3=\mathbf{k}_4=\mathbf{k}_5=0$. For clarity we write the zero final momenta in (V.150) explicitly as 0.

In Fig. 8 we represent (Ai) by a graph, called a numbered $(0,0)_x$-graph.[13] In a similar way, every term (V.16)′ which satisfies (V.148) can be represented by a numbered $(0,0)_x$-graph constructed according to the following procedures:

[13] The term $(\mu,\nu)_x$-graph refers to any graph where a zero momentum is represented by a wavy line.

Every zero initial momentum $\mathbf{k}_\alpha$ is represented by an incoming wavy line with a labeling number α [e.g., $\alpha=3$, 4, 5 in (Ai)]. Every zero final momentum is represented by an outgoing wavy line *without* a labeling number. Every nonzero momentum $\mathbf{k}_\beta$ is represented by a straight line with number β [e.g., $\beta=1$, 2 in (Ai)]. Since in the sum (V.146) these nonzero momenta are to be summed over, the corresponding straight lines are all internal lines. The topological connectedness between vertices and lines follows the same order as given by the corresponding term (V.16)′.

It is easy to see that if (V.148) is satisfied, then there is a one-to-one correspondence between the terms of (V.16)′ and the different numbered $(0,0)_x$-graphs.

From any numbered $(0,0)_x$-graph with a total of N numbers we can generate $N!$ numbered $(0,0)_x$-graphs by permuting the position of the N numbers. Among these $N!$ graphs there will be a total of, say,

$$\omega \tag{V.151}$$

numbered $(0,0)_x$-graphs (including the original graph) that are identical with the original one; or, a total of

$$D=(N!)/\omega \tag{V.152}$$

numbered $(0,0)_x$-graphs that are different. It is important to note that the different terms (V.16)′ which correspond to these different numbered $(0,0)_x$-graphs give identical contribution to the sum (V.146) after summing over all the nonzero momenta.

For example, starting from (Ai) in Fig. 8, different numbered $(0,0)_x$-graphs (Aii), $(Aiii)$, etc. can be formed. The corresponding terms (V.16)′ are

$$(Aii)=(x\Omega)^3[(3!)]\langle 0,0,0|\Upsilon_3{}^s|\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_4\rangle]\times[\langle\mathbf{k}_1,\mathbf{k}_2|\Upsilon_2{}^s|\mathbf{k}_3,\mathbf{k}_5\rangle], \tag{V.153}$$

where $\mathbf{k}_1\neq 0\neq\mathbf{k}_2$, $\mathbf{k}_3=\mathbf{k}_4=\mathbf{k}_5=0$,

$$(Aiii)=(x\Omega)^3[(3!)^{-1}\langle 0,0,0|\Upsilon_3{}^s|\mathbf{k}_3,\mathbf{k}_4,\mathbf{k}_5\rangle]\times[\langle\mathbf{k}_3,\mathbf{k}_4|\Upsilon_2{}^s|\mathbf{k}_1,\mathbf{k}_2\rangle], \tag{V.154}$$

where $\mathbf{k}_3\neq 0\neq\mathbf{k}_4$, $\mathbf{k}_1=\mathbf{k}_2=\mathbf{k}_5=0$, etc. Altogether including (Ai) we can construct

$$D=5![(2!)(2!)]^{-1}$$

different numbered $(0,0)_x$-graphs by permuting the positions of 1, 2, $\cdots$5. Thus

$$\omega=(2!)(2!).$$

In general, let us consider a numbered $(0,0)_x$-graph with a total of N numbers,

$$N=L+M, \tag{V.155}$$

where the (internal) straight lines are numbered $B_1B_2\cdots B_M$ and the (external) incoming wavy lines are numbered $A_1A_2\cdots A_L$. In this graph there are, say, $\Lambda(s,t;n)$ vertices, each connecting s outgoing straight lines, t incoming straight lines, $(n-s)$ outgoing wavy lines and $(n-t)$ incoming wavy lines. Clearly

$$L=\sum(n-t)\Lambda(s,t;n),$$

and

$$M=\sum t\Lambda(s,t;n)=\sum s\Lambda(s,t;n). \tag{V.156}$$

To give a general expression for ω, let us define a *partially numbered* $(0,0)_x$-graph which is obtained from the numbered $(0,0)_x$-graphs by deleting the numbers $A_1\cdots A_L$ associated with the incoming wavy lines but retaining the numbers $B_1\cdots B_M$ associated with the (internal) straight lines. We then consider $M!$ permutations of $B_1\cdots B_M$ which will generate $M!$ partially numbered $(0,0)_x$-graphs, among which the total number of partially numbered $(0,0)_x$-graphs identical with the original one is defined to be the partial symmetry number S'. It then follows that

$$\omega=S'\prod_{s,t,n}[(n-t)!]^{\Lambda(s,t;n)}, \tag{V.157}$$

where ω is introduced in (V.151).

Next, we define a $(0,0)_x$-graph which is obtained from a numbered $(0,0)_x$-graph by deleting all the numbers. In an entirely similar way we can give the general definition of a $(\mu,\nu)_x$-graph.

A $(\mu,\nu)_x$-graph is a single (i.e., connected) graphical structure which contains two different kinds of lines, straight lines and wavy lines. Every line carries a direction which is indicated by an arrow. All wavy lines are external (incoming or outgoing) lines. The straight lines can be either external or internal lines. A $(\mu,\nu)_x$-graph has ν incoming external straight lines and μ outgoing external straight lines.

These lines are connected at various vertices. Each vertex, called an $(s,t;n)$-vertex, is characterized by three integers s, t, and n where s, t, $(n-s)$, $(n-t)$ are, respectively, the numbers of outgoing straight lines, incoming straight lines, outgoing wavy lines and incoming wavy lines that are connected by this vertex. The number n must be greater or equal to 1 while s and t can be arbitrary integers, including zero. Each $(\mu,\nu)_x$-graph must contain at least one vertex.

To each external straight line we assign a *nonzero* momentum q_i [$i=1, 2, \cdots, (\mu+\nu)$]. All these momenta are considered to be distinguishable. Two $(\mu,\nu)_x$-graphs are different only if they have different topological structures which include the positions of these distinguishable momenta of the external straight lines.

Corresponding to each $(\mu,\nu)_x$-graph we assign a term determined by the following procedures:

(i)‴ Associate with each internal line a different integer i ($i=1\cdots M$) and a corresponding nonzero momentum p_i. Associate with each wavy line a zero momentum.

(ii)‴ To each $(s,t;n)$-vertex we assign a factor

$$[(n-s)!(n-t)!]^{-1}\times\langle\mathbf{p}_{C1}\cdots\mathbf{p}_{Cs},0,\cdots 0|\Upsilon_n{}^S|\mathbf{p}_{D1},\cdots\mathbf{p}_{Dt},0,\cdots 0\rangle,$$

where $\mathbf{p}_{D1}, \cdots \mathbf{p}_{Dt}, 0, \cdots 0$ are the momenta associated with the appropriate incoming (straight and wavy) lines and $\mathbf{p}_{C1}, \cdots \mathbf{p}_{Cs}, 0, \cdots 0$ are those associated with the outgoing lines.

(iii)‴ Assign a factor z to each internal straight line and a factor $(xz\Omega)^{\frac{1}{2}}$ to each (incoming or outgoing) wavy line.

(iv)‴ Assign a factor

$$(S')^{-1} \tag{V.158}$$

to the entire graph where S' is called the *partial symmetry number* defined as follows:

Number the internal lines according to (i)‴ and call the resulting graph a *partially numbered* $(\mu,\nu)_x$*-graph*. Among the $M!$ permutations of these M integers the total number of permutations that yield one particular partially numbered $(\mu,\nu)_x$-graph is defined to be S'.

The term corresponding to a $(\mu,\nu)_x$-graph is then given by[4]

$$\sum_{p_1\cdots p_M} [\text{products of all factors in (ii)‴–(iv)‴}]. \tag{V.159}$$

By using (V.146), Rule C′, (V.152) and (V.157) it follows that

$$\ln \mathcal{Q}_\Omega{}^x = -x\Omega + \sum [\text{all different } (0,0)_x\text{-graphs}]. \tag{V.160}$$

In an entirely similar way we can express $\mathfrak{M}(\mathbf{p})$ as sums over different $(\mu,\nu)_x$-graphs.

$$\mathfrak{M}(\mathbf{p}) = z + z^2 \sum [\text{all different } (1,1)\text{-graphs}]. \tag{V.161}$$

A primary (μ,ν)-graph can be obtained from a $(\mu,\nu)_x$-graph by deleting all the wavy lines. This corresponds to a partial sum over those $(\mu,\nu)_x$-graphs that differ *only* in the number of wavy lines attached at various points. Performing such partial sums on (V.160) and (V.161) we obtain (V.32) and (V.42), respectively. Furthermore, after these partial sums only the combination $\Upsilon_{s,t}{}^x$ occurs.

APPENDIX D

The proof of (V.38) is identical with that given in Appendix B of paper[1] IV except for replacing the superscript α by x, $\mathbf{k}$ by $\mathbf{p}$, and $\langle n_{\mathbf{k}} \rangle$ by $\langle \mathfrak{m}_{\mathbf{p}} \rangle$. (IV.94), then, becomes exactly (V.38).

To prove (V.39) we notice that $\langle \mathfrak{m}_0 \rangle$ is, by definition,

$$[\mathcal{Q}_\Omega{}^x]^{-1}[\exp(x\Omega)]\left[\sum_{N=0}^{\infty} (N!)^{-1} z^N \times \sum_{\mathbf{k}_1\cdots\mathbf{k}_N} L\langle \mathbf{k}_1,\cdots \mathbf{k}_N | W_N{}^x | \mathbf{k}_1,\cdots \mathbf{k}_N \rangle\right],$$

where L is defined by (V.3). The above expression is just the right-hand side of (V.39).

APPENDIX E

To prove Theorem 2, we begin with the contracted graphs. Consider a contracted (μ,ν)-graph where

$$(\mu,\nu) = (1,1), \quad \text{or} \quad (0,2), \quad \text{or} \quad (2,0). \tag{V.49}$$

Such a contracted graph is defined as *improper* if by cutting any one of its internal lines open the entire graph can be separated into two disconnected graphs. Otherwise, it is called a proper contracted (μ,ν)-graph.

We then define $\mathfrak{K}(\mathbf{p})$, $\mathfrak{K}_{\text{in}}(\mathbf{p})$ and $\mathfrak{K}_{\text{out}}(\mathbf{p})$ by

$$\begin{aligned}
\mathfrak{K}(\mathbf{p}) &\equiv \sum [\text{all different proper contracted (1,1)-graphs}],\\
\mathfrak{K}_{\text{in}}(\mathbf{p}) &\equiv \sum [\text{all different proper contracted (0,2)-graphs}],\\
\mathfrak{K}_{\text{out}}(\mathbf{p}) &\equiv \sum [\text{all different proper contracted (2,0)-graphs}],
\end{aligned} \tag{V.162}$$

where each contracted graph contributes a term given by (V.36). In (V.162) the momenta associated with the two external lines are both $\mathbf{p}$ in the (1,1)-graph and $\mathbf{p}, -\mathbf{p}$ in the (0,2)- and (2,0)-graphs.

Lemma 1.—

$$\mathfrak{M}(\mathbf{p}) = m^x(\mathbf{p}) + m^x(\mathbf{p})\mathfrak{K}(\mathbf{p})\mathfrak{M}(\mathbf{p}) + m^x(\mathbf{p})\mathfrak{K}_{\text{in}}(\mathbf{p})\mathfrak{M}_{\text{out}}(\mathbf{p}), \tag{V.163}$$

$$\mathfrak{M}_{\text{in}}(\mathbf{p}) = m^x(\mathbf{p})\mathfrak{K}(\mathbf{p})\mathfrak{M}_{\text{in}}(\mathbf{p}) + m^x(\mathbf{p})\mathfrak{K}_{\text{in}}(\mathbf{p})\mathfrak{M}(-\mathbf{p}), \tag{V.164}$$

and

$$\mathfrak{M}_{\text{out}}(\mathbf{p}) = m^x(-\mathbf{p})\mathfrak{K}(-\mathbf{p})\mathfrak{M}_{\text{out}}(\mathbf{p}) + m^x(-\mathbf{p})\mathfrak{K}_{\text{out}}(\mathbf{p})\mathfrak{M}(\mathbf{p}). \tag{V.165}$$

Proof.—(V.43) can be written as

$$\mathfrak{M}(\mathbf{p}) = m^x(\mathbf{p}) + [m^x(\mathbf{p})]^2\mathfrak{K}(\mathbf{p}) + [m^x(\mathbf{p})]^2 \times \sum [\text{all different improper contracted (1,1)-graphs}]. \tag{V.166}$$

By cutting one of its internal lines open, each of the improper graphs in (V.166) can be separated into two disconnected contracted graphs, one of which contains the original external incoming line and the other contains the original external outgoing line. Furthermore, we can always choose the internal line such that after it is cut open the disconnected graph containing the original external incoming line is a *proper* contracted (μ,ν)-graph where

$$(\mu,\nu) = (1,1) \quad \text{or} \quad (0,2). \tag{V.167}$$

By summing over these two possibilities for (μ,ν) and using the definitions of $\mathfrak{K}(\mathbf{p})$ and $\mathfrak{K}_{\text{in}}(\mathbf{p})$, (V.166) becomes (V.163). Similarly starting from (V.47) one can derive (V.164) and (V.165).

By using the same argument but demanding that, after cutting the internal line of the improper graph in (V.166) open, the resulting disconnected graph con-

taining the external outgoing line must always be a proper contracted (μ,ν)-graph, one obtains

$$\mathfrak{M}(\mathbf{p})=m^x(\mathbf{p})+m^x(\mathbf{p})\mathfrak{K}(\mathbf{p})\mathfrak{M}(\mathbf{p})+m^x(\mathbf{p})\mathfrak{K}_{\text{out}}(\mathbf{p})\mathfrak{M}_{\text{in}}(\mathbf{p}). \quad \text{(V.163)}'$$

Similarly, by interchanging the roles of the two external lines, (V.164) and (V.165) become

$$\mathfrak{M}_{\text{in}}(\mathbf{p})=m^x(-\mathbf{p})\mathfrak{K}(-\mathbf{p})\mathfrak{M}_{\text{in}}(\mathbf{p})+m^x(-\mathbf{p})\mathfrak{K}_{\text{in}}(\mathbf{p})\mathfrak{M}(\mathbf{p}), \quad \text{(V.164}')$$

$$\mathfrak{M}_{\text{out}}(\mathbf{p})=m^x(\mathbf{p})\mathfrak{K}(\mathbf{p})\mathfrak{M}_{\text{out}}(\mathbf{p})+m^x(\mathbf{p})\mathfrak{K}_{\text{out}}(\mathbf{p})\mathfrak{M}(-\mathbf{p}). \quad \text{(V.165)}'$$

These equations (V.163)–(V.165) and (V.163)′–(V.165)′ are illustrated in Fig. 9.

Lemma 2.—

$$\mathcal{K}(\mathbf{p})=\mathfrak{K}(\mathbf{p}),$$
$$\mathcal{K}_{\text{in}}(\mathbf{p})=\mathfrak{K}_{\text{in}}(\mathbf{p}), \quad \text{(V.168)}$$
$$\mathcal{K}_{\text{out}}(\mathbf{p})=\mathfrak{K}_{\text{out}}(\mathbf{p}).$$

[$\mathfrak{K}$'s are defined in (V.162) and $\mathcal{K}$'s are defined in (V.51).]

Proof.—The direct way to prove (V.168) is to express $\mathcal{K}(\mathbf{p})$, $\mathcal{K}_{\text{in}}(\mathbf{p})$ and $\mathcal{K}_{\text{out}}(\mathbf{p})$ as explicit functions of $m^x(\mathbf{p})$ by substituting (V.43) and (V.47) into (V.51). A comparison between these expressions and (V.162) yields Lemma 2.

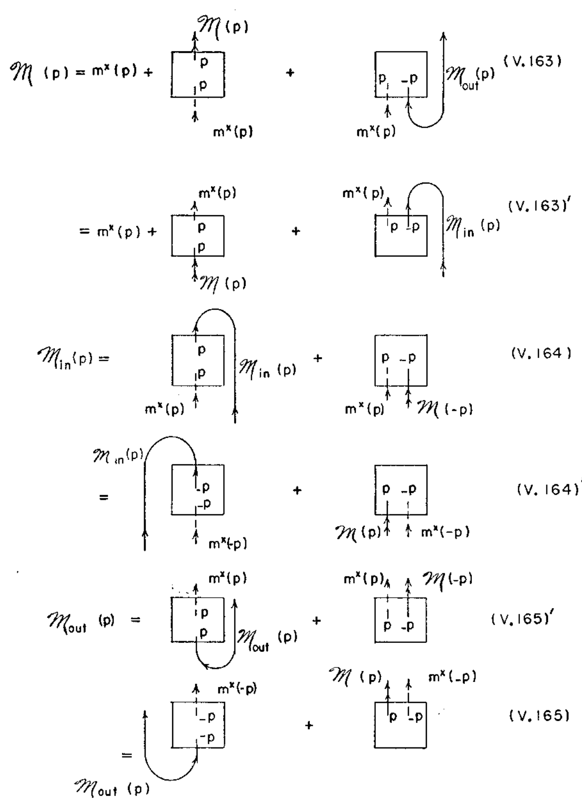

FIG. 9. Graphical representations of (V.163), (V.163)′–(V.165), (V.165)′. The graphical structures of these boxes are illustrated in Fig. 4 and Fig. 5.

Topologically, we may take any proper contracted (μ,ν)-graph where (μ,ν) satisfies (V.49); and then reduce it to an irreducible dual (μ,ν)-graph by replacing, respectively, part of its internal structure that has the same structure as that in $\mathfrak{M}(\mathbf{p})$ by a single line with two parallel arrows, part that has the same structure as $\mathfrak{M}_{\text{in}}(\mathbf{p})$ by a single line with two arrows pointing towards each other, etc. It can then be shown that any such proper contracted (μ,ν)-graph can be reduced to a unique irreducible dual (μ,ν)-graph. Consequently the sums in (V.162) become identical with the corresponding sums in (V.51).

To show Theorem 2, we notice that (V.53) can be written as

$$\mathbf{M}(\mathbf{p})=\mathbf{m}(\mathbf{p})+\mathbf{m}(\mathbf{p})\mathbf{K}(\mathbf{p})\mathbf{M}(\mathbf{p}), \quad \text{(V.169)}$$

or

$$\mathbf{M}(\mathbf{p})=\mathbf{m}(\mathbf{p})+\mathbf{M}(\mathbf{p})\mathbf{K}(\mathbf{p})\mathbf{m}(\mathbf{p}). \quad \text{(V.169)}'$$

By using (V.54), (V.169) is just the matrix form of (V.163)–(V.165) and (V.163)′. Similarly (V.169)′ is the matrix form of (V.163)′–(V.165)′ and (V.163).

APPENDIX F

In this Appendix we shall discuss briefly some miscellaneous properties of $\mathfrak{M}$, $\mathfrak{M}_{\text{in}}$, and $\mathfrak{M}_{\text{out}}$.

1. Let a_k and $a_k^\dagger$ be the annihilation operator and creation operators of momentum k, $\mathcal{H}$ be the Hamiltonian operator (in terms of $a_\mathbf{k}$ and $a_\mathbf{k}^\dagger$) and $\mathfrak{n}$ the total particle number operator

$$\mathfrak{n}=\sum a_\mathbf{k}^\dagger a_\mathbf{k}.$$

We define O_Ω^x to be the operator

$$O_\Omega^x\equiv[\Gamma(a_0^\dagger a_0+1)]^{-1}(x\Omega)^{a_0^\dagger a_0}z^{\mathfrak{n}}\times\exp[-\beta\mathcal{H}-x\Omega], \quad \text{(V.170)}$$

where Γ is the gamma function. In terms of these operators, we can write

$$\mathcal{Q}_\Omega^x=\text{trace}[O_\Omega^x],$$
$$\mathfrak{M}(\mathbf{p})=(\mathcal{Q}_\Omega^x)^{-1}\,\text{trace}[O_\Omega^x a_\mathbf{p}a_\mathbf{p}^\dagger]z,$$
$$\mathfrak{M}_{\text{in}}(\mathbf{p})=(\mathcal{Q}_\Omega^x)^{-1}\,\text{trace}[O_\Omega^x a_0a_0a_\mathbf{p}^\dagger a_{-\mathbf{p}}^\dagger]z^2,$$

and

$$\mathfrak{M}_{\text{out}}(\mathbf{p})=(\mathcal{Q}_\Omega^x)^{-1}\,\text{trace}[a_\mathbf{p}a_{-\mathbf{p}}a_0^\dagger a_0^\dagger O_\Omega^x]z^2. \quad \text{(V.171)}$$

2. As remarked in reference 6, without eliminating the (1,1)-vertices in the primary graphs it is also possible to lead directly from the primary graphs to the irreducible graphs.

To see this it is easiest to start from (V.53) and from Figs. 4 and 5, which give the $\mathcal{K}$ functions explicitly in terms of the $\mathfrak{M}$'s. The left-hand side of (V.53) does not contain the vertex $\Upsilon_{1,1}$ at all. The right-hand side of (V.53) contains $\Upsilon_{1,1}$ only in the term $[\mathbf{m}^x(\mathbf{p})]^{-1}$ and contains it linearly. Moving this linear term to the left-hand side means the inclusion of an additional

diagram in $\mathcal{K}(\mathbf{p})$ containing the $\Upsilon_{1,1}$ vertex. The resultant equation then reads

$$\mathfrak{K}'(\mathbf{p}) = z^{-1} - \mathfrak{M}^{-1}(\mathbf{p}), \tag{V.172}$$

where

$$\mathfrak{K}'(\mathbf{p}) = \mathfrak{K}(\mathbf{p}) + \begin{pmatrix} \langle \mathbf{p}|\Upsilon_{1,1}^{x}|\mathbf{p}\rangle & 0 \\ 0 & \langle -\mathbf{p}|\Upsilon_{1,1}^{x}|-\mathbf{p}\rangle \end{pmatrix}.$$

It can be shown that this is exactly what one obtains by directly reducing the primary graphs without first going through the process of partial summation into contracted graphs.

3. We can also reverse the discussion of the last subsection by observing that the vertices $\Upsilon_{2,0}$ and $\Upsilon_{0,2}$ are contained in (V.53) only on the left-hand side in two very simple terms corresponding to the simplest diagram for $\mathcal{K}_{\text{in}}$ and that for $\mathcal{K}_{\text{out}}$ in Fig. 5. Moving these two terms to the right-hand side of (V.53) and combining them with $\mathbf{m}^{x}(\mathbf{p})$ results in an equation of the form

$$\mathfrak{K}''(\mathbf{p}) = [\mathbf{m}''(\mathbf{p})]^{-1} - \mathfrak{M}^{-1}(\mathbf{p}), \tag{V.173}$$

where $\mathfrak{K}''(\mathbf{p})$ is the same as $\mathfrak{K}(\mathbf{p})$ except that all terms containing $\Upsilon_{0,2}$ and $\Upsilon_{2,0}$ are deleted, and

$$\mathbf{m}''(\mathbf{p}) = \begin{pmatrix} z^{-1} - \langle \mathbf{p}|\Upsilon_{1,1}^{x}|\mathbf{p}\rangle & -\langle\ |\Upsilon_{0,2}|\mathbf{p},-\mathbf{p}\rangle \\ -\langle \mathbf{p},-\mathbf{p}|\Upsilon_{2,0}^{x}|\ \rangle & z^{-1} - \langle -\mathbf{p}|\Upsilon_{1,1}^{x}|-\mathbf{p}\rangle \end{pmatrix}.$$

It can be shown that this is exactly what one obtains by first further contracting the contracted graphs through a partial summation over the (0,2) and (2,0) vertices, and then performing the reduction operation.

APPENDIX G

The proof of (V.58) and (V.59) is similar to, but more complicated than the discussion given in Appendix C of paper IV.

Let us consider any dual (0,0)-graph. By cutting any one of the internal lines open but retaining the arrows of its two ends, we can obtain a dual (μ,ν)-graph, called a corresponding (μ,ν)-graph, where

$$(\mu,\nu) = (1,1)$$

if this particular internal line has two parallel arrows; otherwise,

$$(\mu,\nu) = (0,2) \quad \text{or} \quad (2,0),$$

depending on whether the two arrows are pointing away from each other or towards each other. Furthermore, if the original dual (0,0)-graph is irreducible, then the corresponding (μ,ν)-graph is also an irreducible dual graph.

Similar to the discussion given in paper IV [see Eq. (IV-103)] there is a relationship between the symmetry number of any irreducible dual (0,0)-graph and its corresponding (μ,ν)-graph. To study such a relationship we first introduce the definition of equivalent arrows. Two arrows in an irreducible dual graph are considered equivalent if the labeling of these two arrows, respectively, as α, β and leaving all other arrows unlabeled lead to the same topological structure, (which includes the positions of these two labels), as the labeling of these two arrows, respectively, as β, α. To each arrow we define an *equivalence number*

$$n, \tag{V.174}$$

which is the total number of equivalent arrows including itself. It is clear that two arrows on the same line must have the same equivalence number n.

Next, we consider any irreducible dual (0,0)-graph with symmetry number S. By cutting one of its lines open one obtains an irreducible (μ,ν)-graph with symmetry number, say, σ.

Let n be the equivalence number of an arrow which is on the line that is being cut. The following lemma relates n with the two symmetry numbers S and σ.

Lemma 1.—

$$nS^{-1}\sigma = 1. \tag{V.175}$$

*Proof.—*In Figs. 10 and 11 we list various examples to illustrate (V.175). Although (V.175) is fairly self-evident, like most combinational problems its proof is somewhat clumsy.

We number every arrow of the irreducible dual (0,0)-graph with M lines by an integer i, where

$$i = 1, 2, \cdots (2M).$$

The result is called a *numbered* irreducible dual (0,0)-graph. Let us fix the position of one of the integers,

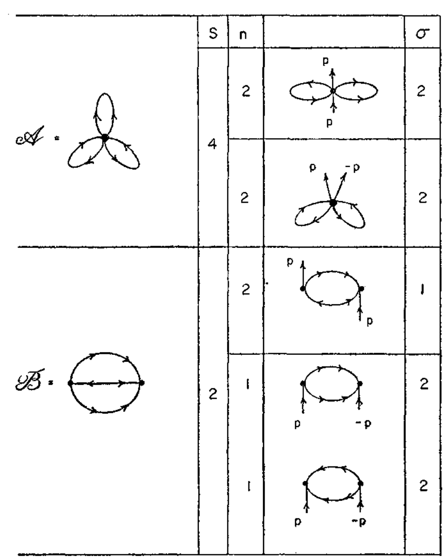

FIG. 10. Examples of symmetry numbers and equivalence numbers. If n is the equivalence number of an arrow in an irreducible dual (0,0)-graph with symmetry number S, then by cutting open the line which contains this arrow and assigning a momentum $\mathbf{p}$ to this arrow one obtains a corresponding (μ,ν)-graph with symmetry number $\sigma = n^{-1}S$ [see (V.175)].

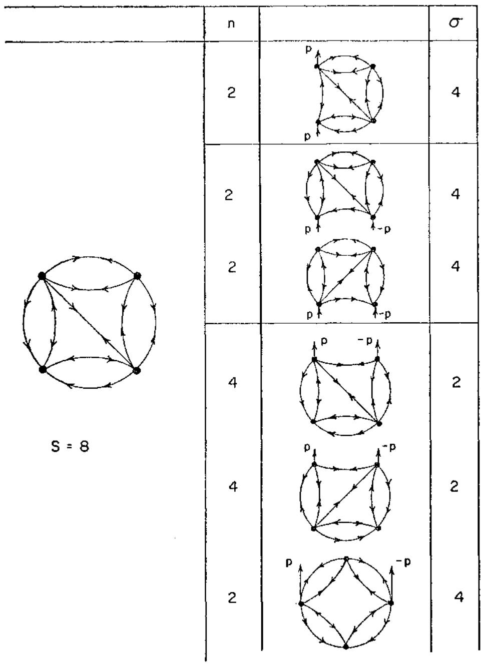

FIG. 11. Further examples of symmetry numbers and equivalence numbers.

say, A, but consider the $(2M-1)!$ permutations of the positions of the other $(2M-1)$ integers. By using the definitions of equivalence number and symmetry number it can be shown that among these $(2M-1)!$ permutations the total number of *numbered* irreducible dual (0,0)-graphs that have identical structures is given by

$$n^{-1}S, \tag{V.176}$$

where n is the equivalence number of the arrow which is associated with the integer A.

On the other hand, we can evaluate the same number (V.176) by considering the corresponding (μ,ν)-graph which is obtained by cutting open the line that contains this particular arrow (which has the equivalence number n), and assign to this arrow a momentum $\mathbf{p}$. It is easy to see that the number (V.176) is identical with the symmetry number σ of this corresponding (μ,ν)-graph. Thus, we find

$$n^{-1}S=\sigma,$$

which is Lemma 1.

Now in

$$\mathfrak{P}'(xz,\mathfrak{M},\mathfrak{M}_{\text{in}},\mathfrak{M}_{\text{out}}) \equiv \sum [\text{all different irreducible dual (0,0)-graphs}] \tag{V.57}$$

we can consider $\mathfrak{P}'$ to be an explicit functional of $\mathfrak{M}(\mathbf{p})$, $\mathfrak{M}_{\text{in}}(\mathbf{p})$, $\mathfrak{M}_{\text{out}}(\mathbf{p})$, and the variable (xz), where the dependence on (xz) is implicitly through the factors $\Upsilon_{S,t}{}^{x}$.

Lemma 2.—

$$[\delta\mathfrak{P}'(xz,\mathfrak{M},\mathfrak{M}_{\text{in}},\mathfrak{M}_{\text{out}})]_{(xz)} = \sum_{\mathbf{p}} \mathcal{K}(\mathbf{p})\delta\mathfrak{M}(\mathbf{p}) + \sum_{\mathbf{p}}{}' \mathcal{K}_{\text{in}}(\mathbf{p})\delta\mathfrak{M}_{\text{out}}(\mathbf{p}) + \sum_{\mathbf{p}}{}' \mathcal{K}_{\text{out}}(\mathbf{p})\delta\mathfrak{M}_{\text{in}}(\mathbf{p}), \tag{V.177}$$

where $\sum_{\mathbf{p}}{}'$ extends over the half $\mathbf{p}$-plane. In (V.177) the variation $\delta\mathfrak{M}$, $\delta\mathfrak{M}_{\text{in}}$, and $\delta\mathfrak{M}_{\text{out}}$ are completely arbitrary provided

$$\delta\mathfrak{M}_{\alpha}(\mathbf{p}) = \delta\mathfrak{M}_{\alpha}(-\mathbf{p}), \tag{V.178}$$

where $\alpha=$ in or out.

Proof.—To show (V.177) let us consider, e.g., the first irreducible dual (0,0)-graph in Fig. 10:

$$\mathcal{A} = \tfrac{1}{4} \sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_3} \langle \mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3 | \Upsilon_{3,3}{}^{x} | \mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3\rangle \mathfrak{M}(\mathbf{p}_1)\mathfrak{M}(\mathbf{p}_2)\mathfrak{M}_{\text{in}}(\mathbf{p}_3).$$

The functional derivatives of $\mathcal{A}$ [subject to (V.178)] are given by

$$\left[\frac{\delta\mathcal{A}}{\delta\mathfrak{M}(\mathbf{p})}\right]_{\mathfrak{M}_{\text{in}},(xz)} = \tfrac{1}{2} \sum_{\mathbf{p}_1\mathbf{p}_2} \langle \mathbf{p},\mathbf{p}_1,\mathbf{p}_2 | \Upsilon_{3,3}{}^{x} | \mathbf{p},\mathbf{p}_1,\mathbf{p}_2\rangle \mathfrak{M}(\mathbf{p}_1)\mathfrak{M}_{\text{in}}(\mathbf{p}_2),$$

and

$$\left[\frac{\delta\mathcal{A}}{\delta\mathfrak{M}_{\text{in}}(\mathbf{p})}\right]_{\mathfrak{M},(xz)} = \tfrac{1}{2} \sum_{\mathbf{p}_1\mathbf{p}_2} \langle \mathbf{p}_1,\mathbf{p}_2,\mathbf{p} | \Upsilon_{3,3}{}^{x} | \mathbf{p}_1,\mathbf{p}_2,\mathbf{p}\rangle \mathfrak{M}(\mathbf{p}_1)\mathfrak{M}(\mathbf{p}_2),$$

where these two expressions are identical with the corresponding (1,1)-graph and (2,0)-graph of $\mathcal{A}$, as shown in Fig. 10.

As another example, we consider the second irreducible dual (0,0)-graph in Fig. 10.

$$\mathcal{B} = \tfrac{1}{2} \sum_{\mathbf{p}_1\mathbf{p}_2\mathbf{p}_3} \langle \mathbf{p}_1\mathbf{p}_2 | \Upsilon_{2,1}{}^{x} | \mathbf{p}_3\rangle\langle\, | \Upsilon_{0,3}{}^{x} | \mathbf{p}_1, \mathbf{p}_2, -\mathbf{p}_3\rangle \times \mathfrak{M}(\mathbf{p}_1)\mathfrak{M}(\mathbf{p}_2)\mathfrak{M}_{\text{out}}(\mathbf{p}_3).$$

The functional derivative of $\mathcal{B}$ [subject to (V.178)] is given by

$$\left[\frac{\delta\mathcal{B}}{\delta\mathfrak{M}(\mathbf{p})}\right]_{\mathfrak{M}_{\text{out}},(xz)} = \sum_{\mathbf{p}_1\mathbf{p}_2} \langle \mathbf{p},\mathbf{p}_1 | \Upsilon_{2,1}{}^{x} | \mathbf{p}_2\rangle \times \langle\, | \Upsilon_{0,3}{}^{x} | \mathbf{p}, \mathbf{p}_1, -\mathbf{p}_2\rangle \mathfrak{M}(\mathbf{p}_1)\mathfrak{M}_{\text{out}}(\mathbf{p}_2), \tag{V.179}$$

and

$$\left[\frac{\delta\mathcal{B}}{\delta\mathfrak{M}_{\text{out}}(\mathbf{p})}\right]_{\mathfrak{M},(xz)} = \tfrac{1}{2} \sum_{\mathbf{p}_1\mathbf{p}_2} \langle \mathbf{p}_1,\mathbf{p}_2 | \Upsilon_{2,1}{}^{x} | \mathbf{p}\rangle\langle\, | \Upsilon_{0,3}{}^{x} | \mathbf{p}_1, \mathbf{p}_2, -\mathbf{p}\rangle \times \mathfrak{M}(\mathbf{p}_1)\mathfrak{M}(\mathbf{p}_2) + \tfrac{1}{2} \sum_{\mathbf{p}_1\mathbf{p}_2} \langle \mathbf{p}_1, \mathbf{p}_2 | \Upsilon_{2,1}{}^{x} | -\mathbf{p}\rangle \times \langle\, | \Upsilon_{0,3}{}^{x} | \mathbf{p}_1,\mathbf{p}_2,\mathbf{p}\rangle \mathfrak{M}(\mathbf{p}_1)\mathfrak{M}(\mathbf{p}_2). \tag{V.180}$$

Comparing with Fig. 10, one finds that (V.179) is identical with the corresponding (1,1)-graph of $\mathfrak{B}$ and (V.180) is equal to the sum of the two corresponding (0,2)-graphs of $\mathfrak{B}$.

In general, let λ_1 be the total number of lines, each of which has two parallel arrows, in an irreducible dual (0,0)-graph. The functional derivative of such a graph with respect to $\delta\mathfrak{M}_{(\mathbf{p})}$ is a sum of λ_1 terms each of which can be obtained by cutting one of the λ_1 lines open and then assigning to both arrows of the opened line a momentum $\mathbf{p}$. Each term, therefore, is equal to $S^{-1}\sigma$ times the value of the corresponding (1,1)-graph where S and σ are the symmetry numbers of the irreducible dual (0,0)-graph and its corresponding (1,1)-graph, respectively. By cutting open, one at a time, these λ_1 different lines one would obtain n such identical terms where n is the equivalence number of the arrow which is on the line that is being opened. By using Lemma 1, one finds

$$\left\{\frac{\delta}{\delta\mathfrak{M}(\mathbf{p})}[\text{any irreducible dual (0,0)-graph}]\right\}_{\mathfrak{M}_{\text{in}},\mathfrak{M}_{\text{out}},(xz)} =\sum[\text{all its different corresponding (1,1)-graphs}]. \quad \text{(V.181)}$$

In this irreducible dual (0,0)-graph, let λ_2 be the total number of internal lines that have two arrows pointing towards each other. The functional derivative of such a graph with respect to $\delta\mathfrak{M}_{\text{in}}(\mathbf{p})$ [subject to (V.178)] is a sum of

$$2\lambda_2 \quad \text{(V.182)}$$

terms, each of which can be obtained by cutting one of these λ_2 lines open and assigning to these two arrows momenta $\mathbf{p}$ and $-\mathbf{p}$, respectively. The factor 2 in (V.182) is due to the two ways of assigning $\mathbf{p}$ and $-\mathbf{p}$ to these two arrows. Again, if n is the equivalence number of the arrow of the opened line then every such term would appear n times in the sum, and each term is equal to $S^{-1}\sigma$ times the value of the corresponding (2,0)-graph whose symmetry number is σ. By using Lemma 1, one finds

$$\left\{\frac{\delta}{\delta\mathfrak{M}_{\text{in}}(\mathbf{p})}[\text{any irreducible dual (0,0)-graph}]\right\}_{\mathfrak{M},\mathfrak{M}_{\text{out}},(xz)} =\sum[\text{all its different corresponding (2,0)-graphs}]. \quad \text{(V.183)}$$

Similarly, one finds

$$\left\{\frac{\delta}{\delta\mathfrak{M}_{\text{out}}(\mathbf{p})}[\text{any irreducible (0,0)-graph}]\right\}_{\mathfrak{M},\mathfrak{M}_{\text{in}},(xz)} =\sum[\text{all its different corresponding (0,2)-graphs}]. \quad \text{(V.184)}$$

By using (V.181), (V.183), (V.184) and summing over all irreducible dual (0,0)-graphs, one proves Lemma 2.

Lemma 3.—If in

$$\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')=\sum_{\mathbf{p}}\ln\{z^{-1}[\mathfrak{M}^2(\mathbf{p})-\mathfrak{M}'^2(\mathbf{p})]^{\frac{1}{2}}\} -\sum_{\mathbf{p}}[m^x(\mathbf{p})]^{-1}[\mathfrak{M}(\mathbf{p})-m^x(\mathbf{p})]+\mathfrak{P}'+\mathfrak{X}, \quad \text{(V.59)}$$

$\mathfrak{P}$ is regarded as an explicit functional of x, z, $\mathfrak{M}$ and $\mathfrak{M}'$, then at constant x and z

$$\begin{aligned}[\delta\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')]_{x,z} &=\sum_{\mathbf{p}}\{\mathfrak{K}(\mathbf{p})+[\mathfrak{M}^2(\mathbf{p})-\mathfrak{M}'^2(\mathbf{p})]^{-\frac{1}{2}}\mathfrak{M}(\mathbf{p}) \\ &\quad -[m^x(\mathbf{p})]^{-1}\}\delta\mathfrak{M}(\mathbf{p})+2\sum_{\mathbf{p}}{}'\{\mathfrak{K}'(\mathbf{p}) \\ &\quad -[\mathfrak{M}^2(\mathbf{p})-\mathfrak{M}'^2(\mathbf{p})]^{-\frac{1}{2}}\mathfrak{M}'(\mathbf{p})\}\delta\mathfrak{M}'(\mathbf{p}), \end{aligned} \quad \text{(V.185)}$$

where

$$\delta\mathfrak{M}'(\mathbf{p})=\delta\mathfrak{M}'(-\mathbf{p}).$$

Proof.—Lemma 3 is a direct consequence of Lemma 2 and (V.55).

We remark that if

$$[\delta\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')]_{x,z}=0,$$

then $\mathfrak{M}$ and $\mathfrak{M}$ satisfy (V.53) and vice versa. (V.186)

To prove (V.58), one regards $\mathfrak{M}$ and $\mathfrak{M}'$ as given by (V.53). They are expressible in terms of x and z. Substituting these expressions into (V.59) one considers $\mathfrak{P}$ to be a function of z and (xz),

$$\mathfrak{P}(x,z,\mathfrak{M},\mathfrak{M}')\equiv\boldsymbol{\mathfrak{P}}(z,xz),$$

where z and (xz) are treated as independent variables. By using (V.59), (V.33), and (V.186), one finds

$$\left[z\frac{\partial}{\partial z}\boldsymbol{\mathfrak{P}}(z,xz)\right]_{(xz)}=\sum_{\mathbf{p}}[z^{-1}\mathfrak{M}(\mathbf{p})-1]+x\Omega. \quad \text{(V.187)}$$

Furthermore, as $z\rightarrow 0$ but keeping $(xz)=$constant

$$[\boldsymbol{\mathfrak{P}}(z,xz)+x\Omega]\rightarrow\sum_{n=1}^{\infty}(n!)^{-2}(xz\Omega)^n \times\langle 0,\cdots 0|\Upsilon_n{}^s|0,\cdots 0\rangle. \quad \text{(V.188)}$$

By using (V.34) it can be verified readily that $\ln\mathcal{Q}_\Omega{}^x$ satisfies the same equations (V.187) and (V.188) as $\boldsymbol{\mathfrak{P}}(z,xz)$. Consequently,

$$\ln\mathcal{Q}_\Omega{}^x=\boldsymbol{\mathfrak{P}}(z,xz). \quad \text{(V.189)}$$

The variational principles [(V.61)–(V.63)] follow directly from (V.186) and (V.189).

APPENDIX H

To prove Theorem 3 it is necessary to discuss some detailed properties of the $(\mu,\nu)_x$-graphs introduced in Appendix C.

We first observe that rules (i)‴–(iv)‴ used in determining (V.159) can be stated in an alternative form:

(i)^x In each $(\mu,\nu)_x$-graph, assign a different integer j to every line (internal or external, straight or wavy) where

$$j=1,\,2,\,\cdots N,$$

and

$$N=m+l_0+l_i+\mu+\nu,$$

where m, l_0, l_i are, respectively, the total number of internal lines, wavy outgoing lines and wavy incoming lines. Since the total number of the external incoming lines in a $(\mu,\nu)_x$-graph must be equal to that of the external outgoing lines, we have

$$l_0+\mu=l_i+\nu.$$

Next, assign to each internal line a nonzero momentum p_{A_i} $(i=1,\cdots m)$ where A_i is the integer associated with that internal line, and to each wavy line a zero momentum.

(ii)^x To each $(s,t;n)$-vertex we assign a factor

$$\langle \mathbf{p}_{C1},\cdots \mathbf{p}_{Cs},0,\cdots 0|\Upsilon_n{}^S|\mathbf{p}_{D1},\cdots \mathbf{p}_{Dt},0,\cdots 0\rangle,$$

where $(\mathbf{p}_{D1},\cdots \mathbf{p}_{Dt},0,\cdots 0)$ and $(\mathbf{p}_{C1},\cdots \mathbf{p}_{Cs},0,\cdots 0)$ are, respectively, the appropriate momenta of the incoming and outgoing lines connected at this vertex.

(iii)^x Assign a factor z to each internal line and a factor $(xz\Omega)^{\frac{1}{2}}$ to each wavy line.

(iv)^x Assign a factor

$$(\text{total symmetry number})^{-1}$$

to the entire $(\mu,\nu)_x$-graph where the total symmetry number is defined as follows:

Number the $(\mu,\nu)_x$-graph according to (i)^x, and call the resulting graph a "*completely numbered* $(\mu,\nu)_x$-*graph*." Two completely numbered $(\mu,\nu)_x$-graphs are different only if they have different topological structures which include the positions of these N integers. It is important to remember that the external straight lines are always considered to be distinguishable from each other. Among the $N!$ permutations of these N integers, the total number of "completely numbered $(\mu,\nu)_x$-graphs" identical to any given one is defined to be the "*total symmetry number*" of the $(\mu,\nu)_x$-graph.

The term corresponding to a $(\mu,\nu)_x$-graph is, then, given by

$$\sum_{\mathbf{p}_{A1}\cdots\mathbf{p}_{Am}}[\text{product of all factors in (ii)}^x\text{–(iv)}^x].\qquad\text{(V.190)}$$

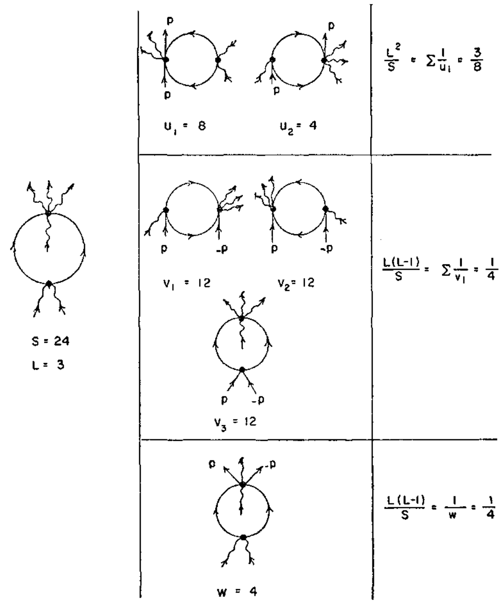

FIG. 12. Examples of total symmetry numbers for a $(0,0)_x$-graph and its related $(\mu,\nu)_x$-graphs [see (V.196) and (V.197)]. Notice that in this example $S^{-1}L=\sum_i u_i^{-1}-\frac{1}{2}\sum_j v_j^{-1}-\frac{1}{2}\sum_k w_k^{-1}=\frac{1}{8}$.

We remark that the differences between (ii)^x and (ii)‴ precisely cancels the differences between (iv)^x and (iv)‴. Consequently (V.190) is identical to (V.159).

Some examples of the total symmetry numbers are given in Fig. 12.

Similar to the discussions given in Appendix E we classify all $(\mu,\nu)_x$-graphs into two groups, proper and improper. A $(\mu,\nu)_x$-graph is called improper if by cutting any one of its internal lines open the entire graph can be separated into two disconnected graphs. Otherwise, it is called a proper $(\mu,\nu)_x$-graph. It is clear that all $(0,0)_x$-graphs are proper.

In terms of these proper $(\mu,\nu)_x$-graphs we can use (V.162) and (V.168) to express $\mathcal{K}(\mathbf{p})$, $\mathcal{K}_{\text{in}}(\mathbf{p})$, and $\mathcal{K}_{\text{out}}(\mathbf{p})$.

$$\begin{aligned}
&\mathcal{K}(\mathbf{p})\\
&\quad=\sum[\text{all different proper }(1,1)_x\text{-graphs}]\\
&\qquad\qquad-\langle\mathbf{p}|\Upsilon_{1,1}{}^x|\mathbf{p}\rangle,\\
&\mathcal{K}_{\text{in}}(\mathbf{p})\qquad\qquad\qquad\qquad\qquad\qquad\text{(V.191)}\\
&\quad=\sum[\text{all different proper }(0,2)_x\text{-graphs}],\\
&\mathcal{K}_{\text{out}}(\mathbf{p})\\
&\quad=\sum[\text{all different proper }(2,0)_x\text{-graphs}],
\end{aligned}$$

where each graph contributes a term given by (V.190).

The presence of $-\langle\mathbf{p}|\Upsilon_{1,1}{}^x|\mathbf{p}\rangle$ in (V.191) is due to the fact that a (1,1)-vertex is not present in the contracted (1,1)-graph but the corresponding $(1,1;n)$-vertices are present in the $(1,1)_x$-graphs.

There exists a close relationship between $(0,0)_x$-graphs and proper $(\mu,\nu)_x$-graphs where

$$(\mu,\nu)=(1,1),\ (0,2),\quad\text{and}\quad(2,0).$$

Starting from a $(0,0)_x$-graph we can generate a set of proper $(1,1)_x$-graphs by changing any one of the outgoing wavy lines in the $(0,0)_x$-graph to an external outgoing straight line associated with momentum $\mathbf{p}$, and by changing any one of the incoming wavy lines to an external incoming straight line also associated with momentum $\mathbf{p}$. The resulting graph is a proper $(1,1)_x$-graph. The totality of all different proper $(1,1)_x$-graphs constructed this way is called the set of all *related* proper $(1,1)_x$-graphs.

Similarly, we can take any two of the incoming (outgoing) wavy lines in a $(0,0)_x$-graph and change them to two external incoming (outgoing) lines associated with momenta $\mathbf{p}$ and $-\mathbf{p}$, respectively. The resulting graph is a proper $(0,2)_x[(2,0)_x]$-graph. The totality of all different proper $(0,2)_x[(2,0)_x]$-graphs thus constructed is called the set of all related proper $(0,2)_x[(2,0)_x]$-graphs.

Lemma 1.—

$$S^{-1}L=\sum_i u_i^{-1}-\tfrac{1}{2}\sum_j v_j^{-1}-\tfrac{1}{2}\sum_k w_k^{-1}, \quad \text{(V.192)}$$

where $2L$ is the total number of wavy lines in any $(0,0)_x$-graph, S is its total symmetry number, u_i, v_j, w_k are, respectively, the total symmetry number of its ith related proper $(1,1)_x$-graph, the jth related proper $(0,2)_x$-graph and the kth related proper $(2,0)_x$-graph. In (V.192) the sum extends to all appropriate related graphs.

An example of (V.192) is given in Fig. 12.

Proof.—From any $(0,0)_x$-graph we can construct "completely numbered $(0,0)_x$-graphs" according to $(\mathrm{i})^x$. From the definition of the "total symmetry number," the total number of such different completely numbered $(0,0)_x$-graphs is given by

$$g=N!S^{-1}, \quad \text{(V.193)}$$

where N is the total number of lines (straight or wavy and internal or external) in the $(0,0)_x$-graph. From each of these different "completely numbered $(0,0)_x$-graphs" we can choose an incoming wavy line and an outgoing wavy line; change both to straight lines; label both with the momentum $\mathbf{p}$ but retain their numbers. The resulting graph is a "completely numbered proper $(1,1)_x$-graph." The total number of such different "completely numbered proper $(1,1)_x$-graph" is

$$L^2g=L^2N!S^{-1}, \quad \text{(V.194)}$$

where the factor L^2 represents the different ways to choose these two wavy lines among the L numbered incoming wavy lines and the L numbered outgoing wavy lines. The same set of "completely numbered $(1,1)_x$-graphs" can also be constructed by numbering the related set of proper $(1,1)_x$-graphs. By using the definition of the "total symmetry number" u_i, the number of such different "completely numbered $(1,1)_x$-graphs" is found to be

$$N!\sum u_i^{-1}. \quad \text{(V.195)}$$

Equating (V.194) with (V.195), we find

$$L^2S^{-1}=\sum_i u_i^{-1}. \quad \text{(V.196)}$$

In an entirely similar way, by considering the related set of proper $(0,2)_x$-graphs and $(2,0)_x$-graphs it can be shown that

$$L(L-1)S^{-1}=\sum_j v_j^{-1}=\sum_k w_k^{-1}, \quad \text{(V.197)}$$

where $L(L-1)$ represents the different ways to choose two among the L appropriate numbered wavy lines and label them $+\mathbf{p}$ and $-\mathbf{p}$, respectively.

Combining (V.196) and (V.197), we prove Lemma 1.

Lemma 2.—If

$$\Omega^{-1}\frac{\partial}{\partial x}\ln \mathcal{Q}_\Omega{}^x=0, \quad \text{(V.198)}$$

then

$$z^{-1}=\mathcal{K}(\mathbf{p}\to 0)-\mathcal{K}'(\mathbf{p}\to 0)+\langle 0|\Upsilon_{1,1}{}^x|0\rangle, \quad \text{(V.199)}$$

where $\mathcal{K}$ and $\mathcal{K}'$ are given by (V.78) and (V.79).

Proof.—From (V.160), we can write

$$\Omega^{-1}\frac{\partial}{\partial x}\ln \mathcal{Q}_\Omega{}^x=-1+\sum (x\Omega)^{-1}L[(0,0)_x\text{-graph}], \quad \text{(V.200)}$$

where $2L$ is the total number of wavy lines in the $(0,0)_x$-graph. In (V.200) the sum extends over all different $(0,0)_x$-graphs. Throughout this appendix, we use the notation $[(\mu,\nu)_x\text{-graphs}]$ to represent the term corresponding to the $(\mu,\nu)_x$-graph as given by (V.190).

By using (V.190) and (V.196) we find

$$(xz\Omega)^{-1}L^2[(0,0)_x\text{-graph}] =\sum_i [i\text{th related proper }(1,1)_x\text{-graph}]_{\mathbf{p}\to 0},$$

where the sum extends over all different related proper $(1,1)_x$-graphs. The factor $(xz\Omega)^{-1}$ on the left-hand side is due to $(\mathrm{ii})^x$. Similarly, by using Lemma 1 we find for any $(0,0)_x$-graph that the following identity holds:

$$\begin{aligned}(xz\Omega)^{-1}L[(0,0)_x\text{-graph}] &=\sum_i [i\text{th related proper }(1,1)_x\text{-graph}]_{\mathbf{p}\to 0}\\ &-\tfrac{1}{2}\sum_j [j\text{th related proper }(0,2)_x\text{-graph}]_{\mathbf{p}\to 0}\\ &-\tfrac{1}{2}\sum_k [k\text{th related proper }(2,0)_x\text{-graph}]_{\mathbf{p}\to 0}.\end{aligned} \quad \text{(V.201)}$$

If (V.198) holds, then by substituting (V.201) into (V.200) and utilizing (V.191) it follows that

$$z^{-1}=\mathcal{K}(\mathbf{p}\to 0)-\tfrac{1}{2}\mathcal{K}_{\mathrm{in}}(\mathbf{p}\to 0)-\tfrac{1}{2}\mathcal{K}_{\mathrm{out}}(\mathbf{p}\to 0) +\langle 0|\Upsilon_{1,1}{}^x|0\rangle.$$

Thus, Lemma 2 is proved.

To prove Theorem 3 we notice that (V.199) is

identical with

$$\{[m^x(\mathbf{p})]^{-1}-\mathcal{K}(\mathbf{p})+\mathcal{K}'(\mathbf{p})\}_{\mathbf{p}\to 0}=0. \quad \text{(V.202)}$$

On the other hand, from (V.77),

$$[\mathfrak{M}'(\mathbf{p})/\mathfrak{M}(\mathbf{p})]=\mathcal{K}'(\mathbf{p})\{[m^x(\mathbf{p})]^{-1}-\mathcal{K}(\mathbf{p})\}^{-1}, \quad \text{(V.203)}$$

and

$$\mathfrak{M}^{-1}(\mathbf{p})=\{[m^x(\mathbf{p})]^{-1}-\mathcal{K}(\mathbf{p})\} -\{[m^x(\mathbf{p})]^{-1}-\mathcal{K}(\mathbf{p})\}^{-1}[\mathcal{K}'(\mathbf{p})]^2. \quad \text{(V.204)}$$

Combining (V.202), (V.203), and (V.204), we complete the proof for Theorem 3.

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Calculations of Total Cross Sections for Scattering from Coulomb Potentials with Exponential Screening*

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Momentum transfer cross sections and total cross sections are calculated for scattering from the potential energy function $V=(Z_1Z_2e^2/r)\exp(-r/a)$. Here the first factor is the Coulomb term and the exponential factor contains a screening length a. The cross sections are obtained by integrating the differential cross section over all angles using a classical calculation or a Born approximation calculation according to whichever is valid. The validity criteria are discussed as they depend on the de Broglie wavelength of the scattered particle. In certain cases the Born approximation solution is valid at small angles and the classical solution is valid at large angles. Graphs and tables are presented showing the results as functions of suitable parameters.

The momentum transfer cross section is finite in all cases and the total cross section is finite except in the classical limit. In this limit, however, calculations are presented showing that portion of the total cross section which arises from scattering through angles greater than a specified small angle.

1. INTRODUCTION

THE screened Coulomb potential energy function is often used to describe the interaction between two colliding atoms. It is useful in an energy range extending from a few hundred electron volts to several hundred thousand electron volts. The function under consideration is

$$V=(Z_1Z_2e^2/r)\exp(-r/a), \quad (1)$$

where Z_1e and Z_2e are the nuclear charges of the colliding atoms and a is a screening length. Differential cross sections were computed classically for scattering from this potential energy function in a paper,[1] hereinafter called reference I, and similar calculations which agree well have been made by Firsov.[2] Experimental measurements of differential cross section for ion-atom collisions by Fuls *et al.*[3] agree very well with the calculated values. Evidently one may use the classical calculations of I with some confidence to obtain values of impact parameter and distance of closest approach, as well as differential cross section at various scattering angles. It was, therefore, thought desirable to extend the calculations to obtain certain total scattering cross sections for this potential.

It has long been recognized that the Coulomb potential gives rise to an infinite total cross section both classically and quantum mechanically. The addition of the exponential screening factor, however, makes this total cross section finite except in the purely classical limit, as seen in the values to be presented in Sec. 4 below.

Although the total elastic scattering cross section is a well-established concept, it is not particularly useful because it cannot be measured. The reason, of course, is that extremely gentle collisions make up a large part of the total cross section, and one cannot experimentally tell the difference between an unscattered particle and one which has been scattered through a minute angle. One way of avoiding this difficulty is to calculate, as in Sec. 5 below, only that portion of the total cross section which results from scattering in excess of a specified angle.

Perhaps a more useful cross section is that for momentum transfer. This incorporates a $1-\cos\theta$ factor in the integrand, which gives a low weight to the gentle forward collisions and a proportionally higher weight to the more violent collisions. The momentum transfer cross section enters into calculation of diffusion coeffi-

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