CLUSTER DEVELOPMENTS FOR JASTROW WAVE FUNCTIONS

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STELLINGEN

I

Variatie van de energie van een fermionengas beschreven door een Jastrow-golffunctie, levert in eerste orde een gemodificeerde tweedeeltjes-vergelijking, die verwant is met de zgn. Bethe-Goldstone vergelijking.

H. A. Bethe en J. Goldstone, Proc. Roy. Soc. A **238** (1957) 551.

II

De generalisatie van Jastrow-golffuncties tot mengsels van fermionen levert de mogelijkheid (naast de volume-energie) de symmetrie-energie van kernmaterie, althans qualitatief, te berekenen.

Hoofdstuk III van dit proefschrift.

III

Het is te verwachten dat de in dit proefschrift gegeven methode ook kan worden toegepast op de grondtoestand van een mengsel van fermionen en bosonen en bovendien, dat de clusterontwikkelingen van de distributiefuncties uitsluitend irreducible clusterintegralen bevatten.

Hoofdstuk II van dit proefschrift.

IV

De splitsing van de quantummechanische configuratie-integrand van een Bose- of Fermigas in een 'statistisch' en een 'dynamisch' deel, maakt het mogelijk meer gedetailleerde clusterintegralen in te voeren. Deze zijn van belang bij de fugaciteitsontwikkeling van druk en dichtheid in geval van lage temperatuur.

K. Huang, C. N. Yang en J. M. Luttinger, Phys. Rev. **105** (1957) 776.
Hoofdstuk III, appendix, van dit proefschrift.

V

De invloed van de kernspinprecessie ten gevolge van voorafgaande K-vangst op de hoekverdeling van γ-straling, uitgezonden door gerichte atoomkernen, is verwaarloosbaar klein.

H. A. Tolhoek, C. D. Hartogh en S. R. de Groot, J. Phys. Rad. **16** (1955) 615.

VI

Bij een γ-γ-overgang levert het waarnemen van de polarisatie van een der stralingen, naast het meten van de hoekcorrelatie tussen die twee stralingen, de mogelijkheid het teken van het electrische quadrupoolmoment van de tussentoestand te bepalen.

VII

De beschouwing van Bethe en de Hoffmann over de tekenkeuze bij de afleiding van de Kemmer-interactie tussen mesonen en nucleonen, is onjuist.

H. A. Bethe en J. de Hoffmann, Mesons and Fields II, § 31, Row, New-York, 1955.

VIII

Het gebruik van de door Abe ingevoerde pseudopotentiaal voor een gas van harde bollen verdient de voorkeur boven de pseudopotentiaal ingevoerd door Huang en Yang.

R. Abe, Progr. theor. Phys. **19** (1958) 1,699.
K. Huang en C. N. Yang, Phys. Rev. **105** (1957) 767.

IX

De door Rose gegeven formulering van het eerste decompositietheorema voor tensoren van de eerste rang is niet geheel juist.

M. E. Rose, Elementary Theory of Angular Momentum, § 20, Chapman, London, 1957.

X

Tegen de door Cooper en Henley gebruikte uitdrukking voor de Coulombenergie (ter berekening van de kernstraal uit het energieverschil tussen spiegelkernen) kunnen bezwaren worden aangevoerd.

L. M. Cooper en E. M. Henley, Phys. Rev. **92** (1953) 810.

CLUSTER DEVELOPMENTS FOR JASTROW WAVE FUNCTIONS

PROEFSCHRIFT

TER VERKRIJGING VAN DE GRAAD VAN DOCTOR IN DE WIS- EN NATUURKUNDE AAN DE RIJKSUNIVERSITEIT TE LEIDEN OP GEZAG VAN DE RECTOR MAGNIFICUS DR H. J. LAM, HOOGLERAAR IN DE FACULTEIT DER WIS- EN NATUURKUNDE, TEGEN DE BEDENKINGEN VAN DE FACULTEIT DER WIS- EN NATUURKUNDE TE VERDEDIGEN OP DONDERDAG 18 DECEMBER 1958 TE 14 UUR

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CHRISTIAAN DIRK HARTOGH

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Promotor: PROF. DR S. R. DE GROOT

Aan mijn ouders

INTRODUCTION

The purpose of this thesis is the study of the ground state, described by a Jastrow wave function, of a fermion gas with short range interactions (which may have a hard core). The influence of the introduction of forces is represented by a correlation factor multiplying the unperturbed ground state wave function; this correlation factor is a function of the position coordinates of the particles and may contain variational parameters.

In chapter I cluster-like expansions for the k-particle distribution functions are derived in a general form for fermions without spin, provided a certain condition has been satisfied. This condition, imposed on the correlation factor, is of importance when using the wave function as a trial wave function in a variational calculation. In chapter II a reduction of the result, generalized to mixtures of fermions, is carried out by means of the introduction of irreducible cluster functions and the use of certain combinatorial methods. In chapter III the method is extended to particles with spin and explicit results are given for the distribution functions and the energy, including the case of fermion mixtures. A discussion is given of the application of the method to nuclear matter. In the appendix to this chapter, the method is applied to an imperfect Bose or Fermi gas at low temperature and leads to the fugacity expansion of the pressure and the density in terms of more detailed cluster integrals.

The contents of this thesis are also published in Physica (Physica **24** (1958) 721, 875, 896).

CHAPTER I

GENERAL CLUSTER DEVELOPMENT OF THE DISTRIBUTION FUNCTIONS

Synopsis

This chapter is concerned with a form of wave function, which was proposed by Jastrow for the ground state of a fermion gas with short range interactions. The influence of the introduction of forces is represented by a correlation factor F, which is a function of the particle coordinates and which may contain variational parameters, in front of the Slater determinant for the unperturbed ground state wave function. This wave function may be used as a trial function in a variational principle. The evaluation of the energy can make use of cluster-like expansions for the k-particle distribution function $g_k(\boldsymbol{r}^k)$, which are given in this paper in a general form for fermions without spin. The expansion of $g_k(\boldsymbol{r}^k)$ can be made for the limit of large total volume and reads

$$g_k(\boldsymbol{r}^k) = n^k \sum_{l=k}^{\infty} b_{k,l}(\boldsymbol{r}^k),$$

where the $b_{k,l}(\boldsymbol{r}^k)$'s are cluster integrals which depend on the density, n, only, and not on the total number of particles. It seems plausible that this expansion converges rapidly, if $n\delta^3 \ll 1$ (δ range of correlations in the F-factor).

§ 1. *Introduction.* During the last few years the many-body problem of interaction fermions in the ground state has received renewed attention of many authors. Different lines of approach were used by (a) Brueckner, Bethe, Goldstone and Hugenholtz, (b) Lee, Yang and Huang, (c) Jastrow [1]), Iwamoto and Yamada [2]). The application of these developments, which has most interest at present, is to the problem of the structure of nuclear matter. The relative merits of the various approaches may be different in different applications, e.g., the problems of infinite nuclear matter, the theory of the nuclear "surface" and finite nuclei. It seems therefore of interest to make a further investigation of the various methods even if previous methods have met with reasonable success.

In the series of papers, of which this one is the first, we want to give the mathematics of the cluster developments, to be used in connection with Jastrow's wave function (cf. (2.1), (2.4) and (2.8)) in a general form, avoiding a number of objections, which can be raised against Jastrow's

calculations and generalizing it in various aspects. Our method differs also substantially from the cluster development method which was used by Iwamoto and Yamada [2]) for this type of wave functions.

Jastrow's method was applied to nuclear matter by Emery [3]) and Dabrowski [4]). We want further to point to the paper by Gomes, Walecka and Weisskopf [5]), in which a clear physical discussion of a number of features of the wave function of nuclear matter and the expression of the correlation between nucleons is given. In our opinion it shows that Jastrow's wave function represents these correlations in a way which seems simple and attractive and hence worthy of further investigation.

We shall give in this chapter the general form of the cluster developments for the k-particle distribution functions for a system of fermions without spin specified by a Jastrow wave function. The estimate of the explicit dependence of the various cluster contributions on the total number of fermions requires a careful handling of the momentum relations originating from the orthogonality of the different plane waves, which describe the unperturbed ground state. In subsequent chapters of this thesis we shall give: (a) a reduction of these expressions by means of the introduction of so called "irreducible cluster functions"; (b) the expressions for the kinetic and potential energy for such a system and a comparison with the work of Jastrow, Iwamoto and Yamada; (c) a generalization to fermions with spin; (d) an application of the methods used to a Bose or Fermi gas of interacting particles at low temperature.

§ 2. *The wave function and the distribution functions.* We consider the problem of N interacting fermions, contained in a volume Ω. We are interested here in volume effects only, so that we shall take the limit for $N \to \infty$, at constant density $n = N/\Omega$. For the sake of formal simplicity we shall limit ourselves in this paper to "fermions without spin" (particles, without spin coordinate, for which the wave function must be antisymmetric in the place coordinates). We shall further assume that the volume, in which the system is contained, is of a cubic shape with sides L ($\Omega = L^3$), and we shall require periodic boundary conditions.

If the particles have no interactions, the normalized wave function for the ground state of the system will simply be given by the Slater determinant

$$\begin{aligned} \Phi_0(\boldsymbol{r}^N, n) &= (\Omega^N N!)^{-\frac{1}{2}} \operatorname{Det} [\exp (i\boldsymbol{k}_i \cdot \boldsymbol{r}_j)] = \\ &= (\Omega^N N!)^{-\frac{1}{2}} \textstyle\sum_P \delta_P \exp [i \sum_i \boldsymbol{k}_{Pi} \cdot \boldsymbol{r}_i] = \\ &= (\Omega^N N!)^{-\frac{1}{2}} \textstyle\sum_P \delta_P \exp [i \sum_i \boldsymbol{k}_i \cdot \boldsymbol{r}_{Pi}], \qquad (21). \end{aligned}$$

which we shall sometimes write as a sum over the permutations P of the subscripts i ($\delta_P = +1$ or -1 for even and odd permutations). $\boldsymbol{r}^N$ represents

the set of N one-particle coordinates $\boldsymbol{r}_j$ $(j = 1, 2, \ldots, N)$. The possible values $\boldsymbol{k}_i$ $(i = 1, 2, \ldots, N)$ for the single particle momenta are given by

$$\boldsymbol{k}_i = (2\pi/L)\boldsymbol{n}_i, \tag{2.2}$$

where the $\boldsymbol{n}_i$ are three-dimensional vectors with integer components $(0, \pm 1, \pm 2, \ldots)$. In the limit of large N, the allowed values for $\boldsymbol{k}_i$ are those values (2.2) lying within the Fermi sphere in momentum space, which has the radius

$$k_F(n) = (6\pi^2)^{\frac{1}{3}} n^{\frac{1}{3}}. \tag{2.3}$$

The wave functions for interacting fermions, which will be studied in this paper, are of the form

$$\Phi(\boldsymbol{r}^N, n) = F(\boldsymbol{r}^N, n)\, \Phi_0(\boldsymbol{r}^N, n), \tag{2.4}$$

where $F(\boldsymbol{r}^N, n)$ is a symmetrical function in the N one particle coordinates. It is then seen that $\Phi(\boldsymbol{r}^N, n)$ again satisfies the requirement of antisymmetry in the particle coordinates. The correlations of the nucleons caused by the interaction are expressed by the factor $F(\boldsymbol{r}^N, n)$. The interest of the approach using such wave functions, which must be considered as approximate trial wave functions, was explained in § 1. We shall suppose in all our developments that we have short range forces and also that the nucleon correlations expressed by the F-factor have a short range, δ. We shall always require the following properties for $F(\boldsymbol{r}^N)$:

I. *The product property*:

$$F(\boldsymbol{r}^N) = F_{N_1}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_{N_1})\, F_{N_2}(\boldsymbol{r}_{N_1+1}, \ldots, \boldsymbol{r}_N)\ (N = N_1 + N_2),$$
$$\text{if } r_{ij} \equiv |\boldsymbol{r}_i - \boldsymbol{r}_j| > \delta \text{ for every } i = 1,2, \ldots, N_1 \text{ and}$$
$$\text{every } j = N_1 + 1, \ldots, N. \tag{2.5}$$

The functions F_{N_1} $(N_1 < N)$ are defined by this equation.

II. *Normalization to one* for separate configurations:

$$F_1(\boldsymbol{r}_i) = 1, \tag{2.6}$$

where $F_1(\boldsymbol{r}_i)$ is defined according to (2.5) if $N_1 = 1$. It should be noted that the wave function $\Phi(\boldsymbol{r}^N, n)$ according to (2.4) is generally not normalized, if $F(\boldsymbol{r}^N)$ is normalized according to (2.6). The value of the normalization constant, which has to be added, is derived in § 4 (cf. (4.28) and (4.32)).

It is an immediate consequence of (2.5) and (2.6) that the F-factor equals one, for a configuration in which no two points are closer than δ:

$$F(\boldsymbol{r}^N) = 1, \text{ if } r_{ij} > \delta \text{ for every } i, j = 1, \ldots, N.\ (i \neq j). \tag{2.7}$$

The wave function $\Phi(\boldsymbol{r}^N, n)$ deviates from the wave function $\Phi_0(\boldsymbol{r}^N, n)$ for non-interacting fermions as soon as any two particles approach each other within the distance δ.

The simplest and most important example of an F-factor satisfying (2.5) and (2.6) is given by [1])

$$F(\boldsymbol{r}^N) = \prod_{i>j=1}^{N} f(r_{ij}), \tag{2.8}$$

where $f(r)$ satisfies

$$f(r) = 1, \text{ if } r > \delta. \tag{2.9}$$

The introduction of a correlation factor of this type yields, already in first order, a finite result for the energy in case of a hard core potential.

The F-factor (2.8) introduces explicitly only two-particle correlations. Of course it is easy to generalize (2.8) so that also explicit 3-particle correlations are added:

$$F(\boldsymbol{r}^N) = [\prod_{i>j=1}^{N} f(r_{ij})][\prod_{k>l>m=1}^{N} g(\boldsymbol{r}_k, \boldsymbol{r}_l, \boldsymbol{r}_m)], \tag{2.10}$$

where $g(\boldsymbol{r}_k, \boldsymbol{r}_l, \boldsymbol{r}_m)$ must satisfy

$$g(\boldsymbol{r}_k, \boldsymbol{r}_l, \boldsymbol{r}_m) = 1, \text{ if } r_{kl} > \delta, r_{lm} > \delta, r_{km} > \delta. \tag{2.11}$$

The functions f and g (and hence the F-factor) may depend on one or more parameters α, which may be used as adjustable parameters when taking (2.4) as trial wave function in a quantum mechanical variational principle.

The expectation values of operators such as the energy can be calculated simply for a given wave function (2.4) once we have obtained the values of the so-called k-particle distribution function $g_k(\boldsymbol{r}^k)$. These are defined by the equation

$$g_k(\boldsymbol{r}^k) = a_k \int \Phi^*(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})\, \Phi(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})\, \mathrm{d}\boldsymbol{r}^{N-k}. \tag{2.12}$$

$\boldsymbol{r}^k$ stands for the set of k coordinates forming the basis; $\boldsymbol{r}^{N-k}$ stands for the other variables, over which the integration is performed ($k \ll N$). a_k is a normalization constant, which is chosen in such a way that

$$\int g_k(\boldsymbol{r}^k)\, \mathrm{d}\boldsymbol{r}^k = N!/(N-k)!. \tag{2.13}$$

This normalization makes $g_k(\boldsymbol{r}^k) \approx n^k$ for configurations in which the k particle coordinates lie sufficiently far apart.

The distribution functions can be generalized to expressions, which are non-diagonal in the coordinates:

$$g_k(\boldsymbol{r}^k, \boldsymbol{r}'^k) = a_k \int \Phi^*(\boldsymbol{r}'^k, \boldsymbol{r}^{N-k})\, \Phi(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})\, \mathrm{d}\boldsymbol{r}^{N-k}. \tag{2.14}$$

Although such distribution functions are needed for the evaluation of the kinetic energy ($k = 1$), we shall limit our attention in the following section mainly to expressions (2.12) for the sake of simplicity of the presentation.

§ 3. *Introduction of the correlation functions.* In the following section a cluster-like expansion for the distribution functions $g_k(\boldsymbol{r}^k)$ will be deduced. The methods which are used have a certain analogy to those which are used

in statistical mechanics [6][7]). In this section we shall introduce or summarize a number of definitions and notions, which will be employed in the further developments, also for avoiding too frequent references to papers in the field of statistical mechanics.

We start by considering the k-particle distribution function for non-interacting fermions; this function is a special case of (2.12)

$$g_k^{(0)}(\boldsymbol{r}^k) = a^k \int \Phi^*_0(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})\, \Phi_0(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})\, \mathrm{d}\boldsymbol{r}^{N-k}. \tag{3.1}$$

It is easily shown, according to standard methods, that this can be reduced to

$$g_k^{(0)}(\boldsymbol{r}^k) = n^k\, L_k^{(N)}(\boldsymbol{r}^k), \tag{3.2}$$

where $L_l^{(N)}$ is generally defined as

$$L_l^{(N)}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_l) = \mathrm{Det}\,(l_{ij}^{(N)}) \quad (i, j = 1, 2, \ldots, l), \tag{3.3}$$

with

$$l_{ij}^{(N)} = N^{-1} \sum_{\lambda=1}^{N} e^{i\boldsymbol{k}_\lambda \cdot (\boldsymbol{r}_i - \boldsymbol{r}_j)} \text{ (hence } l_{ii}^{(N)} = 1). \tag{3.4}$$

The summation should be performed over all $\boldsymbol{k}_\lambda$ within the Fermi sphere. The summation may be replaced by an integration (which is then easily carried out) for small values of $\boldsymbol{r}$ and in the limit of large Ω. This provides $l_{ij}^{(N)} = l(r_{ij})$ with

$$l(r) = 3\,(\sin y - y \cos y) y^{-3} \text{ with } y = k_F r = (6\pi^2)^{\frac{1}{3}}\, n^{\frac{1}{3}} r. \tag{3.5}$$

We shall indicate below when $l_{ij}^{(N)}$ may be replaced by the expression (3.5) (for convenience we shall mostly omit the superscript N).

As an illustration we may specialize to $k = 2$. We then find the pair distribution function for non-interacting fermions

$$g_2^{(0)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = n^2\, L_2^{(N)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = n^2[1 - l^2(r_{12})]. \tag{3.6}$$

We shall say that the function $g_k^{(0)}(\boldsymbol{r}^k)$ expresses the *statistical correlation* of fermions (the correlation due to Fermi statistics only) and we shall call $L_l^{(N)}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_l)$ the *statistical correlation function* for l fermions.

The part of the correlation of interacting fermions, which exists in deviations from the correlation given by $L_l^{(N)}$, as a consequence of their interaction, will be designated as the *dynamical correlation*. The dynamical correlation is expressed by means of the F-factor, if wave functions of the type (2.4) are used. We shall introduce a number of functions (W, U, R, V), which depend directly on the F-factor, and which we shall call (*dynamical*) *correlation functions*. They will be used for the cluster developments. We shall often use correlation functions for a certain basis $\boldsymbol{r}^k$, which means that a set of functions is used which all depend on some given set of k place coordinates $\boldsymbol{r}_\lambda$ and mostly also on other variables.

The *general correlation function* $W_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_l)$ (for the basis $\boldsymbol{r}^k$, and containing l variables) is defined by the equation

$$W_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_l) = F_l^*(\boldsymbol{r}^k, \boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_l)\, F_l(\boldsymbol{r}^k, \boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_l). \quad (3.7)$$

This function can be introduced for an N-particle system, because F_l is defined for such a system according to (2.5). In case the F-factor has the explicit form (2.8), we can immediately give the expression for F_l for this example

$$F_l(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_l) = \prod_{i>j=1}^{l} f(r_{ij}). \quad (3.8)$$

It follows directly from the definition (3.7) that $W_{k,l}$: (a) satisfies the *product property* (2.5), (b) is normalized to one for separate configurations. Hence one has in particular

$$W_{0,1} = 1. \quad (3.9)$$

It follows further from the definition of $W_{k,l}$ that it is symmetric in all variables $\boldsymbol{r}_1, \ldots, \boldsymbol{r}_l$. The general correlation function $W_{k,l}$ is analogous to a certain extent to the cluster functions $W_{k,l} = \exp(-\sum_{i>j=1}^{l} V_{ij}/kT)$ occurring as configurational integrands in the statistical mechanics of an imperfect classical gas with short range interactions [6][7]). If the wave function $\Phi(\boldsymbol{r}^N, n)$ according to (2.4) would not have the factor $\Phi_0(\boldsymbol{r}^N, n)$, cluster expansions for the quantum mechanical system in the ground state could be given by the methods already known from statistical mechanics [6][7]). This applies to the case of bosons, where we may put $\Phi_0 = 1$. Jastrow has given the cluster development for a system of bosons in the ground state [1]). However, a procedure which is appreciably more complicated must be followed for a system of fermions in the ground state (cf. § 4). This finds expression in the more complicated dependence of the final result on the density, in contrast with bosons, where the final result for $g_k(\boldsymbol{r}^k)$ can be written as a power series in the density. This is a consequence of the $k_F = (6\pi^2)^{\frac{1}{3}} n^{\frac{1}{3}}$ occurring in the statistical correlation function (cf. 3.5)).

The *separated correlation functions* $U_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_l)$ are defined in terms of the $W_{k,l}$-functions by the following equations, which are known in statistical mechanics as the Ursell-Mayer development [6][7]).

$$\begin{aligned}
&W_{k,k}(\boldsymbol{r}^k) = U_{k,k}(\boldsymbol{r}^k),\\
&W_{k,k+1}(\boldsymbol{r}^k, \boldsymbol{r}_\nu) = U_{k,k}(\boldsymbol{r}^k)\, U_{0,1}(\boldsymbol{r}_\nu) + U_{k,k+1}(\boldsymbol{r}^k, \boldsymbol{r}_\nu),\\
&W_{k,k+2}(\boldsymbol{r}^k, \boldsymbol{r}_\nu, \boldsymbol{r}_\lambda) = U_{k,k}(\boldsymbol{r}^k)\, U_{0,1}(\boldsymbol{r}_\nu) U_{0,1}(\boldsymbol{r}_\lambda) + \quad (3.10)\\
&+ U_{k,k}(\boldsymbol{r}^k)\, U_{0,2}(\boldsymbol{r}_\nu, \boldsymbol{r}_\lambda) + U_{k,k+1}(\boldsymbol{r}^k, \boldsymbol{r}_\nu)\, U_{0,1}(\boldsymbol{r}_\lambda) +\\
&+ U_{k,k+1}(\boldsymbol{r}^k, \boldsymbol{r}_\lambda) U_{0,1}(\boldsymbol{r}_\nu) + U_{k,k+2}(\boldsymbol{r}^k, \boldsymbol{r}_\nu, \boldsymbol{r}_\lambda),\\
&\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots
\end{aligned}$$

The general form of these equations may be written in an abbreviated form as (containing $k = 0$ as a special case)

$$W_{k,l}(\boldsymbol{r}_k, \boldsymbol{r}^{l-k}) = S'_{l(l_i)}\, U_{k,l_1}(\boldsymbol{r}^k, \boldsymbol{r}^{l_1-k}) \prod_{i>1}^{i'} U_{0,l_i}(\boldsymbol{r}^{l_i}). \tag{3.11}$$

The summation $S'_{l(l_i)}$ should be extended over all possible partitions of the $l - k$ non-basis coordinates over the different U_{k,l_i}-functions, hence the summation over the numbers l_i must be such that $l = \sum_{i=1}^{i'} l_i$, while k basis coordinates always remain concentrated in one U_{k,l_1}-function. The equations (3.10) can be solved for the U-functions. One obtains for $k = 0$.

$$\begin{aligned} &U_{0,1}(\boldsymbol{r}_\nu) = W_{0,1}(\boldsymbol{r}_\nu) = 1, \\ &U_{0,2}(\boldsymbol{r}_\nu, r_\lambda) = W_{0,2}(\boldsymbol{r}_\nu, \boldsymbol{r}_\lambda) - W_{0,1}(\boldsymbol{r}_\nu) W_{0,1}(\boldsymbol{r}_\lambda), \end{aligned} \tag{3.12}$$

.....

The $U_{k,l}$-functions for $k > 0$ are obtained as

$$\begin{aligned} &U_{k,k}(\boldsymbol{r}^k) = W_{k,k}(\boldsymbol{r}^k), \\ &U_{k,k+1}(\boldsymbol{r}^k, \boldsymbol{r}_\nu) = W_{k,k+1}(\boldsymbol{r}^k, \boldsymbol{r}_\nu) - W_{k,k}(\boldsymbol{r}^k)\, W_{0,1}(\boldsymbol{r}_\nu), \end{aligned} \tag{3.13}$$

.....

It is easily seen that the $U_{k,l}$-functions are (a) symmetric in the k basis coordinates, (b) symmetric in the $l - k$ non-basis coordinates. Further one can deduce rather easily from the defining equations (3.10), and from the product property and normalization of the W-functions that the U-functions satisfy the following property, which we call the *separation property*:

A $U_{k,l}$-function approaches zero for a configuration in which the coordinates are divided into two groups with a mutual distance of at least δ (the basis coordinates should occur in one group only).

This can be expressed by the formula (3.14). This formula expresses a special division, from which the general case follows directly from the symmetry of $U_{k,l}$:

$$U_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_l) = 0, \text{ if } r_{ij} > \delta \text{ for every } i = 1, 2, \ldots, p$$

and for every

$$j = p + 1, \ldots, l \quad (p \text{ may have any value } k \leqslant p < l). \tag{3.14}$$

We shall call a correlation function, which has this separation property, a *cluster function.*

It is easily seen from the equations (3.11) defining the relation of the $U_{k,l}$ to the $W_{k,l}$ that $W_{k,q}$ can be expanded according to

$$W_{k,q}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k}) = \sum_{l=k}^{q} \sum_{(\lambda_i)} U_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{\lambda_{k+1}}, \ldots, \boldsymbol{r}_{\lambda_l})\, W_{0,q-l}(\boldsymbol{r}_{\lambda_{l+1}}, \ldots, \boldsymbol{r}_{\lambda_q}). \tag{3.15}$$

The summation $\sum_{(\lambda_i)}$ represents a summation over the different possible ways in which the coordinates $\boldsymbol{r}^{q-k}$ can be divided into two sets of coordinates $(\boldsymbol{r}_{\lambda_{k+1}}, \ldots, \boldsymbol{r}_{\lambda_l})$ and $(\boldsymbol{r}_{\lambda_{l+1}}, \ldots, \boldsymbol{r}_{\lambda_q})$, which occur in the $U_{k,l}$-function and the $W_{0,q-l}$-function respectively.

In view of the developments of the next section we define the *incomplete correlation functions* $V_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{k+1} \ldots \boldsymbol{r}_l)$ in the following way. $V_{k,l}$ is defined by an expansion similar to the expansion (3.11) for $W_{k,l}$; however, we omit all terms of (3.11) which contain a factor U_{0,l_i} with $l_i = 1$ (in other words all terms with $U_{0,1}$ are omitted), or written in a similar way as (3.11)

$$V_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k}) = S'_{l(l_i)}\, U_{k,l_1}(\boldsymbol{r}^k, \boldsymbol{r}^{l_1-k}) \prod_{1<i\leqslant t}^{(l_i>1)} U_{0,l_i}(\boldsymbol{r}^{l_i}). \tag{3.16}$$

It follows immediately from the definitions (3.11) and (3.16) and the fact that $U_{0,1} = 1$, if we arrange (3.11) according to powers of $U_{0,1}$, that

$$W_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k}) = \sum_{q=k}^{l} \sum_{(\lambda_n)} V_{k,q}(\boldsymbol{r}^k, \boldsymbol{r}_{\lambda_{k+1}}, \ldots, \boldsymbol{r}_{\lambda_q}). \tag{3.17}$$

The summation $\sum_{(\lambda_n)}$ indicates that we should take as non-basis coordinates in $V_{k,q}$ every possible set of $(q - k)$ coordinates, which can be selected from the $(l - k)$ non-basis coordinates in $W_{k,l}$. This can be done in

$$N_{k,q}{}^{(l)} = \binom{l-k}{q-k} = \frac{(l-k)!}{(q-k)!\,(l-q)!} \tag{3.18}$$

possible ways.

The $V_{k,q}$ can be expanded in an entirely analogous way as the $W_{k,q}$ according to (3.15); we see that the following formula for the $V_{k,q}$ follows from (3.16), exactly as (3.15) follows from (3.11)

$$V_{k,q}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k}) = \sum_{l=k}^{q} \sum_{(\lambda_l)} U_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{\lambda_{k+1}}, \ldots, \boldsymbol{r}_{\lambda_l})\, V_{0,q-l}(\boldsymbol{r}_{\lambda_{l+1}}, \ldots, \boldsymbol{r}_{\lambda_q}). \tag{3.19}$$

Representation of correlation functions by means of graphs. It is often useful to visualize correlation functions by means of graphs, in particular if the F-factor has the form (2.8). We summarize the definitions concerning graphs, which will be used here: A *graph* is a figure built from numbered *points* and *lines* (connecting the points) as elements. A graph is *connected*, if any two points are connected directly or indirectly by one or more lines. An *articulation point* of a graph is a point, where a graph may be cut into two or more parts, which are not mutually connected. An *irreducible graph* is a connected graph without articulation points. A *complete star* is a graph, which contains all possible lines connecting the points.

$U_{k,l}$-functions may be represented by graphs. In the general case we represent a $U_{k,l}$-function simply by the complete star with the l coordinate points. We distinguish between *basis-lines*, connecting two points of the basis, and *U-lines*, being all other connections. The expansion (3.11) can be expressed as related to a certain set of graphs, the different terms in the right-hand member correspond to all possible partitions of the l points over a number of (mutually not connected) complete stars, the k basis-points always being situated in the same complete star. Each term of the right-hand member of (3.11) is a product of U-functions, each U-function corresponding to a complete star resulting from a certain partition, and not being connected to other points.

In case the F-factor is given by (2.8) we shall write

$$h(r_{ij}) = |f(r_{ij})|^2 - 1. \tag{3.20}$$

We can then write the correlation function $W_{k,l}$ as

$$W_{k,l} = \Pi_{i>j=1}^{l} |f_{ij}|^2 = \Pi_{i>j=1}^{k} |f_{ij}|^2 \, \Pi'_{n,m=1}(1 + h_{nm}). \tag{3.21}$$

Π' indicates that no term with both $n, m \leqslant k$ should be included; we write f_{ij} for $f(r_{ij})$ and h_{ij} for $h(r_{ij})$. In this case of two-particle correlations given by (3.21) more specific representations of functions then for the general case can be given: a function, which is a product of a number of h_{ij}-factors may now be represented by a graph if we make every h_{ij}-factor correspond to a line connecting the points numbered i and j. We may introduce the following "types" of lines: *f-lines* corresponding to $|f_{ij}|^2$-factors; *h-lines* corresponding to h_{ij}-factors. We then obtain graphs (which may contain 2 types of lines) which can represent any product of $|f_{ij}|^2$- and h_{ij}-factors. The f-lines will correspond to the basis lines of the general case. A $U_{k,l}$-function is now represented by the collection of all *connected* graphs formed with h-lines, the basis points being mutually connected by f-lines.

The expressions for the $U_{k,l}$-functions for the form (3.21) for $W_{k,l}$ are easily deduced from the equations (3.10), ..., (3.13); we give some simple examples

$$U_{0,2}(\boldsymbol{r}_1, \boldsymbol{r}_2) = h_{12}; \; U_{0,3}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = h_{12}h_{23} + h_{21}h_{13} + h_{13}h_{32} + h_{12}h_{23}h_{31}.$$
$$U_{2,2}(\boldsymbol{r}_1, \boldsymbol{r}_2) = |f(r_{12})|^2; \; U_{2,3}(\boldsymbol{r}_1, \boldsymbol{r}_2; \boldsymbol{r}_3) = |f(r_{12})|^2(h_{13} + h_{23} + h_{13}h_{32}). \tag{3.22}$$

The graphs corresponding to these functions are shown in Fig. 1.

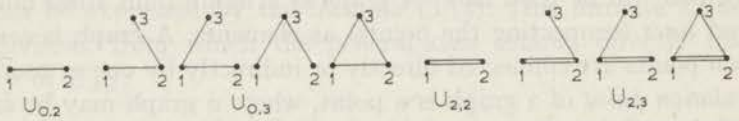

Fig. 1. Some examples of graphs representing U-functions, (cf. (3.22)); a single line represents a h-connection, a double line represents a basis-connection ($|f|^2$-factor).

It is sometimes useful to introduce the *irreducible correlation functions* $R_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_l)$ defined by the equations

$$U_{k,k}(\boldsymbol{r}^k) = R_{k,k}(\boldsymbol{r}^k),$$
$$U_{k,k+1}(\boldsymbol{r}^k, \boldsymbol{r}_\nu) = \textstyle\sum_{\lambda=1}^{k} R_{k,k}(\boldsymbol{r}^k) \, R_{0,2}(\boldsymbol{r}_\lambda, \boldsymbol{r}_\nu) + R_{k,k+1}(\boldsymbol{r}^k, \boldsymbol{r}_\nu), \ldots . \tag{3.23}$$

$R_{k,l}$-functions may be represented in the general case by complete stars, entirely analogous to $U_{k,l}$-functions. The general form of the expansion (3.23) for $U_{k,l}$ can then be expressed in the following way by means of graphs: consider all possible connected graphs of l points of the following type:

(1) the k basis-points should all be contained in the same complete star,

(2) the graphs may be reducible, but the irreducible parts should be complete stars.

Each term of a right-hand member of (3.23) is a product of R-functions, each R-function corresponding to an irreducible part of a graph.

It is seen that the R-functions have the same separation property (3.14) as the U-function and are also symmetric in the basis coordinates and symmetric in the non-basis coordinates.

As an example we write down some equations for $k = 0$

$$\begin{aligned} U_{0,2}(\boldsymbol{r}_1, \boldsymbol{r}_2) &= R_{0,2}(\boldsymbol{r}_1, \boldsymbol{r}_2); \\ U_{0,3}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) &= R_{0,2}(\boldsymbol{r}_1, \boldsymbol{r}_2)\, R_{0,2}(\boldsymbol{r}_2, \boldsymbol{r}_3) + R_{0,2}(\boldsymbol{r}_1, \boldsymbol{r}_3)\, R_{0,2}(\boldsymbol{r}_3, \boldsymbol{r}_2) + \\ &\quad + R_{0,2}(\boldsymbol{r}_2, \boldsymbol{r}_1)\, R_{0,2}(\boldsymbol{r}_1, \boldsymbol{r}_3) + R_{0,3}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3). \end{aligned} \tag{3.24}$$

In case $W_{k,l}$ is given by (3.21) one can derive the expressions for the $R_{k,l}$ functions in terms of f_{ij} and h_{ij} functions. We give some examples:

$$\begin{aligned} &R_{0,2}(\boldsymbol{r}_1, \boldsymbol{r}_2) = h_{12}; \; R_{0,3}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = h_{12}h_{23}\, h_{31}; \\ &R_{0,4}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \boldsymbol{r}_4) = h_{12}h_{23}h_{34}h_{41} + h_{13}h_{32}h_{24}h_{41} + \ldots; \\ &R_{2,2}(\boldsymbol{r}^2) = |f_{12}|^2; \; R_{2,3}(\boldsymbol{r}^2, \boldsymbol{r}_3) = |f_{12}|^2\, h_{13}h_{23}; \\ &R_{2,4}(\boldsymbol{r}^2, \boldsymbol{r}_3, \boldsymbol{r}_4) = |f_{12}|^2\, (h_{14}h_{43}h_{32} + \ldots.). \end{aligned} \tag{3.25}$$

Fig. 2 shows graphs representing some of these functions by means of the more specific representation by graphs, which is possible in the case that $W_{k,l}$ is given by (3.21). It can be shown in general for this case that the $R_{k,l}$-functions are sums of all possible terms represented by the different *irreducible* graphs formed with h-lines and f-lines between the basis points.

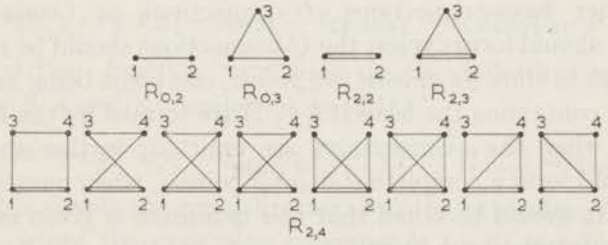

Fig. 2. Some examples of graphs representing irreducible correlation functions R (cf. (3.25)); a single line represents a h-connection, a double line represents a basis-connection ($|f|^2$-factor).

Mixed correlation functions will be used in the following section for the expansion of $V_{k,q}\, L_q^{(N)}$. These functions are introduced as functions containing dynamical correlations as well as statistical correlations. We shall give their definitions by means of graphs containing different kinds of connections. A statistical correlation function $L_q^{(N)}$ is given by a determinant, which can be written as a sum over permutations, while permutations

can be analyzed in terms of *cyclic* permutations; examples

$$\begin{array}{lll} \text{cycle } (1) & \text{corresponds to} & l_{11} = 1, \\ \text{cycle } (1, 2) & \text{corresponds to} & -l_{12}l_{21}, \\ \text{cycle } (1, 2, 3) & \text{corresponds to} & l_{12}l_{23}l_{31}, \\ \text{cycle } (1, 3, 2) & \text{corresponds to} & l_{13}l_{32}l_{21}, \\ \text{cycle } (1, 2, 4, 3) & \text{corresponds to} & -l_{12}l_{24}l_{43}l_{31}. \end{array} \tag{3.26}$$

The total number of cycles for a given group of s coordinates is $(s-1)!$; each function representing such a cycle has the sign $(-1)^{s-1}$, which indicates whether the cycle is an even or odd permutation. Hence, if we make every l_{ij}-factor with $i \neq j$ correspond to a line connecting the points i and j, we can obtain all terms for the statistical correlations by confining ourselves to l-connections which connect certain numbered coordinates in a cycle of definite order. Fig. 3 shows the graphs representing the terms of (3.26) for $s > 1$; the different orders of the cycles can be distinguished by arrows.

Fig. 3. Some examples of graphs representing cycles of l-connections, (cf. (3.26)); a dotted line represents a l-connection.

We now define the *mixed correlation function* $B_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})$ as the correlation function corresponding to all *connected* graphs formed with k basis-coordinates and $l-k$ non-basis coordinates; the connections in the graph may be either basis-connections, U-connections or l-connections; the l-connections should form cycles; the U-connections should be such that one or more complete stars (of *at least two points*, one point being admitted only in the cluster containing the basis if $k = 1$) are formed by the U- and basis-connections, when the l-connections are omitted; further the basis connections should form a complete star (of k points), when omitting the other connections. It should be noted that this definition is given in such a way that no $U_{0,1}$-factors occur in the expression for $B_{k,l}$.

In general the $B_{k,l}$-functions will have a number of terms, each of which can be specified by a graph. Sometimes it is useful to take a number of terms together and define $B_{k,l}{}^{(m)}$- and $B_{k,l}{}^{(m,p)}$-functions in the following way:

The function $B_{k,l}{}^{(m)}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})$ is defined in the same way as $B_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})$ except that only those graphs are considered, which fall apart in a number m of U-clusters, if the l-connections are omitted. We indicate a set of points as a U-cluster, if the points are connected by U-lines and (or) basis-lines.

The function $B_{k,l}{}^{(m,p)}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})$ is defined in the same way as

$B_{k,l}{}^{(m)}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})$ except for a further restriction for the graphs: only the graphs with a number p of l-connections should be considered here.

It is an immediate consequence of the definitions that one can write

$$B_{k,l} = \sum_{m=1}^{\frac{1}{2}(k-l)+1} B_{k,l}^{(m)} \quad \text{and} \quad B_{k,l} = \sum_{m,p} B_{k,l}{}^{(m,p)}. \tag{3.27}$$

It is seen from the definitions that the $B_{k,l}$-functions are symmetric in the basis coordinates and symmetric in the non-basis coordinates. In Fig. 4 some examples are given of graphs, which are used for the definition of

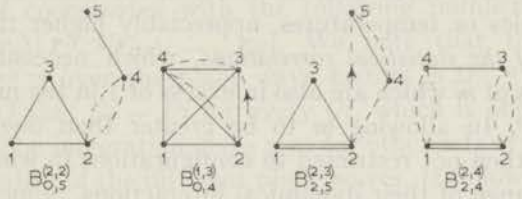

Fig. 4. Examples of graphs corresponding to terms of mixed correlation functions $B_{k,l}{}^{(m,p)}$. Each graph represents one of the many terms, belonging to the $B_{k,l}{}^{(m,p)}$, which is indicated. A single line represents a U-connection; a double line represents a basis-connection; a dotted line represents an l-connection.

$B_{k,l}{}^{(m,p)}$-functions. We also write down the explicit formulae for some $B_{k,l}$-functions

$$\begin{aligned}
B_{0,2}(\boldsymbol{r}^2) &= U_{0,2}(\boldsymbol{r}^2)\, L_2{}^{(N)}(\boldsymbol{r}^2), \\
B_{0,3}(\boldsymbol{r}^3) &= U_{0,3}(\boldsymbol{r}^3)\, L_3{}^{(N)}(\boldsymbol{r}^3), \\
B_{0,4}(\boldsymbol{r}^4) &= U_{0,4}(\boldsymbol{r}^4)\, L_4{}^{(N)}(\boldsymbol{r}^4) + \\
&+ U_{0,2}(\boldsymbol{r}_1, \boldsymbol{r}_2) U_{0,2}(\boldsymbol{r}_3, \boldsymbol{r}_4)\{- l_{13} l_{31} + l_{13} l_{34} l_{41} - l_{14} l_{43} l_{32} l_{21} + \ldots\} + \ldots
\end{aligned} \tag{3.28}$$

Mixed correlation functions are used in the following expansion of $V_{k,q}\, L_q{}^{(N)}$ which is entirely analogous to (3.16)

$$V_{k,q}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k})\, L_q{}^{(N)}(\boldsymbol{r}^q) = S'_{q(l_i)} B_{k,l_1}(\boldsymbol{r}^k, \boldsymbol{r}^{l_1-k}) \prod_{1<i\leq i'}^{(l_i>1)} B_{0,l_i}(\boldsymbol{r}^{l_i}). \tag{3.29}$$

This expansion is simply the generalization of (3.16), expanding $V_{k,q} L_q{}^{(N)}$ instead of $V_{k,q}$, where the expansion corresponds to all possible partitions into connected graphs; the difference of (3.29) and (3.16) being formed by the addition of the l-connections as possible elements for the graphs.

The mixed correlation functions further occur in the following expansion analogous to (3.19), which is easily proved by consideration of the graphs involved, and which will be used in the following section

$$\begin{aligned}
&V_{k,q}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k})\, L_q{}^{(N)}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k}) = \\
&\quad = \sum_{l=k}^{q} \sum_{(\lambda_l)} B_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}_{\lambda_{k+1}}, \ldots, \boldsymbol{r}_{\lambda_l})\, V_{0,q-l}(\boldsymbol{r}_{\lambda_{l+1}}, \ldots, \boldsymbol{r}_{\lambda_q}) \\
&\qquad L_{q-l}{}^{(N)}(\boldsymbol{r}_{\lambda_{l+1}}, \ldots, \boldsymbol{r}_{\lambda_q}).
\end{aligned} \tag{3.30}$$

§ 4. *The cluster expansion for the distribution functions.* We shall develop in this section a general method, which provides a cluster expansion for the distribution function $g_k(\boldsymbol{r}^k)$, if the wave function is given by (2.4). As mentioned before the methods which are used are analogous in many respects to the cluster expansion methods of statistical mechanics [6)7)]. However, the analogy is often primarily a formal one, while physical interpretations of formally corresponding quantities are different. We first mention some general points, before going into the details of the derivation:

(1) A new element, which does not occur in the usual developments (for classical mechanics or temperatures, appreciably higher than zero) is the *large influence of the statistical correlations*, which necessitates the introduction of values of m which are also in excess of 1 in the mixed correlation functions $B_{k,l}^{(m)}$. In allowing m to be greater than one, the statistical correlations are then not restricted to configurations in which the particles are within the range of their dynamical interactions. Something analogous will hold for an imperfect gas at such temperatures, T, where the De Broglie wave length $(\lambda = [h^2/2\pi mkT]^{\frac{1}{2}})$, which is a measure for the range of the "statistical" correlations, is not small compared to the range of the dynamical correlations, δ, caused by the short-ranged interactions.

(2) The integrations over the momentum variables must be carried out with care: the orthogonality of the plane waves with different $\boldsymbol{k}_i$ has to be taken into account and gives rise to a number of relations between the momenta, which occur. Only *after satisfying such momentum relations* the transition to the limit of continuously varying $\boldsymbol{k}$ (transition from sum to integral) can be made.

(3) It is *essential for the convergence* of the cluster expansions with the mixed correlation functions $B_{k,l}$ to require for the U-clusters, which are obtained by omitting the l-connections, that they *contain at least two points* (cf. the estimate (4.13) below; if separate points should be admitted as U-clusters, the factor $[n\delta^3]^{l-m}$ should not necessarily decrease for increasing l, as $m \approx l$ would be possible; however, for U-clusters with at least two points: $m \leqslant \frac{1}{2}l$ and $[n\delta^3]^{l-m}$ must decrease for increasing l),

We start the reduction of the expression for the distribution function $g_k(\boldsymbol{r}^k)$ by inserting (2.4) into (2.12) and writing out the determinants as sums over permutations according to (2.1)

$$g_k(\boldsymbol{r}^k) = a_k \int \Phi_0^*(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})\, W_{k,N}(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})\, \Phi_0(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})\, \mathrm{d}\boldsymbol{r}^{N-k} =$$
$$= a_k\, \Omega^{-N}\, (N!)^{-1} \int \sum_Q^{(N)} \delta_Q [\prod_{i=1}^N \exp(-i\boldsymbol{k}_i \cdot \boldsymbol{r}_{Qi})]\, W_{k,N}(\boldsymbol{r}^k, \boldsymbol{r}^{N-k})$$
$$\sum_P^{(N)} \delta_P [\prod_{i=1}^N \exp(i\boldsymbol{k}_i \cdot \boldsymbol{r}_{Pi})]\, \mathrm{d}\boldsymbol{r}^{N-k}. \qquad (4.1)$$

The superscripts (N) indicate that P and Q are to be understood as all permutations of N coordinates. A reduction of (4.1) is made by inserting the expansion (3.17) for $W_{k,N}$. Because of the symmetry of the $V_{k,q}$-functions

in the non-basis coordinates, all $N_{k,q}^{(l)}$ (cf. (3.18)) similar $V_{k,q}$ terms give the same result in the integral, and we may substitute for $W_{k,N}$ in (4.1)

$$W_{k,N}(\boldsymbol{r}^k, \boldsymbol{r}^{N-k}) \to \sum_{q=k}^{N} \frac{(N-k)!}{(q-k)!\,(N-q)!} V_{k,q}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k}). \tag{4.2}$$

After this substitution, we can carry out the integration over the variables $\boldsymbol{r}^{N-q}$, for which the integrand has only plane wave factors. We write: $\int \mathrm{d}\boldsymbol{r}^{N-k} \ldots = \int \mathrm{d}\boldsymbol{r}^{q-k} \int \mathrm{d}\boldsymbol{r}^{N-q} \ldots$; we designate by $\boldsymbol{r}^k$, $\boldsymbol{r}^{q-k}$, $\boldsymbol{r}^{N-q}$ the three groups of coordinates with the following numbers $\boldsymbol{r}^k(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_k)$; $\boldsymbol{r}^{q-k}(\boldsymbol{r}_{k+1}, \ldots, \boldsymbol{r}_q)$; $\boldsymbol{r}^{N-q}(\boldsymbol{r}_{q+1}, \ldots, \boldsymbol{r}_N)$. We note that the result of the integration $\int \mathrm{d}\boldsymbol{r}^{N-q}$ over the plane wave factors is Ω^{N-q} for such permutations P and Q that $Qi = Pi$ for every Qi, which is one of the numbers $q+1, \ldots, N$. The integration gives zero for other sets of P and Q because of the orthogonality of the different plane waves. It follows that the double sum $\sum_{Q,P}$ gives $(N-q)!$ times the result Ω^{N-q}, as far as one is concerned with permutations of the coordinates $\boldsymbol{r}^{N-q}$. The following result is deduced in this way from (4.1)

$$g_k(\boldsymbol{r}^k) = \frac{a_k}{\Omega^N N!} \sum_{q=k}^{N} \frac{(N-k)!}{(q-k)!\,(N-q)!} \Omega^{N-q}\,(N-q)!$$

$$\int \mathrm{d}\boldsymbol{r}^{q-k}\, V_{k,q}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k})\, X(\boldsymbol{r}^q), \tag{4.3}$$

with (the superscript (q) indicating that P and Q are now permutations of the q coordinates)

$$X(\boldsymbol{r}^q) = \sum_Q^{(q)} \sum_P^{(q)} \delta_Q\, \delta_P \sum_{(\lambda_1, \ldots, \lambda_q)} \prod_{i=1}^{q} \exp\left[i\boldsymbol{k}_{\lambda_i} \cdot (\boldsymbol{r}_{Pi} - \boldsymbol{r}_{Qi})\right]. \tag{4.4}$$

The summation over $(\lambda_1, \ldots, \lambda_q)$ should be extended over all possible sets of momenta $\boldsymbol{k}_{\lambda_1}, \ldots, \boldsymbol{k}_{\lambda_q}$. It can further be seen that the following reduction can be made in (4.4) concerning the $\sum$-signs

$$\sum_{(\lambda_1, \ldots, \lambda_q)} \prod_{i=1}^{q} = (q!)^{-1} \sum_{\lambda_1=1}^{N} \sum_{\lambda_2=1}^{N} \cdots \sum_{\lambda_q=1}^{N} \prod_{i=1}^{q} = (q!)^{-1} \prod_{i=1}^{q} \sum_{\lambda_i=1}^{N}. \tag{4.5}$$

The first equality contained in (4.5) is seen to be valid by noting that (4.4) can be considered a product of two determinants, over which the sum $\sum_{(\lambda_1, \ldots, \lambda_q)}$ is taken. It then follows from the property of determinants to be zero, if any two rows are equal, that terms of the sum $\sum_{\lambda_1=1}^{N} \cdots \sum_{\lambda_q=1}^{N}$ with some $\lambda_i = \lambda_j$ are zero, so that the latter sum is $q!$ times (number of permutations of $\lambda_1, \ldots, \lambda_q$) the sum $\sum_{(\lambda_1, \ldots, \lambda_q)}$. It follows from (4.4) and (4.5) that (cf. also (3.3))

$$\begin{aligned} X(\boldsymbol{r}^q) = (q!)^{-1} \sum_Q^{(q)} \sum_P^{(q)} \delta_Q \delta_P \prod_{i=1}^{q} \sum_{\lambda_i=1}^{N} \exp\left[i\boldsymbol{k}_{\lambda_i} \cdot (\boldsymbol{r}_{Pi} - \boldsymbol{r}_{Qi})\right] = \\ = N^q (q!)^{-1} \sum_Q^{(q)} \sum_P^{(q)} \delta_Q \delta_P \prod_{i=1}^{q} l(\boldsymbol{r}_{Pi} - \boldsymbol{r}_{Qi}) = \\ = N^q \sum_P^{(q)} \delta_P \prod_{i=1}^{q} l(\boldsymbol{r}_{Pi} - \boldsymbol{r}_i) = N^q L_q^{(N)}(\boldsymbol{r}^q). \end{aligned} \tag{4.6}$$

Combining (4.3) and (4.6), we obtain:

$$g_k(\boldsymbol{r}^k) = \frac{a_k}{N!} \sum_{q=k}^{N} \frac{(N-k)!}{(q-k)!} N^q \Omega^{-q} \int V_{k,q}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k}) L_q^{(N)}(\boldsymbol{r}^k, \boldsymbol{r}^{q-k}) \, \mathrm{d}\boldsymbol{r}^{q-k}. \quad (4.7)$$

A further reduction of (4.7) can be made by inserting (3.30) for the integrand in (4.7). The summation $\sum_{(\lambda_i)}$ in (3.30) simply provides a factor $\binom{q-k}{l-k}$ after carrying out the integration, because the result of the integration is independent of the names of the integration variables. Hence the integral in (4.7) may be written as

$$\int V_{k,q} L_q^{(N)} \, \mathrm{d}\boldsymbol{r}^{q-k} = \sum_{l=k}^{q} \binom{q-k}{l-k} \int \mathrm{d}\boldsymbol{r}^{l-k} B_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k}) \int \mathrm{d}\boldsymbol{r}^{q-l} V_{0,q-l}(\boldsymbol{r}^{q-l}) L_{q-l}^{(N)}(\boldsymbol{r}^{q-l}). \quad (4.8)$$

We have now to study some *properties of integrals with correlation functions*. We first consider an integral of the type

$$\int \exp\left[-i \sum_{i=1}^{l} \boldsymbol{k}_{\lambda_i} \cdot \boldsymbol{r}_i\right] U_{0,l}(\boldsymbol{r}^l) \exp\left[i \sum_{i=1}^{l} \boldsymbol{k}_{\mu_i} \cdot \boldsymbol{r}_i\right] \mathrm{d}\boldsymbol{r}^l. \quad (4.9)$$

It is easily shown that this integral vanishes, unless

$$\sum_{i=1}^{l} \boldsymbol{k}_{\lambda_i} = \sum_{i=1}^{l} \boldsymbol{k}_{\mu_i}. \quad (4.10)$$

The expression (4.9) has the form of a matrix element of the operator $U_{0,l}(\boldsymbol{r}^l)$; when considering it as such, (4.10) can be expressed as the conservation of the total momentum. The proof of (4.10) is given by introducing relative coordinates and one reference coordinate (with respect to which the $l-1$ relative coordinates are taken) and integrating over the reference coordinate, of which $U_{0,l}$ is then independent. It is easily seen that the value of the integral (4.9) is of the order

$$\Omega \, \delta^{3(l-1)}, \quad (4.11)$$

if (4.10) is satisfied, as is seen by noting that $U_{0,l}$ differs from zero in a volume of the order δ^3 for each of the $(l-1)$ relative coordinates.

An analogous estimate of the order of magnitude can be made for the integral

$$\int B_{0,l}^{(m,p)}(\boldsymbol{r}^l) \, \mathrm{d}\boldsymbol{r}^l. \quad (4.12)$$

The integrand contains p statistical correlation factors $l_{ij} (i \neq j)$ defined by (3.4). If we should consider the U-factors of the integrand only, we should obtain the order of magnitude $\Omega^m \delta^{3(l-m)}$ for the integral, as we should then have m unconnected U-clusters, each U-cluster providing a factor $\Omega \delta^{3(l_j-1)}$ after integration (with $\sum_{j=1}^{m} l_j = l$). As to the p $\boldsymbol{k}_\lambda$-values occurring in the l_{ij}-factors, we can obtain momentum relations analogous to (4.10) by first carrying out m integrations taking one reference coordinate for each of the

m U-clusters. This provides m momentum relations which must be satisfied in order that the integral should differ from zero. The definition of the l_{ij}'s and the fact that they form cycles, ensures the conservation of the "total momentum" of such a cycle. This reduces the number of momentum relations to $m - 1$, since the "total momentum" of $B_{k,l}{}^{(m,p)}$ is now automatically conserved. It follows moreover that the remaining $m - 1$ momentum relations involve only those summation variables $\boldsymbol{k}_\lambda$ occurring in l_{ij}-factors connecting points i and j of different U-clusters. The normalization of l_{ij} according to (3.4) is such that the result of a summation over an independent $\boldsymbol{k}_\lambda$-variable gives a result of order unity, while each momentum relation restricts a sum to one term and provides a factor N^{-1}. It follows that the order of magnitude for a term of the integral (4.12) is given by

$$\Omega^m \delta^{3(l-m)} N^{-m+1} = \Omega^l N^{-l+1} [n\delta^3]^{l-m}. \tag{4.13}$$

The estimates (4.11) and (4.13) are order of magnitude estimates for one term of the integral. It should be remembered that a further combinatiorial factor will enter for the number of different graphs contributing to a certain $B_{k,l}$. After the momentum relations (such as (4.10)) have been taken into account, one can see that the remaining l-factors can be replaced by the result (3.5) found by passing to the limit $N \to \infty$ and carrying out an integration.

In order to pass to the limit $N \to \infty$ in the expression (4.7) we define $b_{0,l}{}^{(m)}$ as the integral (4.12) provided with such a factor that it remains finite for $N \to \infty$ (cf. (4.13)):

$$b_{0,l}{}^{(m)} = \lim_{N\to\infty}^{(n=\text{const})} \Omega^{-l} N^{l-1} (l!)^{-1} \int B_{0,l}{}^{(m)}(\boldsymbol{r}^l)\, \mathrm{d}\boldsymbol{r}^l . (m \geqslant 1, l \geqslant 2) \tag{4.14}$$

Considerations of entirely the same type may be given for integrals with $B_{k,l}{}^{(m)}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})$; we then define

$$b_{k,l}{}^{(m)} = \lim_{N\to\infty}^{(n=\text{const})} \Omega^{-l+k} N^{l-k} [(l-k)!]^{-1} \int B_{k,l}{}^{(m)}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})\, \mathrm{d}\boldsymbol{r}^{l-k}.$$
$$(m > 1; l > k \geqslant 1) \tag{4.15}$$

We write down some examples of (4.14)

$$\begin{aligned}
&b_{0,2}{}^{(1)} = \tfrac{1}{2} n\, \Omega^{-1} \int U_{0,2}(\boldsymbol{r}^2)\, L_2(\boldsymbol{r}^2)\, \mathrm{d}\boldsymbol{r}^2 = \tfrac{1}{2} n \int U_{0,2}(r_{12})[1 - l^2(r_{12})]\, \mathrm{d}\boldsymbol{r}_{12},\\
&b_{0,3}{}^{(1)} = \tfrac{1}{6} n^2 \int U_{0,3}(\boldsymbol{r}_{12}, \boldsymbol{r}_{13})\, L_3(\boldsymbol{r}_{12}, \boldsymbol{r}_{13})\, \mathrm{d}\boldsymbol{r}_{12}\, \mathrm{d}\boldsymbol{r}_{13},\\
&b_{0,4}{}^{(2)} = -\tfrac{1}{2} n^2 \int U_{0,2}(r_{12})\, U_{0,2}(r_{13})\, \mathrm{d}\boldsymbol{r}_{12}\, \mathrm{d}\boldsymbol{r}_{13} +\\
&+ n^2 \int U_{0,2}(r_{12})\, U_{0,2}(r_{13}) l^2(r_{12})\, \mathrm{d}\boldsymbol{r}_{12}\, \mathrm{d}\boldsymbol{r}_{13} -\\
&- \tfrac{1}{2} n^2 \int U_{0,2}(r_{12})\, U_{0,2}(r_{13})\, l(r_{12})\, l(r_{23})\, l(r_{31})\, \mathrm{d}\boldsymbol{r}_{12}\, \mathrm{d}\boldsymbol{r}_{13} + \ldots\ldots
\end{aligned} \tag{4.16}$$

We can now reduce the expression (4.7) for $g_k(\boldsymbol{r}^k)$, making use of (4.8) and (4.15); we obtain

$$g_k(\boldsymbol{r}^k) = (a_k (N-k)!\, N^k / \Omega^k N!) \sum_{l=k}^{N} b_{k,l}(\boldsymbol{r}^k)\, Q_l{}^{(N)}, \tag{4.17}$$

with
$$Q_l{}^{(N)} = \sum_{M=0}^{N-l} (N^M / \Omega^M M!) \int \mathrm{d}\boldsymbol{r}^M\, V_{0,M}(\boldsymbol{r}^M)\, L_M{}^{(N)}(\boldsymbol{r}^M). \tag{4.18}$$

In order to obtain (4.17), we have reduced the summations, according to $\sum_{q=k}^{N}\sum_{l=k}^{q} = \sum_{l=k}^{N}\sum_{q=l}^{N} = \sum_{l=k}^{N}\sum_{M=0}^{N-l}$, putting $M = q - l$. It is seen from (3.27) and (4.15) that $b_{k,l}(\boldsymbol{r}^k)$ may be expanded as

$$b_{k,l}(\boldsymbol{r}^k) = \sum_{m=1}^{\frac{1}{2}(l-k+2)} b_{k,l}^{(m)}(\boldsymbol{r}^k). \tag{4.19}$$

The expression for $Q_l^{(N)}$ can be reduced by substituting the expansion (3.29) (for $k = 0$) into the integral $\int d\boldsymbol{r}^M V_{0,M}(\boldsymbol{r}^M)\, L_M^{(N)}(\boldsymbol{r}^M)$, which provides the following result, using (4.14) and characterizing a partition into clusters by numbers m_s, specifying the number of clusters of s coordinates

$$Q_l^{(N)} = \sum_{M=0}^{N-l} \frac{N^M}{\Omega^M M!}\, S'_{M(m_s)} \prod_{s=2}^{M} \frac{M!}{m_s!(s!)^{m_s}} [b_{0,s}\, \Omega^s N^{-s+1}\, s!]^{m_s}, \tag{4.20}$$

where $S'_{M(m_s)}$ indicates the sum over all partitions such that

$$\sum_{s=2}^{M} s m_s = M \ . \ (m_s = 0,1, \ldots) \tag{4.21}$$

In view of (4.21), we see that (4.20) can be written as

$$Q_l^{(N)} = \sum_{M=0}^{N-l} F_M^{(N)}, \tag{4.22}$$

with

$$F_M^{(N)} = S'_{M(m_s)} \prod_{s=2}^{M} (N b_{0,s})^{m_s} (m_s!)^{-1}. \tag{4.23}$$

In order to arrive at the cluster development for $g_k(\boldsymbol{r}^k)$, there is a problem of convergence of these expansions. It seems plausible for physical reasons that expansions should exist, which approach the limit of no dynamical correlation at all, if $\delta^3 n \to 0$. In a similar way as (4.13) is obtained, one sees that $b_{k,l}^{(m)}$ should contain a factor $[n\delta^3]^{l-m-k+1}$ $(m \leqslant \frac{1}{2}(l-k)+1)$, so that it seems reasonable to consider series of the type $\sum_{l,m} b_{k,l}^{(m)}$, ordered to increasing l or $l - m$ if $n\delta^3 \ll 1$. However, it is a notorious problem of cluster developments in statistical mechanics to obtain rigorous mathematical proofs for the convergence of such expansions and at the moment the problem is still unsolved, although it has received much attention [8]). Hence we shall content ourselves here simply by assuming that the following series converges

$$b = b_0(\alpha, n) = \sum_{s=2}^{\infty} b_{0,s}. \tag{4.24}$$

In order to be able to derive explicit expressions for $g_k(\boldsymbol{r}^k)$, we have to know how $Q_l^{(N)}$ and $Q_0^{(N)}$ are related. On the basis of the expression (4.22) we have been led to assume

$$\lim_{N\to\infty} (Q_l^{(N)}/Q_0^{(N)}) = 1. \ (l : \text{some fixed number}) \tag{4.25}$$

This is seen by noting that $Q_l^{(N)}$ differs from $Q_0^{(N)}$ according to (4.22) only by the omission of l terms in a number of N terms. This difference will become relatively negligible for $N \to \infty$ under certain conditions. A more

detailed discussion of these points is given in the appendix, where the validity of (4.25) is shown, provided the (sufficient) condition

$$\sum_s' s b_{0,s} + \sum_s'' 4s\,|b_{0,s}| < 1 \tag{4.26}$$

is satisfied. The first summation in (4.26) is extended over values of $s(\geqslant 2)$ for which $b_{0,s}$ is positive, the second summation over all values $s(\geqslant 2)$ for which $b_{0,s}$ is negative. *Hence one should limit the choice of the functions* $f(r, \alpha)$, when using Jastrow wave functions in a variational principle, to such functions for which (4.26) is statisfied.

Specializing (2.12), (2.13) and (4.7) for $k = 0$, one sees that

$$\begin{aligned} g_0 \equiv 1 &= a_0 \int \Phi^* \Phi \, \mathrm{d}\boldsymbol{r}^N = \\ &= a_0 \, (N!)^{-1} \sum_{q=0}^{N} N!(q!)^{-1} N^q \, \Omega^{-q} \int V_{k,q}\,(\boldsymbol{r}^q)\, L_q^{(N)}\,(\boldsymbol{r}^q)\, \mathrm{d}\boldsymbol{r}^q. \end{aligned} \tag{4.27}$$

Comparing this with (4.18) for $l = 0$, one sees that

$$Q_0^{(N)} = \int |\Phi(\boldsymbol{r}^N)|^2 \, \mathrm{d}\boldsymbol{r}^N. \tag{4.28}$$

The value of the normalization constant a_k is then obtained by writing according to (2.12) and (2.13)

$$N![(N-k)!]^{-1} = \int g_k(\boldsymbol{r}^k)\, \mathrm{d}\boldsymbol{r}^k = a_k \int |\Phi|^2 \, \mathrm{d}\boldsymbol{r}^N = a_k Q_0^{(N)}. \tag{4.29}$$

The normalized expression for $g_k(\boldsymbol{r}^k)$ is now obtained from (4.17) and (4.29)

$$g_k(\boldsymbol{r}^k) = (N/\Omega)^k \sum_{l=k}^{N} b_{k,l}(\boldsymbol{r}^k)(Q_l^{(N)}/Q_0^{(N)}). \tag{4.30}$$

The transition to the limit $N \to \infty$ according to (4.25) provides us with a form for the cluster development such as we wanted to obtain

$$g_k(\boldsymbol{r}^k) = n^k \sum_{l=k}^{\infty} b_{k,l}(\boldsymbol{r}^k). \tag{4.31}$$

The different $b_{k,l}$ contain increasing powers of $n\delta^3$. However, they also contain a dependence on n in a different way, as the $l(r)$-functions occurring in the integral expression for $b_{k,l}$ depend on the Fermi limit $k_F = (6\pi^2)^{\frac{1}{3}} n^{\frac{1}{3}}$.

The knowledge of the k-particle distribution function of a system has an interest in itself. However, the primary interest of obtaining these cluster expansions is that they also provide us with a way to calculate the potential and kinetic energy of the system. We shall give the expressions for the energy in a subsequent paper.

Equation (4.28) provides us with the meaning of $Q_0^{(N)}$ as the normalization constant of the Jastrow wave function $\Phi(\boldsymbol{r}^N)$, which was not normalized before: a factor $[Q_0^{(N)}]^{-\frac{1}{2}}$ should be added to $\Phi(\boldsymbol{r}^N)$ in order to normalize it. The considerations, which led us to (4.25) (see appendix) lead also to an expression for the principal behaviour of $Q_0^{(N)}$ for $N \to \infty$, namely

$$Q_0^{(N)} = e^{Nb}\,(1 + \varepsilon), \text{ where } \varepsilon \to 0 \text{ for } N \to \infty. \tag{4.32}$$

This provides us with the meaning of the constant b, given by (4.24), which can be considered as the result (4.31) for the value $k = 0$. It should be noted that the normalization constant for $\Phi(\boldsymbol{r}^N)$ is not a quantity dependent on the density only, but a factor depending roughly exponentially on the total number of particles.

The preceding developments can be extended in an entirely analogous way to distribution functions $g_k(\boldsymbol{r}^k, \boldsymbol{r}'^k)$ (cf. (2.14)), which are not diagonal in the basis coordinates. One has to replace $\boldsymbol{r}^k$ by $\boldsymbol{r}'^k$ in those parts originating from the complex conjugate wave function. A "doubled" basis has then to be considered as one unit in the definition of the spatial cluster functions $U_{k,l}$ and $R_{k,l}$. The cycles of l-connections retain the same formal expression, if the l_{ij} are now defined by

$$l_{ij} = l(\boldsymbol{r}_i - \boldsymbol{r}_j^*) \text{ with } \boldsymbol{r}_j^* = \boldsymbol{r}_j', \text{ if } j \leq k \qquad (4.33)$$

$$\boldsymbol{r}_j^* = \boldsymbol{r}_j, \text{ if } j > k.$$

In a subsequent chapter, we shall further give a reduction of the expressions for $b_{k,l}(\boldsymbol{r}^k)$ making use of the irreducible cluster functions. We note that equation (4.31) reads

$$1 = \Sigma_{l=1}^{\infty} b_{1,l} = 1 + \Sigma_{l=2}^{\infty} b_{1,l} \qquad (4.34)$$

for the special case $k = 1$. The introduction of the irreducible cluster functions will provide a direct and independent proof of this equation.

Appendix

The magnitude of the expressions $Q_l^{(N)}$. The derivation in § 4 required the limiting value of $Q_l^{(N)}/Q_0^{(N)}$ for large N. It follows from (4.22) and (4.23) that

$$Q_l^{(N)} = S^*_{N-l(m_s)} \prod_s (Nb_{0,s})^{m_s}(m_s!)^{-1}, \qquad (A.1)$$

where $S^*_{N-l(m_s)}$ indicates the sum over all sets of m_s, such that

$$\Sigma_{s\geq 2}\, sm_s \leqslant N - l. \qquad (A.2)$$

We introduce a quantity $\bar{Q}^{(N)}$, which is defined by the right member of (A. 1) in case the summations over m_s are not restricted. Hence

$$\bar{Q}^{(N)} = \prod_s e^{Nb_{o,s}} = e^{Nb}, \qquad (A.3)$$

where b is given by (4.24). In the following we shall only consider s values for which $b_{o,s} \neq 0$. If the cluster development is not too slowly convergent, only a very limited number of terms $b_{o,s}$ will differ essentially from zero;

we shall think of this case. Suppose we have a set of positive numbers, α_s, such that for large values of N the following inequality is satisfied:

$$\Sigma_s (\alpha_s N)s < N - l. \tag{A.4}$$

It follows then from the definition of $\bar{Q}^{(N)}$, (A.1) and (A.2), that

$$|\bar{Q}^{(N)} - Q_l{}^{(N)}| < |S''_{(m_s)} \prod_s (N b_{0,s})^{m_s} (m_s!)^{-1}|, \tag{A.5}$$

if we denote by $S''_{(m_s)}$ the summation over all sets of m_s values such that m_s is larger than $\alpha_s N$ for at least one value of s. The right member of (A.5) can be written as

$$\bar{Q}^{(N)} |1 - \prod_s (1 - e^{-N b_{0,s}} f_{\alpha_s}{}^{(N)})| \tag{A.6}$$

where we have abbreviated

$$f_{\alpha_s}{}^{(N)} = \Sigma_{m_s \geq \alpha_s N + 1}^{\infty} (N b_{0,s})^{m_s} (m_s!)^{-1}. \tag{A.7}$$

Suppose that it is possible to find a set of α_s values, such that $\alpha_s > |b_{0,s}|$. In this case, one easily sees that

$$\begin{aligned} |f_{\alpha_s}{}^{(N)}| &< (N|b_{0,s}|)^{\alpha_s N} [(\alpha_s N)!]^{-1} \Sigma_{k=1}^{\infty} (|b_{0,s}|/\alpha_s)^k = \\ &= (N |b_{0,s}|)^{\alpha_s N} [(\alpha_s N)!]^{-1} (|b_{0,s}|/\alpha_s)(1 - |b_{0,s}|/\alpha_s)^{-1}. \end{aligned} \tag{A.8}$$

Using the Stirling formula for $(\alpha_s N)!$, it follows from (A.8) that

$$\lim_{N \to \infty}^{\alpha_s = const.} |e^{-N b_{0,s}} f_{\alpha_s}{}^{(N)}| = 0, \tag{A.9}$$

if the following inequalities hold

$$\alpha_s > |b_{0,s}| \quad \text{and} \quad 1 - (b_{0,s}/\alpha_s) + \ln (|b_{0,s}|/\alpha_s) < 0. \tag{A.10}$$

The conditions (A.10) can be written in the following simpler form

$$\alpha_s > b_{0,s} \quad \text{if} \quad b_{0,s} > 0 \quad \text{and} \quad \alpha_s \geqslant 4 |b_{0,s}| \quad \text{if} \quad b_{0,s} < 0. \tag{A.11}$$

((A.11) implies (A.10); the coefficient 4 may be replaced by $c = 3.5\ ..$, being the root of $\ln c = c^{-1} + 1$).

Combining the preceding results, one finds, from (A.5) and (A.6), using (A.4) and (A.11), that

$$\lim_{N \to \infty} |\bar{Q}^{(N)} - Q_l{}^{(N)}|(\bar{Q}^{(N)})^{-1} = 0 \ (l\text{: some fixed number}), \tag{A.12}$$

provided the condition ($s \geqslant 2$)

$$\Sigma_s' \, s b_{0,s} + \Sigma_s'' \, 4s \, |b_{0,s}| < 1 \tag{A.13}$$

is satisfied. The first summation in (A.13) is extended over all values of s for which $b_{0,s} > 0$; the second summation over s values for which $b_{0,s} < 0$.

The inequality (A.13) serves as a (sufficient) condition for the validity of (4.25), which follows immediately from (A.12). One finds moreover ($l = 0$)

$$Q_0^{(N)} = e^{Nb}(1 + \varepsilon) \quad \text{with} \quad \varepsilon \to 0 \quad \text{for} \quad N \to \infty. \tag{A.14}$$

Finally, we just want to mention, that another less restrictive condition can be derived, in case it would be known that $F_M^{(N)}$ is positive for large M and N; one can then derive (using certain results of app. XI of [7]))

$$\sum_{s \geq 2} s b_{0,s} < 1. \tag{A.15}$$

However, it should be realized that $F_M^{(N)}$ is not always positive if $b_{0,2} < 0$ and if the behavior of $F_M^{(N)}$ would be mainly determined by $b_{0,2}$, which case may very well occur in real applications.

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CHAPTER II

INTRODUCTION OF IRREDUCIBLE CLUSTER FUNCTIONS

Synopsis

In the previous chapter a cluster development of the k-particle distribution function, $g_k(\boldsymbol{r}^k)$, for a system of interacting fermions in the ground state represented by a Jastrow wave function was considered. It was written as

$$g_k(\boldsymbol{r}^k) = n^k \sum_{l=k}^{\infty} b_{k,l}(\boldsymbol{r}^k)$$

(n particle density), where the $b_{k,l}(\boldsymbol{r}^k)$ denote the cluster integrals. In this chapter a reduction is carried out by means of the introduction of irreducible cluster functions and the use of certain combinatorial methods. The reduction results in a development of $g_k(\boldsymbol{r}^k)$, in which the $b_{k,l}(\boldsymbol{r}^k)$ are replaced by simpler terms, which are sums of cluster integrals involving irreducible cluster functions only. The presentation includes a generalization to mixtures of fermions of different types.

§ 1. *Introduction.* The cluster expansion method which was developed in the previous chapter [1]) (further cited as I) is carried further in this chapter by means of the introduction of irreducible cluster functions (notations will be the same as in paper I, unless otherwise stated). In this way the result I (4.31) for the k-particle distribution function, $g_k(\boldsymbol{r}^k)$, for a system of interacting fermions, represented by a Jastrow wave function can be reduced considerably: it will be shown that the cluster integrals $b_{k,l}(\boldsymbol{r}^k)$ can be replaced by terms $\beta_{k,l}$ which are sums of cluster integrals containing only certain irreducible cluster functions. We want to mention here two things about the introduction of irreducible cluster functions:

(*a*) This introduction is *similar* to a certain extent to *the introduction of the irreducible cluster functions in statistical mechanics* by Mayer [2]). If our wave function I (2.4) would contain only the F-factor but not the Slater determinant Φ_0 (this could be applied to interacting bosons), this would result in the introduction of the irreducible cluster functions $R_{k,l}$ instead of the cluster functions $U_{k,l}$ (see I § 3). The $R_{k,l}$-functions are represented by graphs without articulation points.

(*b*) However, the presence of the Slater determinant Φ_0 in the case of interacting fermions resulted in the introduction of the $B_{k,l}$-functions, which

then replace the $U_{k,l}$-functions to a certain extent (see I § 3). We now have to introduce new "mixed" irreducible correlation functions $S_\nu^{(k)}$, containing also statistical correlations. The presence of the Φ_0-factor requires a *renewed consideration of relations between momenta contained in the plane wave part* Φ_0.

We shall present the reduction in this chapter immediately for a somewhat more general system than in I (no essential complications are caused by this generalization). We assume a mixture of fermions of *different types, indicated by the index t* (we may think, for instance, of protons and neutrons indicated by $t = 1$ and $t = 2$, respectively). However, the particles are still "fermions without spin". The extension to real fermions shall be given in the subsequent chapter. We first mention the generalization of the result I (4.31)

$$g_k(\boldsymbol{r}^k) = n^k \sum_{l=k}^{\infty} b_{k,l}(\boldsymbol{r}^k) \tag{1.1}$$

for one type of fermions, without repeating any derivation as the generalization is straightforward. We indicate by N_t the total number of particles of type t and by n_t the partial density of this type: $n_t = N_t/\Omega$. We further put: $N = \sum_t N_t$ and $n = \sum_t n_t$. Note that each type of fermions will in general have its own fermi limit $k_{F,t}$. We indicate by k and l the sets of k_t and l_t values, e.g. $k = (k_1, k_2)$ and $l = (l_1, l_2)$ if there are two types of fermions (we shall often give the examples for *two* types of particles below, although this number of types is by no means essential for the method). The trial wave function taken as a starting point (instead of I (2.4)) will now be (for two types of particles)

$$\Phi(\boldsymbol{r}^N) = F(\boldsymbol{r}^N)\, \Phi_0^{(1)}(\boldsymbol{r}^{N_1})\, \Phi_0^{(2)}(\boldsymbol{r}^{N_2}), \qquad (N_1 + N_2 = N) \tag{1.2}$$

where $\Phi_0^{(1)}$ and $\Phi_0^{(2)}$ are the Slater determinants for particles of type 1 and 2 respectively. The F-factor should now be symmetrical in the 1-particles and in the 2-particles. The special form of the F-factor corresponding to I (2.8) may now be written as

$$F(\boldsymbol{r}^N) = F_{11}(\boldsymbol{r}^{N_1})\, F_{22}(\boldsymbol{r}^{N_2})\, F_{12}(\boldsymbol{r}^N), \tag{1.3}$$

with:

$$\begin{aligned} F_{11}(\boldsymbol{r}^{N_1}) &= \prod_{i>j=1}^{N} f^{(11)}(r_{ij}), \\ F_{22}(\boldsymbol{r}^{N_2}) &= \prod_{i>j=N_1+1}^{N} f^{(22)}(r_{ij}), \\ F_{12}(\boldsymbol{r}^N) &= \prod_{i=1}^{N_1} \prod_{j=N_1+1}^{N} f^{(12)}(r_{ij}), \end{aligned} \tag{1.4}$$

containing 3 functions $f^{(11)}(r)$, $f^{(22)}(r)$, $f^{(12)}(r)$, which may be different. The total wave function Φ is, as is required, antisymmetrical in the 1-particles and in the 2-particles, but not in all particles together. The generalization of the result (1.1) for a system specified by the wave function (1.2) can now be given by the equation

$$g_k(\boldsymbol{r}^k) = (\prod_t n_t^{k_t}) \sum_{l \geq k}^{\infty} b_{k,l}(\boldsymbol{r}^k) \tag{1.5}$$

with (cf. I (4.14) and (4.15))

$$b_{0,l} = \lim_{N\to\infty}^{(n_t=const.)} N^{-1} \left[\prod_t (N_t/\Omega)^{l_t}(l_t!)^{-1}\right] \int B_{0,l}(\boldsymbol{r}^l)\, \mathrm{d}\boldsymbol{r}^l \tag{1.6}$$

and for $k \neq 0$ $(l \geqslant k)$

$$b_{k,l} = \lim_{N\to\infty}^{(n_t=const.)} \{\prod_t (N_t/\Omega)^{l_t-k_t}[(l_t - k_t)!]^{-1}\} \int B_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k}) \mathrm{d}\boldsymbol{r}^{l-k}. \tag{1.7}$$

The normalization of the distribution function g_k is now fixed according to (cf. I (2.13))

$$\int g_k(\boldsymbol{r}^k)\, \mathrm{d}\boldsymbol{r}^k = \prod_t N_t!/(N_t - k_t)!. \tag{1.8}$$

It should be noted that the $B_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})$-functions are generalizations of the $B_{k,l}$-functions used before as k, l, $\boldsymbol{r}^k$ and $\boldsymbol{r}^{l-k}$ represent in fact (k_1, k_2), (l_1, l_2), $\boldsymbol{r}^{k_1}\boldsymbol{r}^{k_2}$ and $\boldsymbol{r}^{l_1-k_1}\,\boldsymbol{r}^{l_2-k_2}$, respectively.

The functions $R_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k})$, defined by I (3.10) and I (3.23), can be generalized in the same way. The generalized $R_{k,l}$-functions can again be represented by *complete stars*, which have as elements:

(*a*) 2 types of points for type $t = 1$ and $t = 2$,

(*b*) basis-connections of 3 types: (11), (22) and (12),

(*c*) R-connections (being all other connections) of 3 types: (11), (22) and (12). R or basis-connections are said to be of type (t_1t_2), when connecting two points of type t_1 and t_2.

In the general case we shall express the dynamical part of the $B_{k,l}$-functions in terms of R-functions. If we represent the $l^{(t)}(\boldsymbol{r}_i, \boldsymbol{r}_j)$-factors (if $i \neq j$) by $l^{(t)}$ connections (only between particles of the same type t), the function $B_{k,l}$ corresponds to all *connected* graphs, formed with the set of k basis points and the set of $l - k$ non-basis points. The connections in the graph may be either basis-connections, R-connections or l-connections; the l-connections should form cycles. The basis- and R-connections should be such, that the irreducible parts of each of the connected graphs, which are obtained when omitting the l-connections, are complete stars R (one of them containing all the basis coordinates; $R_{0,1}$ should not occur, as a non-basis point with only l-connections is not admitted).

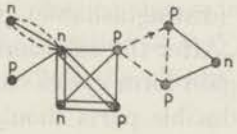

Fig. 1. Example of a graph representing a term of a generalized $B_{k,l}$-function in case two types of fermions exist. A single line represents an R-connection; a double line a basis-connection; a dotted line an l-connection; n: neutron; p: proton.

In case the F-factor is given by (1.3), (1.4) the function $B_{k,l}$ corresponds to all connected graphs formed with l-connections $(l^{(1)}(r_{ij}),\ l^{(2)}(r_{ij}))$, h-connections $(h^{(11)}(r_{ij}) = |f^{(11)}(r_{ij})|^2 - 1;\ h^{(22)}(r_{ij}) = |f^{(22)}(r_{ij})|^2 - 1;$ $h^{(12)}(r_{ij}) = |f^{(12)}(r_{ij})|^2 - 1)$ and with f-connections between the basis points

($|f^{(11)}(r_{ij})|^2$, $|f^{(22)}(r_{ij})|^2$, $|f^{(12)}(r_{ij})|^2$). The l-connections must again form cycles, while no points with l-connections only may occur.

The generalization to mixtures of fermions can also be made for distribution functions, $g_k(\boldsymbol{r}^k, \boldsymbol{r}'^k)$, not diagonal in the basis coordinates.

In § 2 we shall explain the definition and introduction of the irreducible correlation functions. In § 3 the general combinatorial methods, which are used for a further reduction, are explained. They are applied to the present problem in § 4. A discussion of the result is given in § 5.

§ 2. *The introduction of irreducible correlation functions.* In order to introduce irreducible correlation functions in the case that as well dynamical as statistical correlations exist (and possibly different types of fermions) we first discuss some notions useful for the characterization of the general type of graphs we have to consider:

We introduce three numbers (t, a, b), each expressing a characteristic of a certain *point* of a graph and often denoted in abbreviated form by $\tau \equiv (t, a, b)$. $t = 1, 2, \ldots$ indicates the type of fermion specified by the point. $a = 1, 2, 3$; $a = 1$ indicates a point with R- or basis-connections only; $a = 2$ indicates a point with as well R- or basis-connections as l-connections; $a = 3$ indicates a point with l-connections only. $b = 1, 2$; $b = 1$ indicates a basis point; $b = 2$ indicates a non-basis point.

A graph may be characterized by a function i_τ specifying the numbers of points of the different types $\tau = (t, a, b)$. The total number of points is denoted as $i = \sum_\tau i_\tau$; while we write further $i_a = \sum_{t,b} i_{tab}$; $i_{ta} = \sum_b i_{tab}$.

We have often to consider different functions i_τ, which we shall distinguish by an index ν (we might put $\nu = 1, 2, 3, \ldots$), so that we can then write $i^\nu{}_\tau$, i^ν, $i^\nu{}_a$, $i^\nu{}_{ta}$.

We now define S-functions corresponding to certain irreducible graphs as follows:

$S_\nu(\boldsymbol{r}^{i^\nu})$ is the function corresponding to all *irreducible* graphs formed with l-, R-, and basis-connections and characterized by a definite $i^\nu{}_\tau$-function, if the (distinguishable) points of the type τ are given for each value of τ. After the omission of the l-connections (which connections should again form cycles connecting only points of the same type t) the irreducible parts should be complete stars, R, one of them containing all the $\sum_{t,a} i^\nu{}_{ta1}$ basis coordinates. S_ν is a symmetrical function in the variables corresponding to points of the same type $\tau = (t, a, b)$. (2.1)

Note, that we admit in this definition (contrary to the definition of the $B_{k,l}$-functions) that points may occur with l-connections only.

The expansion I (3.23) of $U_{k,l}$-functions in terms of irreducible cluster functions $R_{k,l}$ has a certain analogue in an expansion of the $B_{k,l}$-functions

in terms of the S-functions. We can write ($k \neq 0$)

$$B_{k,l}(\boldsymbol{r}^k, \boldsymbol{r}^{l-k}) = \sum_{l(\nu)} S_{\nu_0}{}^{(k)}(\boldsymbol{r}^k, \boldsymbol{r}^{i\nu_0-k}) \prod_\nu S_\nu(\boldsymbol{r}^{i\nu}). \tag{2.2}$$

The S-factor $S_{\nu_0}{}^{(k)}$ should contain all basis variables; the other S-factors S_ν may contain 0 or 1 basis variables. $\sum_{l(\nu)}$ indicates a sum of all possible products of S-functions, subject to the following conditions: (*a*) the graph corresponding to each product of S-factors is a graph of l points, which may be reducible, (*b*) the irreducible parts correspond to the different S-factors, (*c*) the graphs of $B_{k,l}$ should contain no points of the type $\tau = (t, 3, 2)$. One should note, that a variable corresponding to an articulation point of the graph, occurs in two or more S-factors.

We shall distinguish two types of cluster integrals, β_ν, according to the definitions (the superscript k indicates the number of basis variables, which occur)

$$\beta_\nu{}^{(k)}(\boldsymbol{r}^k) = \{\prod_\tau (N_t/\Omega)^{i\nu_\tau}[i^\nu{}_\tau!]^{-1}\} \int S_\nu{}^{(k)}(\boldsymbol{r}^k, \boldsymbol{r}^{i\nu-k})\, \mathrm{d}\boldsymbol{r}^{i\nu-k} \text{ if } k \neq 0, \tag{2.3}$$

$$\beta_\nu{}^{(0)} = \{\prod_\tau (N_t/\Omega)^{i\nu_\tau}[i^\nu{}_\tau!]^{-1}\} \int S_\nu{}^{(0)}(\boldsymbol{r}^{i\nu})\, \mathrm{d}\boldsymbol{r}^{i\nu-1} \text{ if } k = 0. \tag{2.4}$$

After substitution of (2.2) in the expressions (1.6) and (1.7) for the cluster integrals $b_{k,l}$, a reduction is obtained in case of a large system, as the integrations over the different S-factors can be carried out separately in the same way as was indicated by Mayer in statistical mechanics[2]). This is possible, because $\beta_\nu{}^{(0)}$ can be taken as independent of the value of the variable, over which no integration is performed, if the total volume is large.

We shall restrict ourselves to distribution functions, $g_k(\boldsymbol{r}^k)$, which are diagonal in the basis coordinates, $\boldsymbol{r}^k$ ($\boldsymbol{r} = \boldsymbol{r}'$). The cluster integrals $\beta_\nu{}^{(1)}(\boldsymbol{r}_i)$, occurring if the basis coordinate $\boldsymbol{r}_i$ corresponds to an articulation point in the graph, are independent of $\boldsymbol{r}_i$ in this case. It follows from (2.3) and (2.4) that $\beta_\nu{}^{(1)}(\boldsymbol{r}_i)$ is (apart from a difference in the normalization factor) equal to $\beta_\mu{}^{(0)}$, if μ is such, that $i^\mu{}_{ta2} = \sum_b i^\nu{}_{tab}$ and $i^\mu{}_{ta1} = 0$. As far as the combinatorial problem is concerned, the difference between basis coordinates and non-basis coordinates (expressed by the index b) is now no longer essential and may be eliminated by the following change in the notation: (1) $\bar{\tau} = (t,a)$; (2) $\bar{\nu}$ characterizes as well the function $i^{\bar{\nu}}_{\bar{\tau}} = \sum_b i^\nu{}_{tab}$ as the set of values $k_t{}^{\bar{\nu}} = \sum_{a=1,2} i^\nu{}_{ta1}$; (3) we introduce the cluster integral $\beta_{\bar{\nu}}$, defined by the following equation if $k^{\bar{\nu}} \neq 0$

$$\beta_{\bar{\nu}} = [\prod_{\bar{\tau}} (N_t/\Omega)^{i\bar{\nu}\bar{\tau}}] \sum_\nu [\prod_{t,a,b} [i^\nu{}_{tab}!]^{-1}] \sum_P \int S_\nu{}^{(k)}(\boldsymbol{r}^k, \boldsymbol{r}^{i\nu-k})\, \mathrm{d}\boldsymbol{r}^{i\nu-k}. \tag{2.5}$$

$\sum_\nu$ indicates a summation over all values of ν, which give the same $\bar{\nu}$; $\sum_P$ is the summation over all permutations P, which permute the basis coordinates of the same type t. $\beta_{\bar{\nu}}$ is a symmetrical function in the basis coordinates. If $k_t = 1$ for $t = t'$ and $k_t = 0$ for $t \neq t'$, the only irreducible cluster integral is $\beta = n_{t'}$. In case $k^{\bar{\nu}} = 0$, $\beta_{\bar{\nu}}$ is defined by (2.4) for that value of ν, for which $i^{\bar{\nu}}{}_{ta} = i^\nu{}_{ta2}$. If we want to indicate the set of basis variables for $\beta_{\bar{\nu}}$, we write

$\beta_{\bar{\nu}}^{(k)}$, if $\sum_t k_t^{\bar{\nu}} \geqslant 1$ and $\beta_{\bar{\nu}}^{(0)}$ if $\sum_t k_t^{\bar{\nu}} = 0$ (so that $\beta_{\bar{\nu}}^{(0)}$ is just a constant).

A reducible graph may be characterized by numbers $m_{\bar{\nu}}$, indicating the number of irreducible parts of the type $\bar{\nu}$. We shall denote by $K_{l\{m_{\bar{\nu}}\}}$ the *number of different (connected) graphs of l points, which have irreducible parts, specified by the numbers $m_{\bar{\nu}}$*. $\{m_{\bar{\nu}}\}$ denotes the set of numbers $m_{\bar{\nu}}$, of which $K_{l\{m_{\bar{\nu}}\}}$ is therefore a function *). l represents a set of numbers l_t. To an irreducible part, characterized by $\bar{\nu}$, there corresponds a set of points, for each value of $\bar{\tau} = (t, a)$, the number of points for the different sets are given by $i_{\bar{\tau}}^{\bar{\nu}}$. In the total graph no points of the type $\bar{\tau} = (t, 3)$ should occur. One should note, that in the determination of $K_{l\{m_{\bar{\nu}}\}}$, only the numbers $i_{\bar{\tau}}^{\bar{\nu}}$ are essential; but that there may be different $\bar{\nu}$ values with the same function $i_{\bar{\tau}}^{\bar{\nu}}$, distinguished by different values of $k_t^{\bar{\nu}}$.

The formula (1.5) for $g_k(\boldsymbol{r}^k)$ may now be brought in a different shape by substituting the expansion (2.2) in the expression (1.6), (1.7) for $b_{k,l}(\boldsymbol{r}^k)$ and introducing the $\beta_{\bar{\nu}}$'s according to (2.4) and (2.5). The result for $\sum_t k_t \geqslant 1$ can be written as

$$g_k(\boldsymbol{r}^k) = \sum_l \sum'_{\{m_{\bar{\nu}}\}} g_{l\{m_{\bar{\nu}}\}}(\boldsymbol{r}^k) = \sum_l \sum'_{\{m_{\bar{\nu}}\}} K_{l\{m_{\bar{\nu}}\}} \left[\prod_t (N_t/\Omega)^{l_t} (l_t!)^{-1}\right] \prod_{\bar{\nu}} \left[\beta_{\bar{\nu}} \prod_{\bar{\tau}} (\Omega/N_t)^{i_{\bar{\tau}}^{\bar{\nu}}} (i_{\bar{\tau}}^{\bar{\nu}}!)\right]^{m_{\bar{\nu}}}. \tag{2.6}$$

The summation $\sum'_{\{m_{\bar{\nu}}\}}$ is a summation restricted in the following way: Each set of $\{m_{\bar{\nu}}\}$ values, over which the summation is extended, should be such that the corresponding term contains one and only one factor $\beta_{\bar{\nu}}$ with $\sum_t k_t^{\bar{\nu}} > 0$. For this factor, $\{k_t^{\bar{\nu}}\}$ should equal the value of k specified in $g_k(\boldsymbol{r}^k)$. If $k_t = 1$ for $t = t'$ and $k_t = 0$ for $t \neq t'$, g_1 equals $n_{t'}$ (cf. (1.8)).

If $\sum_t k_t = 0$, we can still consider the expression (2.6), defining the summation $\sum'_{\{m_{\bar{\nu}}\}}$ by the requirement that $m_{\bar{\nu}} = 0$ if $\sum_t k_t^{\bar{\nu}} > 0$. For this case the right member of (2.6) equals nb (cf. I (4.24)).

The result $g_k(\boldsymbol{r}^k)$ is of the form (if $\sum_t k_t \geqslant 1$)

$$g_k(\boldsymbol{r}^k) = \sum_{l\{m_{\bar{\nu}}\}} A_{l\{m_{\bar{\nu}}\}} \beta_{\bar{\nu}_0}{}^{(k)}(\boldsymbol{r}^k) \prod_{\bar{\nu}} (\beta_{\bar{\nu}}^{(0)})^{m_{\bar{\nu}}} \tag{2.7}$$

and the problem is to reduce $A_{l\{m_{\bar{\nu}}\}}$ to its simplest form. For this purpose we have to insert an expression for $K_{l\{m_{\bar{\nu}}\}}$. The general combinatorial methods to be used for determining $K_{l\{m_{\bar{\nu}}\}}$ are discussed in the next section. In order to simplify the notation we shall omit below the bar of $\bar{\nu}$ and $\bar{\tau}$ and write simply ν and τ.

§ 3. *The general combinatorial problem.* In our derivation of the value of the coefficients of the different $\prod_\nu \beta_\nu{}^{m_\nu}$ factors, we shall use the terminology of Mayer (cf. [2]), App. X and also I § 3). We speak of a *graph* as a figure with numbered points, obtained by filling the *holes* of a *frame* (figure in

*) We shall use the notation with { } parentheses also in other cases for distinguishing a dependence on a set of values $\{m_{\bar{\nu}}\}$ from a dependence on a particular $m^{\bar{\nu}}$.

which the points are not numbered) by *bolts*, representing numbered coordinates. A certain term of the expansion (2.2) is represented by a graph, which is in general *reducible* (graph with articulation points), and can be *dissociated*. The *dissociated arrangement* consists of a number of *frames* (representing the irreducible parts) in which each hole, or all holes except one, are filled with the numbered *bolts*. We can determine the dissociated arrangement uniquely, by choosing some irreducible part as the *root* and removing it first with all its bolts. In case of a reducible graph, the dissociated arrangement consists now of one or more connected graphs, each of them with one hole. If the hole is of character τ, such a part is called a *branch* of character τ. The further dissociation is carried out by dissociating the branches, in such a way that each irreducible part gets only *one empty hole*. If $\sum_t k_t \neq 0$. we may choose the irreducible part containing all basis variables as the root, but this is by no means necessary.

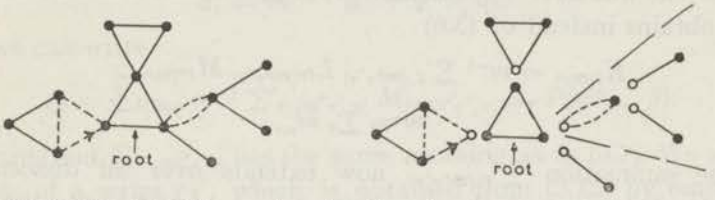

Fig. 2. Example of a reducible graph and a dissociated arrangement, resulting from it.

In order to reduce the result (2.6) for $g_k(\boldsymbol{r}^k)$ we have to find a value for $K_{l\{m_\nu\}}$. For this purpose we consider the different reducible graphs and different dissociated arrangements, which lead to a definite set of values m_ν. Each irreducible part may be characterized by ν. In the dissociated arrangement each irreducible part may be characterized in addition by the character, τ', of the hole, which is not filled by a bolt, and by the character, τ, of the branch to which it belongs. We introduce numbers $m^\nu{}_{\tau'\tau}$ for a dissociated arrangement, specifying the number of irreducible parts ν, with hole τ', in a branch of character τ. Let ν_r be the type of the root. We have

$$m_\nu = \sum_{\tau',\tau} m^\nu{}_{\tau'\tau} \text{ if } \nu \neq \nu_r \tag{3.1}$$

and

$$m_\nu = 1 + \sum_{\tau',\tau} m^\nu{}_{\tau'\tau} \text{ if } \nu = \nu_r. \tag{3.2}$$

Further one sees immediately that

$$\sum_t l_t = 1 + \sum_\nu m_\nu (i^\nu - 1). \tag{3.3}$$

We put further

$$m^\nu{}_{\tau'} = \sum_\tau m^\nu{}_{\tau'\tau}. \tag{3.4}$$

The total number of points of character t may be written as

$$l_t = \sum_a i^{\nu_r}{}_\tau + \sum_{\nu,a,\tau'} m^\nu{}_{\tau'} [i^\nu{}_\tau - \delta_{\tau,\tau'}]. \quad (\tau = t, a) \tag{3.5}$$

The numbers $m^{\nu}{}_{\tau'\tau}$ depend obviously on the choice of the root. If the root is of the type ν_r (while a number m_{ν_r} of frames of this type exist), the number $K_{l\{m_\nu\}}$ (see § 2, e.g., (2.6)) can be written as[2])

$$K_{l\{m_\nu\}} = (m_{\nu_r})^{-1} \sum'_{\{m^{\nu}{}_{\tau'\tau}\}} L_{l\{m^{\nu}{}_{\tau'\tau}\}} M_{l\{m^{\nu}{}_{\tau'\tau}\}}. \tag{3.6}$$

In this formula $L_{l\{m^{\nu}{}_{\tau'\tau}\}}$ is the number of different dissociated arrangements, characterized by the set $\{m^{\nu}{}_{\tau'\tau}\}$ and a root ν_r, which can be formed with a set of l (numbered) bolts. $M_{l\{m^{\nu}{}_{\tau'\tau}\}}$ is the number of ways in which each dissociated arrangement can be bolted together. The type of bolt is characterized by t, the type of hole by $\tau' = (t, a)$. The summation $\sum'_{\{m^{\nu}{}_{\tau'\tau}\}}$ is meant as a summation over all values of $m^{\nu}{}_{\tau'\tau}$, which are in agreement with a reducible graph characterized by $\{m_\nu\}$ and a root of the type ν_r (cf. (3.1), (3.2)).

It is often preferable to use a generalization of (3.6), in which a set $\{\nu_r\}$ is given, such that any frame of some type ν_r ($r = 1,2,\ldots$) may be chosen as a root. One will have certain numbers $m^{\nu}{}_{\tau'\tau}$ if a root is chosen of the type ν_r. One obtains instead of (3.6)

$$K_{l\{m_\nu\}} = m^{-1} \sum'_{r,\{m^{\nu}{}_{\tau'\tau}\}} L_{lr\{m^{\nu}{}_{\tau'\tau}\}} M_{lr\{m^{\nu}{}_{\tau'\tau}\}} \tag{3.7}$$

with

$$m = \sum_r m_{\nu_r}, \tag{3.8}$$

while the summation $\sum'_{r,\{m^{\nu}{}_{\tau'\tau}\}}$ now extends over all dissociated arrangements belonging to the composition $\{m_\nu\}$, also choosing the roots of all different types ν_r.

The value $L_{lr\{m^{\nu}{}_{\tau'\tau}\}}$ is easily found by considering its definition: the number of ways that the l bolts can be distributed over the frames of the dissociated arrangement characterized by $\{m^{\nu}{}_{\tau'\tau}\}$, taking a root of type ν_r:

$$L_{lr\{m^{\nu}{}_{\tau',\tau}\}} = \frac{\prod_t (l_t)!}{[\prod_{\tau''} i^{\nu}{}_{\tau''\tau''}!] \prod_{\nu,\tau',\tau} (m^{\nu}{}_{\tau'\tau})! \{[i^{\nu}{}_{\tau'} - 1]! \prod_{\tau'' \neq \tau'} [i^{\nu}{}_{\tau''}]!\}^{m^{\nu}{}_{\tau'\tau}}}. \tag{3.9}$$

The expressions (3.7) and (3.9) will be used for a reduction of the expression (2.6) for $g_k(\boldsymbol{r}^k)$. It will prove convenient below not to reduce the series (2.6) itself but to reduce a very similar series, in which the basis coordinates do no longer play any particular role. We can write this "symmetrized" series, g_S, as:

$$\begin{aligned} g_S &= \sum_{l\{m_\nu\}} g^S{}_{l\{m_\nu\}} = \\ &= \sum_{l\{m_\nu\}} K_{l\{m_\nu\}} [\prod_t (N_t/\Omega)^{l_t} (l_t!)^{-1}] \prod_\nu [\beta_\nu \prod_\tau (\Omega/N_t)^{i^{\nu}{}_\tau} (i^{\nu}{}_\tau!)]^{m_\nu} = \\ &= \sum_{l\{m_\nu\}} A^S{}_{l\{m_\nu\}} \prod_\nu (\beta_\nu)^{m_\nu}. \end{aligned} \tag{3.10}$$

The summation $\sum_{\{m_\nu\}}$ is not subjected to the restriction, which the summation $\sum'_{\{m_\nu\}}$ has in (2.6). The expression (3.10) is considered as a polynomial in the β_ν's. The β_ν's are considered here simply as variables depending on ν (for which it is not necessary to specify any particular value). The extension

of the summation from (2.6) to (3.10) is possible, because $K_{l\{m_\nu\}}$ was already defined for the more general $\{m_\nu\}$-sets occurring in the summation (3.10). The expression for $g_k(\boldsymbol{r}^k)$ can be derived in a simple way from the series for g_S by recalling the meaning of the accent of the summation sign in (2.6). By substitution of (3.7) and (3.9) into (3.10), we obtain an expression for $g^S{}_{l\{m_\nu\}}$, which may be written as

$$g^S{}_{l\{m_\nu\}} = m^{-1} \sum'_{r,\{m^\nu{}_{\tau'\tau}\}} M_{lr\{m^\nu{}_{\tau'\tau}\}} \beta_{\nu r} P\{m^\nu{}_{\tau'\tau}, \beta\}, \tag{3.11}$$

if we introduce the abbreviations

$$P\{m^\nu{}_{\tau'\tau}, \beta\} = \prod_{\nu,\tau'} \frac{[\sigma_{\tau'} i^\nu{}_{\tau'} \beta_\nu]^{m^\nu{}_{\tau'}}}{\prod_\tau (m^\nu{}_{\tau'\tau})!} = \prod_\tau P_\tau \{m^\nu{}_{\tau'\tau}, \beta\}, \tag{3.12}$$

$$P_\tau\{m^\nu{}_{\tau'\tau}, \beta\} = \prod_{\nu,\tau'} \frac{[\sigma_{\tau'} i^\nu{}_{\tau'} \beta_\nu]^{m^\nu{}_{\tau'\tau}}}{(m^\nu{}_{\tau'\tau})!}, \tag{3.13}$$

$$\sigma_\tau = n_t^{-1} \quad \text{if} \quad \tau = (t, a). \tag{3.14}$$

Hence we can write

$$g_S = \sum_{l\{m_\nu\}} m^{-1} \sum'_{r,\{m^\nu{}_{\tau',\tau}\}} M_{lr\{m^\nu{}_{\tau',\tau}\}} \beta_{\nu r} P\{m^\nu{}_{\tau'\tau}, \beta\}. \tag{3.15}$$

The summation $\sum'_{r,\{m^\nu{}_{\tau'\tau}\}}$ has the same meaning as in (3.7). We shall also make use of a series g_S', which is obtained from (3.15) by omitting the factor m^{-1},

$$g_S' = \sum_{l\{m_\nu\}} \sum_{r,\{m^\nu{}_{\tau'\tau}\}} M_{lr\{m^\nu{}_{\tau'\tau}\}} \beta_{\nu r} P\{m^\nu{}_{\tau'\tau}, \beta\}. \tag{3.16}$$

It is clear that the expression for g_S can be found immediately, once the expression for g_S' is obtained (one has only to add the factor $m^{-1} = [\sum_r m_{\nu r}]^{-1}$ in each term).

We are now going to consider the problem of determining $M_{lr\{m^\nu{}_{\tau'\tau}\}}$ and reducing the expression (3.16) for g_S'. We solve this problem first in a general form, and specialize in the next section to the case considered in § 2. We denote by $n\{\lambda_{\tau'}\}$ *the number of ways, that a set of holes specified by* $\{\lambda_{\tau'}\}$ *can be bolted together with a "neutral" bolt.* $\lambda_{\tau'}$ specifies the number of holes of character τ' (not considering any other characteristic of the graph in which the hole is contained). In the problem of § 2 we have $n\{\lambda_{\tau'}\} = 0$ or 1. If not all holes are of the same type t (either neutrons or protons) $n\{\lambda_{\tau'}\} = 0$; cf. further the beginning of § 4. In the treatment of this section we leave the number $n\{\lambda_{\tau'}\}$ unspecified. We now introduce "counting series" [2] [3] (generating functions) for use in the further developments defined by

$$f(y) = \sum_{\{\lambda_{\tau'}\}} n\{\lambda_{\tau'}\} \prod_{\tau'} [(y_{\tau'})^{\lambda_{\tau'}}/(\lambda_{\tau'})!]. \tag{3.17}$$

We shall use the following notation to indicate the coefficient of $\prod_{\tau'}(y_{\tau'})^{\lambda_{\tau'}}$ in the power series $f(y)$

$$[\prod_{\tau'}(y_{\tau'})^{\lambda_{\tau'}}] : f(y). \tag{3.18}$$

With this notation (3.17) can alternatively be written as

$$n\{\lambda_{\tau'}\} = [\Pi_{\tau'}(\lambda_{\tau'})!\,(y_{\tau'})^{\lambda_{\tau'}}] : f(y). \tag{3.19}$$

If the numbers $n\{\lambda_{\tau'}\}$ are assumed to be known, certain combinatorial factors depending on them can be derived and expressed by means of counting series. In the first place the *number of ways, $n_\tau\{\lambda_{\tau'}\}$, that a set of holes, specified by $\{\lambda_{\tau'}\}$ can be attached to a bolt of character τ* is given by

$$n_\tau\{\lambda_{\tau'}\} = n\{\bar{\lambda}_{\tau'}\} \text{ with } \bar{\lambda}_{\tau'} = \begin{cases} \lambda_{\tau'} & \text{if } \tau' \neq \tau, \\ \lambda_{\tau'} + 1 & \text{if } \tau' = \tau. \end{cases} \tag{3.20}$$

This is expressed by means of a counting series as

$$n_\tau\{\lambda_{\tau'}\} = [\Pi_{\tau'}(\lambda_{\tau'})!\,(y_{\tau'})^{\lambda_{\tau'}}] : f_\tau(y), \text{ with } f_\tau(y) = (\partial/\partial y_\tau) f(y). \tag{3.21}$$

Further it is easily deduced that the *number of ways in which a set of $\{\lambda_{\tau'}\}$ holes can be attached to the bolts of a graph of character ν with a τ_0-hole* (any distribution over the different bolts being allowed) is given by

$$[\Pi_{\tau'}(\lambda_{\tau'})!\,(y_{\tau'})^{\lambda_{\tau'}}] : F_{\tau_0\nu}(y) \tag{3.22}$$

with

$$F_{\tau_0\nu}(y) = [f_{\tau_0}(y)]^{i\nu_{\tau_0}-1} \prod_{\tau\neq\tau_0} [f_\tau(y)]^{i\nu_\tau}. \tag{3.23}$$

We want to consider next the *number of ways, $Q_\tau(\{m^\nu{}_{\tau'\tau}\}, N_\tau)$, in which frames belonging to branches of a definite type τ can be bolted together to N_τ branches of this type, if the dissociated arrangement is specified by $\{m^\nu{}_{\tau'\tau}\}$* (these branches are not yet bolted to the root). We use the notation

$$m_{\tau'\tau} = \textstyle\sum_\nu m^\nu{}_{\tau'\tau}. \tag{3.24}$$

A distribution of the holes over the frames is allowed, if such a distribution corresponds to a number of N_τ singly connected structures, each with a hole of character τ. The number of distributions for fixed values of $\{\lambda_{\tau'p}\}$, which is the set of holes such as is used in (3.23) added to frame number p, can be determined by extending the method given in Appendix X, p. 458 of ref. [2]). With (3.23), and after a summation over all possible values of $\{\lambda_{\tau'p}\}$ ($\sum_p \lambda_{\tau'p} = m_{\tau'\tau}$ if $\tau' \neq \tau$; $\sum_p \lambda_{\tau p} = m_{\tau\tau} - N_\tau$), one finds

$$Q_\tau(\{m^\nu{}_{\tau'\tau}\}, N_\tau) = \left[\frac{(m_{\tau\tau}-1)!}{(N_\tau-1)!}(y_\tau)^{m_{\tau\tau}-N_\tau} \prod_{\tau'\neq\tau}(m_{\tau'\tau})!\,(y_{\tau'})^{m_{\tau'\tau}}\right] : [\Pi_{\tau_0\nu}(F_{\tau_0\nu}(y))^{m^\nu{}_{\tau_0\tau}}]. \tag{3.25}$$

If $N_\tau = 0$, we have $\qquad Q_\tau(\{0\}, 0) = 1. \tag{3.25a}$

We shall now denote by $R(\{N_\tau\}, \nu_r)$ the *number of ways, in which the set of $\{N_\tau\}$ branches can be attached to the root ν_r*. It is found to be ($N_\tau \geqslant 0$)

$$R(\{N_\tau\}, \nu_r) = [\Pi_\tau(N_\tau)!\, y_\tau{}^{N_\tau}] : F_{\nu_r}(y), \tag{3.26}$$

with $$F_{\nu r}(y) = \prod_\tau [f_\tau(y)]^{i\nu_r\tau}. \tag{3.27}$$

The number $M_{lr\{m\nu_{\tau'\tau}\}}$, which must be substituted in (3.16), can now be expressed as

$$M_{lr\{m\nu_{\tau'\tau}\}} = \sum_{\{N_\tau\}} R(\{N_\tau\}\nu_r) \prod_\tau Q_\tau(\{m^\nu{}_{\tau'\tau}\}, N_\tau). \tag{3.28}$$

Further, it follows from (3.11), (3.12) and (3.28) that the expression for $g^S{}_{l\{m_\nu\}}$ can be written as

$$g^S{}_{l\{m_\nu\}} = m^{-1} \sum'_{r,\{m\nu_{\tau'\tau}\}} \beta_{\nu r} \sum_{\{N_\tau\}} R(\{N_\tau\}, \nu_r) \prod_\tau Q_\tau(\{m^\nu{}_{\tau'\tau}\}, N_\tau) P_\tau\{m^\nu{}_{\tau'\tau}, \beta\}. \tag{3.29}$$

In order to find a reduced form for $g_S{}'$, (3.16), we calculate first

$$T_\tau(\{m_{\tau'\tau}, \beta\}, N_\tau) = \sum''_{\{m\nu_{\tau'\tau}\}} Q_\tau(\{m^\nu{}_{\tau'\tau}\}, N_\tau) P_\tau\{m^\nu{}_{\tau'\tau}, \beta\}. \tag{3.30}$$

The summation $\sum''_{\{m\nu_{\tau'\tau}\}}$ should be extended here over all sets of $\{m^\nu{}_{\tau'\tau}\}$-values (for a definite τ), such that $\sum_\nu m^\nu{}_{\tau'\tau} = m_{\tau'\tau}$, where the $m_{\tau'\tau}$-values are specified in the left member of (3.30). In case of ambiguity, we shall use a second index τ for the variables $y_{\tau''}$ $(y_{\tau''\tau})$ and $\sigma_{\tau''}$ $(\sigma_{\tau''\tau})$, to indicate the character of the branches, τ, to which the variables belong. From the expressions (3.13) and (3.25) for fixed τ, making use of

$$\sum_{\{m^\nu{}_{\tau'\tau}\}} \prod_{\nu,\tau'} \frac{[\sigma_{\tau'\tau} i^\nu{}_{\tau'} F_{\tau'\nu}(y_{\tau''\tau})\beta_\nu]^{m\nu_{\tau'\tau}}}{(m^\nu{}_{\tau'\tau})!} = \prod_{\tau'} \exp\left[\sigma_{\tau'\tau} \sum_\nu i^\nu{}_{\tau'} F_{\tau'\nu}\beta_\nu\right] \tag{3.31}$$

and putting

$$F_{\tau'}[f(y_{\tau''\tau}), \beta] = \sum_\nu i^\nu{}_{\tau'} F_{\tau'\nu}(y_{\tau''\tau})\beta_\nu, \tag{3.32}$$

we find that $(N_\tau \neq 0)$

$$T_\tau(\{m_{\tau'\tau}, \beta\}, N_\tau) = \left[\frac{(m_{\tau\tau}-1)!}{(N_\tau - 1)!} (y_{\tau\tau})^{m_{\tau\tau}-N_\tau} (\bar\sigma_{\tau\tau})^{m_{\tau\tau}} \prod_{\tau' \neq \tau} (m_{\tau'\tau})! (y_{\tau'\tau})^{m_{\tau'\tau}} (\bar\sigma_{\tau'\tau})^{m_{\tau'\tau}}\right] : \prod_{\tau'} \exp\left[\sigma_{\tau'\tau} F_{\tau'}(f, \beta)\right]. \tag{3.33}$$

In (3.33) we have abbreviated $n_{t'}{}^{-1}\sigma_{\tau'\tau} = \bar\sigma_{\tau'\tau}$ (if $\tau' = (t', a')$, cf. (3.14)) and extended the notation (3.18) to the variables σ (hence $(\bar\sigma_{\tau'\tau})^k := n_{t'}{}^{-k}(\sigma_{\tau'\tau})^k$:). For the special case $N_\tau = 0$, we have $T_\tau = 1$.

The expression (3.16) for $g_S{}'$ can now be simplified by noting that according to (3.30)

$$g_S{}' = \sum_r \sum_{\{m_{\tau'\tau}\}} \sum_{\{N_\tau\}} \beta_{\nu r} R(\{N_\tau\}, \nu_r) \prod_\tau T_\tau(\{m_{\tau'\tau}, \beta\}, N_\tau). \tag{3.34}$$

We introduce the abbreviation (designating the y-variables further as $y_{\tau\tau}$ instead of y_τ)

$$F[f(y), \beta] = \sum_r F_{\nu r}(y)\beta_{\nu r}, \tag{3.35}$$

so that we can write

$$\Sigma_r R(\{N_\tau\}, \nu_r)\beta_{\nu r} = [\Pi_\tau (N_\tau)!\,(y_{\tau\tau})^{N_\tau}] : F[f(y_{\tau\tau}), \beta]. \tag{3.36}$$

We finally introduce

$$G_\tau(y_{\tau\tau}, \sigma_{\tau\tau}) = \Sigma^*_{\{m_{\tau'\tau}\}} [\Pi_{\tau' \neq \tau}(m_{\tau'\tau})!\,(y_{\tau'\tau})^{m_{\tau'\tau}} (\bar{\sigma}_{\tau'\tau})^{m_{\tau'\tau}}] : \Pi_{\tau_0} \exp\{\sigma_{\tau_0\tau} F_{\tau_0}[f(y_{\tau''\tau}), \beta]\}, \tag{3.37}$$

where the summation is over all values of $m_{\tau'\tau} \geqslant 0$ with $\tau' \neq \tau$. Making use of (3.33), (3.34), (3.36), (3.37) and

$$[(N_\tau)!\,(y_{\tau\tau})]^{N_\tau}] : F[f(y_{\tau\tau}), \beta] = [(N_\tau - 1)!\,(y_{\tau\tau})^{N_\tau - 1}] : \frac{\partial}{\partial y_{\tau\tau}} F[f(y_{\tau\tau}), \beta], \tag{3.38}$$

if $N_\tau \neq 0$, we find for $g_{S'}$

$$g_{S'} = \left\{ \Pi_\tau \left[(y_{\tau\tau}{}^0 :) + \Sigma_{m_{\tau\tau} \geqslant 1} [(m_{\tau\tau} - 1)!\,(y_{\tau\tau})^{m_{\tau\tau} - 1} : (\bar{\sigma}_{\tau\tau})^{m_{\tau\tau}} :] \right. \right. \left. \left. G_\tau(y_{\tau\tau}, \sigma_{\tau\tau}) \frac{\partial}{\partial y_{\tau\tau}} \right] \right\} F[(f(y_{\tau'\tau'}), \beta]. \tag{3.39}$$

One should note that the derivations (acting on F) must be carried out, after the Π_τ-sign, but before the :-signs.

§ 4. *Specialization of the combinatorial problem.* We now want to apply the general developments of § 3 to the problem of interacting fermions, as described in § 2. For this specialization we must give in detail the values of $n\{\lambda_{\tau'}\}$ for the different cases and the expressions for $f(y)$. As we do not distinguish in this context whether points are basis points or not, the variable τ is specified merely by giving (t, a) (see § 2 for the definition of $t = 1,2$ and $a = 1, 2, 3$). We first specify the value of $n\{\lambda_{\tau'}\}$ for a pair $(\tau_1, \tau_2) = (t_1 a_1, t_2 a_2)$ of holes, which should be joined. We then have
case (α): $(t_1, t_2) = (1,1)$ or $(2,2)$:

$$n\{\lambda_{\tau'}\} = 1, \text{ if } (a_1, a_2) = (1,1), (1,2), (2,1), (1,3), (3,1), \tag{I}$$
$$n\{\lambda_{\tau'}\} = 0, \text{ if } (a_1, a_2) = (2,2), (2,3), (3,2), (3,3),$$

case (β): $(t_1, t_2) = (1,2)$ or $(2,1)$:

$$n\{\lambda_{\tau'}\} = 0. \tag{4.1}$$

(4.1) expresses that $n\{\lambda_{\tau'}\} = 0$, if holes of different t-value should be joined and that no two holes with l-connections (having $(a_1, a_2) = (2,2), (2,3), (3,2)$ or $(3,3)$) can be joined, as the l-connections should form cycles only. If we consider further only sets where all holes are of the same type t ($n\{\lambda_{\tau'}\}$ being zero for other sets), and specify $\{\lambda_{\tau'}\}$ by the number of holes with $a = 1$, 2 or 3, we have for sets of more than two holes:

$$n\{\lambda_{a=1}, \lambda_{a=2}, \lambda_{a=3}\} = \begin{cases} 1 \text{ if all pairs which may occur are of type (I).} \\ 0 \text{ in any other case.} \end{cases} \tag{4.2}$$

Although, an irreducible frame may contain holes of the type $a = 3$ (cf. (2.1)), it should be noted that in the graph of $B_{k,l}$ no bolts of this type should occur, as they should correspond to points having l-connections only (the hole in the irreducible frame with $k = 1$ is considered to be of the type $a = 1$).

The above statements can be expressed more explicitly as

$$\begin{aligned} &n\{\lambda_1, 0,0\} = 1 \text{ for every } \lambda_1 \geqslant 0, \\ &n\{\lambda_1, 1,0\} = 1 \text{ for every } \lambda_1 \geqslant 0, \\ &n\{\lambda_1, 0,1\} = 1 \text{ for every } \lambda_1 \geqslant 1, \\ &n\{\lambda_1, \lambda_2, \lambda_3\} = 0 \text{ in any other case.} \end{aligned} \tag{4.3}$$

Introducing this in (3.17) we obtain for $f(y)$

$$f(y) = \sum_t [e^{y_{t1}} + y_{t2}\, e^{y_{t1}} + y_{t3}\,(e^{y_{t1}} - 1)] \tag{4.4}$$

and

$$\begin{aligned} f_{t1}(y) &= (1 + y_{t2} + y_{t3})\, e^{y_{t1}}, \\ f_{t2}(y) &= e^{y_{t1}}, \\ f_{t3}(y) &= e^{y_{t1}} - 1. \end{aligned} \tag{4.5}$$

The specialization of the result (3.39) for g_S' requires the introduction of the results (4.4) and (4.5), but a further reduction may be obtained, because in the expressions for the different β_ν *integrations over points with* $a = 3$ (having l-connections only) *can always be carried out*. This is easily seen in the following way: suppose a point j has $l^{(t)}$-connections with the points i and k. We have then according to the definition I (3.4)

$$l_{ij}{}^{(t)}\, l_{jk}{}^{(t)} = N_t{}^{-2} \left[\sum_{\lambda=1}^{N_t} e^{i\boldsymbol{k}\lambda\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j)}\right] \left[\sum_{\mu=1}^{N_t} e^{i\,\boldsymbol{k}_\mu\cdot(\boldsymbol{r}_j - \boldsymbol{r}_k)}\right]. \tag{4.6}$$

In view of the orthogonality of plane waves for different values of λ, the integral over $\boldsymbol{r}_j$ reduces simply to

$$\int l_{ij}\, l_{jk}\, \mathrm{d}\boldsymbol{r}_j = (\Omega/N_t) l_{ik}. \tag{4.7}$$

In a similar way a β_ν for a graph with $a = 3$ points can always be reduced to a $\beta_{\nu'}$ for a graph without $a = 3$ points. The following relation can be derived for this reduction

$$\beta_\nu = \left[\prod_t (-1)^{i^\nu{}_{t3}} \frac{(i^\nu{}_{t2} + i^\nu{}_{t3} - 1)!}{(i^\nu{}_{t2} - 1)!\,(i^\nu{}_{t3})!}\right] \beta_{\nu'} \tag{4.8}$$

where ν' is related in such a way to ν that

$$i^{\nu'}{}_{t1} = i^\nu{}_{t1};\; i^{\nu'}{}_{t2} = i^\nu{}_{t2};\; i^{\nu'}{}_{t3} = 0 \;(k_t{}^{\nu'} = k_t{}^\nu). \tag{4.8a}$$

It is supposed in (4.8) that not all points have $a = 3$. In the derivation one has to take into account the sign of the permutation and the normalization factors according to the definition (2.3), (2.4), (2.5). Further one has to

consider the relation between a frame specified by ν and the frame specified by ν'. It is found that the ν'-frame can be extended to the ν-frame by adding $a = 3$ points on the l-cycles of the ν'-frame in

$$\Pi_t \left[(i^\nu{}_{t2} + i^\nu{}_{t3} - 1)!/(i^\nu{}_{t2} - 1)!\right] \tag{4.9}$$

ways. This number enters as a factor in (4.8).

One special case of irreducible graphs was excluded in (4.8), namely pure permutation cycles for some definite type t of fermions. The integrations over all points except one must now be carried out; one finds in this case ($i^\nu = i^\nu{}_{t3}$)

$$\beta_\nu = (-1)^{i^\nu{}_{t3}-1}\,(n_t/i^\nu{}_{t3}). \tag{4.10}$$

The expressions (4.8) and (4.10) allow to make the following reductions

$$\Sigma'_\nu\, \beta_\nu\, \Pi_t (f_{t3})^{i^\nu{}_{t3}} = \beta_{\nu'}\, \Pi_t (1 + f_{t3})^{-i^{\nu'}{}_{t2}}, \tag{4.11}$$

$$\Sigma'_\nu\, \beta_\nu i^\nu{}_{t'3} (f_{t'3})^{-1}\, \Pi_t (f_{t3})^{i^\nu{}_{t3}} = -\beta_{\nu'} i^{\nu'}{}_{t'2} (1 + f_{t'3})^{-1}\, \Pi_t\, (1 + f_{t3})^{-i^{\nu'}{}_{t2}}. \tag{4.12}$$

The summations Σ'_ν in (4.11) and (4.12) extend over all ν (with $i^\nu{}_{t3} \geqslant 0$) to which the same value of ν' (according to (4.8a)) corresponds

$$\Sigma''_\nu (f_{t3})^{i^\nu{}_{t3}}\, \beta_\nu = -\, n_t[f_{t3} - \ln\,(1 + f_{t3})], \tag{4.13}$$

$$\Sigma''_\nu\, i^\nu{}_{t3}\, (f_{t3})^{i^\nu{}_{t3}-1}\, \beta_\nu = n_t[(1 + f_{t3})^{-1} - 1]. \tag{4.14}$$

The summations Σ''_ν in (4.13) and (4.14) extend over all ν with $i^\nu = i^\nu{}_{t3} \geqslant 2$.

Substituting these results in (3.35) and using (4.5), one obtains, if every type ν_τ is admitted as a possible root

$$F = \Sigma_\nu[\Pi_t (f_{t1})^{i^\nu{}_{t1}}]\beta_\nu - \Sigma_t\, n_t(e^{y_{t1}} - 1 - y_{t1}). \tag{4.15}$$

Substituting the results into (3.32) and using (4.5), leads to the following expressions for $F_{\tau'}$

$$F_{t'1} = \Sigma_\nu\, i^\nu{}_{t'1}\, (f_{t'1})^{-1}\, [\Pi_t\, (f_{t1})^{i^\nu{}_{t1}}]\beta_\nu, \tag{4.16}$$

$$F_{t'2} = \Sigma_\nu\, i^\nu{}_{t'2} (f_{t'2})^{-1}[\Pi_t (f_{t1})^{i^\nu{}_{t1}}]\beta_\nu, \tag{4.17}$$

$$F_{t'3} = -\,\Sigma_\nu\, i^\nu{}_{t'2}\, (f_{t'2})^{-1}\, [\Pi_t (f_{t1})^{i^\nu{}_{t1}}]\, \beta_\nu + n_{t'}\, (e^{-y_{t'1}} - 1). \tag{4.18}$$

The summations Σ_ν in (4.15)–(4.18) are extended over all values ν, for which $\Sigma_t\, i^\nu{}_{t3} = 0$.

It is seen from (4.5) that there is no difference in the number of ways that $a = 2$ and $a = 3$ holes can be connected to some bolt *in a frame*. As far as the holes are concerned, we may therefore combine the indices 2 and 3 to one index, 4 say, and write $y_{t2} + y_{t3} = y_{t4}$, etc. This may also be done for the σ's in formula (3.39), because the value of the parameter $\sigma_{\tau'\tau}$ depends only on t', if $\tau' = (t', a')$. Introducing the abbreviation:

$$\beta\{i_{t1}\} = \Sigma_\nu \beta_\nu \tag{4.19}$$

where the summation $\sum_\nu$ extends over all ν with $i^\nu_{t1} = i_{t1}$ (the i_{t1}-values are specified in the left member of (4.19)) and with $\sum_t i^\nu_{t3} = 0$, the formulae (4.15)–(4.18) can be written as

$$F = \sum_{\{i_{t1}\}} \{\prod_t [e^{y_{t1}}(1 + y_{t4})]^{i_{t1}}\} \beta\{i_{t1}\} - \sum_t n_t[e^{y_{t1}} - 1 - y_{t1}], \quad (4.20)$$

$$F_{t1} = \sum_{\{i_{t1}\}} i_{t1} [e^{y_{t1}}(1 + y_{t4})]^{i_{t1}-1}\{\prod_{t' \neq t}[e^{y_{t'1}}(1 + y_{t'4})]^{i_{t'1}}\} \beta\{i_{t1}\}, \quad (4.21)$$

$$F_{t4} = F_{t2} + F_{t3} = n_t (e^{-y_{t1}} - 1). \quad (4.22)$$

The summation $\sum_{\{i_{t1}\}}$ is over all possible values of $i_{t1} \geqslant 0$.

It is our purpose to obtain a reduced result for g_k by means of the result (3.39) for g_S'. The different terms of the series for g_S correspond to different graphs. In the general formula (3.38) it is not yet specified which type of graphs may be chosen as roots. We shall use different roots for different groups of terms and write

$$g_S = g_I + g_{II,t=1} + g_{III,t=1} + g_{II,t=2} + g_{III,t=2} \quad (4.23)$$

The groups of terms indicated by I, IIt, etc. are chosen in the following way:

I. All graphs containing as irreducible part a frame of a type $\sum_t i^\nu_{t1} = 0$, $\sum_t i^\nu_{t2} \neq 0$, $\sum_t i^\nu_{t3}$ arbitrary. The root is then chosen of such a type.

$II, t = 1$. All graphs, not containing any graphs of a type as specified under I, but containing at least one pure permutation cycle of points with $t = 1$. The root is chosen to be a permutation cycle of type $t = 1$.

$III, t = 1$. All graphs, not containing any irreducible part as mentioned under I or $II, t = 1$, but with at least one bolt of type $t = 1$ which is not contained in a $a = 2$ or $a = 3$ hole. We now choose as a root a single bolt of this type.

$II, t = 2$. All graphs not containing any irreducible parts specified under I; $II, t = 1$; $III, t = 1$, but containing a pure permutation cycle of points $t = 2$.

$III, t = 2$. All graphs not containing any irreducible parts specified under I; ... ; $II, t = 2$. They should then contain at least one bolt of type $t = 2$ which is *not* contained in a $a = 2$ or $a = 3$ hole. We now choose as a root a single bolt of this type.

(In case more values then $t = 1$, 2 are possible the grouping of terms (4.23) should still be supplemented in an obvious way).

We now consider the contributions of the different groups of terms

I. Taking a root of the type specified under I, we find (cf. (4.20) and (3.39); F is found as a part of (4.20), excluding the contribution from the pure permutation cycles, i.e., the second term, and taking only the parts with $i_{t1} = 0$ from the first term)

$$F[f(y_{\tau\tau}), \beta] = \beta\{0\}, \quad (4.24)$$

$$(g_S')_I = [\prod_t \prod_{a=1,4} y^0_{\tau\tau}] : \beta\{0\} = \beta\{0\}. \quad (4.25)$$

$II, t = 1$. In calculating this contribution, we take as a root all pure permutation cycles of the type $t = 1$ (F is obtained from (4.20) taking only the contribution from the second term for the permutation cycles with $t = 1$)

$$F(y_{11}) = -n_1 (e^{y_{11}} - 1 - y_{11}) \quad (y_{11} = y_{11,11}), \tag{4.26}$$

$$(gs')_{II,t=1} = \sum_{m \geqslant 1} [(m_{11}-1)!\,(y_{11})^{m_{11}-1}(\bar{\sigma}_{11})^{m_{11}}] : G_{11}(y_{11}, \sigma_{11}) \frac{\partial}{\partial y_{11}} F(y_{11}). \tag{4.27}$$

The functions F_{t1} and F_{t4}, occurring in G_{11} (cf. (3.37)), are given by (4.21) and (4.22), respectively, if the summation in (4.21) is restricted to values of $\{i_{t1}\}$ for which $\sum_t i_{t1} \neq 0$. We shall use the equality ($m_{t4} \geqslant 0$, $t = 1, 2$)

$$[(m_{t4})!\,(\bar{\sigma}_{t4})^{m_{t4}}] : \exp(\sigma_{t4} F_{t4}(y_{t1})) = (e^{-y_{t1}} - 1)^{m_{t4}}. \tag{4.28}$$

The expression G_{11}, according to (3.37) contains summations over m_{21}, m_{24}, and m_{14}. It follows from (4.28) with $t = 2$, that the summation over m_{24} can be performed by omitting the part $\sum_{m_{24} \geqslant 0} (m_{24})!\,(y_{24})^{m_{24}}\,(\bar{\sigma}_2)^{m_{24}} : \exp[\sigma_{24} F_{24}(y_{21})]$ in G_{11} and substituting for y_{24}

$$y_{24} \to e^{-y_{21}} - 1 \tag{4.29}$$

wherever y_{24} occurs in the part $\prod_{\tau \neq 24} \exp\{\sigma_\tau F_\tau[f, \beta]\}$ of G_{11}. After this substitution, it is seen that the result is independent of y_{21} (cf. result for F_{24} obtained by substituting (4.27) into (4.21)); hence only the term $m_{21} = 0$ remains of the summation over m_{21}. The summation over m_{14} cannot be carried out in the same way as for m_{24}. This is because we have to add a factor $m^{-1} = (m_{14} + 1)^{-1}$ to pass from g_S' to g_S, as follows from (3.8) and the type of root in this case.

The substitution $m = m_{14} + 1$ needs some explanation: According to (3.8) $m = \sum_r m_{v_r}$ is the number of frames which may serve as a root. This number is in the present case the number of pure permutation cycles with $t = 1$ and can be written as $m = 1 + \sum_r m^{v_r}{}_{\tau'\tau}$ with $\tau' = (1,4)$ and $\tau = (1,1)$. Because values were substituted for β_ν for pure permutation cycles according to (4.10), we can no longer count directly the number of such β_ν's which contributed in the result for g_S'. However, it is easily seen that a term of g_S', which results from taking $(\bar{\sigma}_{14})^{m_{14}}$: (cf. (4.31) and (3.37)) had m_{14} factors β_ν contributing to $\sum_\nu m^\nu{}_{14}$. But it follows from the expression for F_{14}, according to (4.22), that the contributions to g_S from frames, which are not pure permutation cycles with $t = 1$, cancel, so that: $\sum_r m^{v_r}{}_{14} = \sum_\nu m^\nu{}_{14}$ and $m = m_{14} + 1$, for the terms in the result for g_S' obtained by taking $(\bar{\sigma}_{14})^{m_{14}} : \exp[\sigma_{14} F_{14}]$.

We now introduce a new (auxiliary) variable ξ_{11} in the expression for G_{11} by replacing $(1 + y_{14})$ (in the part of the expression for G_{11} after the :) by $(1 + y_{14})\xi_{11}$. The notation (3.18) is also used for the variable ξ_{11}. We note that if $A(y) = \sum_k a_k (1 + y)^k$, we may put here $A(y) = \sum_{l \geqslant 0} \xi^l$: $\bar{A}(y, \xi)$

with $\bar{A}(y, \xi) = \sum_k a_k(1 + y)^k \xi^k$. We make further use of the relation ($l_{11} \geqslant 0$; the factor m^{-1} is added)

$$[(m_{14})!\,(m_{14}+1)^{-1}(y_{14})^{m_{14}}(\bar{\sigma}_{14})^{m_{14}}] : (1+y_{14})^{l_{11}} n_1 (1 - e^{y_{11}}) \exp[\sigma_{14} F_{14}(y_{11})] =$$

$$= [(m_{14}+1)!\,(y_{14})^{m_{14}+1}\,(\bar{\sigma}_{14})^{m_{14}+1}] : (1+y_{14})^{l_{11}+1}\,(l_{11}+1)^{-1} n_1\, e^{y_{11}} \exp[\sigma_{14} F_{14}(y_{11})]. \quad (4.30)$$

The expression (4.27) is now reduced to (replacing $(m_{14}+1)$ by m_{14})

$$(gs)_{II,t=1} = \sum_{l_{11}\geqslant 0} [(l_{11}+1)^{-1}(\xi_{11})^{l_{11}}:] \sum_{m_{11}\geqslant 1} [(m_{11}-1)!\,(y_{11})^{m_{11}-1} : (\bar{\sigma}_{11})^{m_{11}}:] \sum_{m_{14}\geqslant 1} [(m_{14})!\,(y_{14})^{m_{14}} : (\bar{\sigma}_{14})^{m_{14}}:]\, n_1\, e^{y_{11}}\,(1+y_{14}) \exp\{\sigma_{11} \sum'_{\{i_{t1}\}} i_{11} [e^{y_{11}}(1+y_{14})\xi_{11}]^{i_{11}-1} \beta\{i_{t1}\} + \sigma_{14} F_{14}(y_{11})\}. \quad (4.31)$$

The summation $\sum'_{\{i_{t1}\}}$ in (4.31) is over all sets $\{i_{t1}\}$, for which $\sum_t i_{t1} \neq 0$.

III, $t = 1$. For calculating the contribution $g_{III,t=1}$, we shall first give a somewhat modified expression for g_S. In the derivation of (3.39), we have dissociated the graph by choosing as root a frame, v_r, of a certain type, $\{v_r\}$. In a similar way, one can start by choosing as root *bolts* of certain types, t_r ($r = 1. \ldots$), specified by a given set of t-values, $\{t_r\}$. The dissociated arrangement then consists of one separate bolt (the root) and frames, which *all* have one hole in this case. The further derivation in this case, is quite analogous to § 3 and the result for g_S' can be written in the same form as (3.39), if we omit the term corresponding to $\prod_\tau [y_{\tau\tau}{}^0]$: (as it would correspond to a bolt without a hole) and replace the function F by a similar function, $\bar{F}$. The function $\bar{F}$ is given by

$$\bar{F}(y_{\tau'\tau'}) = \sum_r n_{t_r} h_{t_r}(y_{\tau'\tau'}), \quad (4.32)$$

$$h_t(y) = \sum_{\{\lambda_{\tau'}\}} n_t\{\lambda_{\tau'}\} \prod_{\tau'} [(y_{\tau'})^{\lambda_{\tau'}}/(\lambda_{\tau'})!]. \quad (4.33)$$

$n_t\{\lambda_{\tau'}\}$ denotes the number of ways that a set of holes, specified by $\{\lambda_{\tau'}\}$, can be bolted together with a bolt of character t. To pass from g_S' to g_S, one has to add a factor $L^{-1} = (\sum_r l_{t_r})^{-1}$ in each term (cf. (3.8)), L specifying the number of bolts which may serve as a root. The factor L^{-1} can be calculated for each term, if one notes that l_t (being the number of bolts of the type t) is equal to the power of ξ_t in such a term, if we replace f_τ and h_t by $\xi_t f_\tau$ and $\xi_t h_t$, respectively ($\tau = (t, a)$; cf. e.g., the expression (3.23) where it is seen that the number of f_τ-factors is also the number of t-bolts in the frame, if $\tau = (t, a)$).

We shall apply these formulae to the graphs, specified in *III*, $t = 1$. However, we use (4.32) and (4.33) in this case, still with a modification in the following sense: as roots we choose bolts of the type $t = 1$ which are not contained in a $\tau = (1,2)$ or $\tau = (1,3)$ hole, hence *not* any bolt of type $t = 1$. The function $\bar{F}$ is then obtained from (4.33) by putting $t = 1$ and restricting

the summations to sets $\{\lambda_{\tau'}\}$ with $\lambda_{\tau'} \geqslant 1$ for $\tau' = (1,1)$ and $\lambda_{\tau'} = 0$ for $\tau' \neq (1,1)$. It is again possible to combine the indices $a = 2$ and $a = 3$, as far as the holes are concerned, to one index, 4. This follows from the fact, that there is no difference in the number of ways that $a = 2$ holes and $a = 3$ holes can be connected to a *bolt in a frame* and the fact, that the bolt, which was chosen as the root is not contained in $a = 2$ or $a = 3$ hole. In order to pass from g_S' to g_S one now has to add a factor L^{-1} in each term, L specifying the number of bolts in the graph of type $t = 1$ and not contained in a $a = 4$ hole. We shall calculate L for terms of g_S', which result from taking $(\bar{\sigma}_{14})^{m_{14}}$: (cf. (3.37) with $\tau' = (1,4)$; $\tau = (1,1)$, because there are only $\tau = (1,1)$-branches) and for which l_{11} is the power of ξ_{11} if the function f_{11} in the branches is replaced by $\xi_{11} f_{11}$ and if $\bar{F}$ is replaced by $\xi_{11}\bar{F}$. It is seen (cf. (3.23)) that l_{11} is the number of $t = 1$ bolts in the dissociated graph which are not contained in a $a = 4$ hole. The number of holes with $t = 1$ and $a = 4$ in the dissociated graph is m_{14}. It follows from the fact that these holes must be attached to bolts with $t = 1$ and $a = 1$ and the fact that only one hole of this type can be attached to such a bolt, that the number of bolts in the non-dissociated graph which can serve as a root is equal to $L = l_{11} - m_{14}$. We can therefore make use of the reduction from (4.18) to (4.22). The values of F_τ are found by taking certain parts of (4.21) and (4.22), namely leaving out the frames admitted as roots under I or II, $t = 1$.

$$\bar{F}(y,\ \xi_{11}) = n_1 \xi_{11} (e^{y_{11}} - 1) \tag{4.34}$$

$$F_{11}(y, \xi_{11}) = \sum'_{\{i_{t1}\}} i_{11}[e^{y_{11}}(1 + y_{14})\xi_{11}]^{i_{11}-1}[e^{y_{21}}(1 + y_{24})]^{i_{21}}\beta\{i_{t1}\} \tag{4.35}$$

$$F_{14}(y, \xi_{11}) = 0 \tag{4.36}$$

$$F_{21}(y, \xi_{11}) = \sum'_{\{i_{t1}\}} i_{21}[e^{y_{21}}(1 + y_{24})]^{i_{21}-1}[e^{y_{11}}(1 + y_{14})\xi_{11}]^{i_{11}}\beta\{i_{t1}\} \tag{4.37}$$

$$F_{24}(y, \xi_{11}) = n_2 (e^{-y_{21}} - 1) \tag{4.38}$$

It follows from (4.36) that the contribution of the 14-holes cancel (y_{14} and m_{14} may be put zero, hence $L = l_{11}$). The summation over m_{24} can be carried out by using (4.28), with $t = 2$, and (4.29), after which the result is independent of y_{21}, so that only the term with $m_{21} = 0$ must be conserved. One finds

$$(gs)_{III,t=1} = \sum_{l_{11}\geqslant 1} [l_{11}^{-1}(\xi_{11})^{l_{11}} :] \sum_{m_{11}\geqslant 1} [(m_{11} - 1)!\,(y_{11})^{m_{11}-1} : (\bar{\sigma}_{11})^{m_{11}} :]$$
$$n_1 \xi_{11}\, e^{y_{11}} \exp [\sigma_{11} \sum'_{\{i_{t1}\}} i_{11}\,(e^{y_{11}}\,\xi_{11})^{i_{11}-1}\,\beta\{i_{t1}\}]. \tag{4.39}$$

It is seen from (4.31), that $[(gs)_{II,t=1} + (gs)_{III,t=1}]$ is expressed by the right member of (4.31), if we extend the summation over $m_{14} \geqslant 0$. Using (4.28) with $t = 1$, one sees that, after the summation over m_{14} has been carried out (in a similar way as the summation over m_{24} for the part $(gs)_{II,t=1}$), the result is independent of y_{11}, so that only the term with $m_{11} = 1$ remains.

$$(gs)_{II,t=1} + (gs)_{III,t=1} =$$
$$= \sum_{l_{11}\geqslant 0} [(l_{11}+1)^{-1}\,(\xi_{11})^{l_{11}}] : \sum'_{\{i_{t1}\}} i_{11}\xi_{11}^{i_{11}-1}\beta\{i_{t1}\} = \sum_{\{i_{t1}\}} \beta\{i_{t1}\}, \quad (4.40)$$

where $\sum''_{\{i_{t1}\}}$ indicates a summation over all sets $\{i_{t1}\}$, with $i_{11} \neq 0$. In an entirely similar way, one finds

$$(gs)_{II,t=2} + (gs)_{III,t=2} = \sum^{*}_{\{i_{t1}\}} \beta\{i_{t1}\}, \quad (4.41)$$

where the summation extends over all sets $\{i_{t1}\}$, for which $i_{21} \neq 0$ and $i_{11} = 0$. Adding the different contributions (4.25), (4.40) and (4.41) to (4.23) and recalling the abbreviation (4.19), one finds

$$g_S = \sum_\nu \beta_\nu, \quad (4.42)$$

where the summation extends over all values of ν (ν is still an abbreviation for $\bar{\nu}$, cf. § 3) for which $\sum_t i^\nu{}_{t3} = 0$. To pass from g_S to $g_k(\boldsymbol{r}^k)$ is now very simple.

§ 5. *Discussion of the result.* In this section we want to give a discussion of the simplification of the expansion for the k-particle distribution, $g_k(\boldsymbol{r}^k)$, obtained in § 4. The general form, with which we started, was given by

$$g_k(\boldsymbol{r}^k) = (\prod_t n_t^{k_t}) \sum_{l=k}^{\infty} b_{k,l}(\boldsymbol{r}^k). \quad (5.1)$$

The simplified result, according to §§ 2, 3, 4 can be written as (cf. (4.42), (3.10), (2.6))

$$g_k(\boldsymbol{r}^k) = \sum_{\bar{\nu}} \beta_{\bar{\nu}}^{(k)} \text{ with } \sum_t i^{\bar{\nu}}{}_{t3} = 0. \quad (5.2)$$

We shall discuss the reduction for the case that the correlation factor, F, is given by (1.3), so that the graphs have h-connections (of the types $h^{(11)}$, $h^{(22)}$, $h^{(12)}$) and basis-connections (of the types $f^{(11)}$, $f^{(22)}$, $f^{(12)}$) and l-connections ($l^{(1)}$ and $l^{(2)}$). The significance of the reduction from (5.1) to (5.2) will be realized if we remember the types of graphs, which correspond to the $b_{k,l}$- and $\beta_{\bar{\nu}}$-terms, respectively:

$b_{k,l}(\boldsymbol{r}^k)$ corresponds to all *connected* graphs (reducible and irreducible) of k (k_1, k_2) basis points and $l - k$ ($l_1 - k_1$, $l_2 - k_2$) non-basis points, formed with h- and l-connections, the basis points being mutually connected by basis lines, and which do not contain any (non-basis) points with l-connections only. If we introduce $b_{k,l}(\boldsymbol{r}^k)_{id}$, defined in the same way as $b_{k,l}(\boldsymbol{r}^k)$ except that only those graphs are considered, which are *irreducible*, it is easily seen, that (cf. (2.1), (2.3) and (2.5))

$$(\prod_t n_t^{k_t})\, b_{k,l}(\boldsymbol{r}^k)_{id.} = \sum_{\bar{\nu}} \beta_{\bar{\nu}}^{(k)}, \quad (5.3)$$

if the summation in the right member of (5.3) is extended over all values of $\bar{\nu}$, for which $i^{\bar{\nu}}{}_{t1} + i^{\bar{\nu}}{}_{t2} = l_t$ and $i^{\bar{\nu}}{}_{t3} = 0$ ($t = 1,2$). We can therefore write the simplified result (5.2) as

$$g_k(\boldsymbol{r}^k) = (\prod_t n_t^{k_t}) \sum_{l=k}^{\infty} b_{k,l}(\boldsymbol{r}^k)_{id}. \quad (5.4)$$

This formulation is valid for an arbitrary correlation factor, if we use the graph representation with basis-, R- and l-connections. If $k = 0$, (5.4) equals b (cf. (4.24) and (4.32)).

We note the following points about the forms (5.2) and (5.4): (1) It is remarkable that the result is *linear* in terms corresponding to irreducible graphs, as the general form of a $b_{k,l}$ will contain *products* of different $\beta_{\bar{\nu}}$'s (cf. (2.2), (2.7)). The reduction from (5.1) to (5.4) was obtained by reordering the different terms of the $b_{k,l}$'s. The terms, which are products of more than one β_ν (and which occur with opposite signs in $b_{k,l}$'s with different values of l) all cancel (cf. Fig. 3).

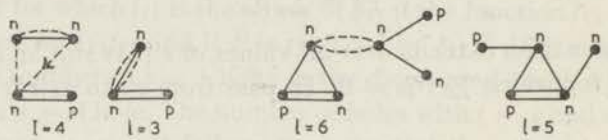

Fig. 3. Graphs corresponding to terms of $b_{k,l}$, but which cancel in the reduction to (5.4); for the notation, cf. fig. 1.

(2) If we omit the l-connections in the graphs corresponding to the $b_{k,l}(\boldsymbol{r}^k)_{id}$'s from (5.4), the resulting graphs of h- and basis-connections may be: A, irreducible; B, reducible and C, unconnected. The results given by Jastrow [4]) for g_k correspond to the type A only, the terms corresponding to the casis B and C were neglected. For an illustration of such graphs cf. Fig. 4.

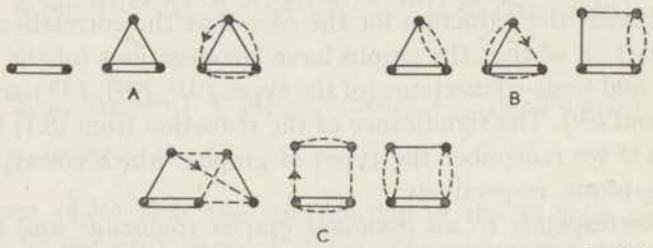

Fig. 4. Graphs, corresponding to different terms occurring in the $b_{id.}$'s of (5.4); leaving out the l-connections, we have: A, irreducible graphs; B, reducible graphs; C, unconnected graphs; for the notation, cf. fig. 1.

(3) It should be noted, that terms of $(b_{k,l})_{id}$ of the type C can be further reduced to some extent, by a further study of the momentum relations.

The equation (5.4) reduces simply to one term (n_t), in case $k_t = \sum_{t'} k_{t'} = 1$, as the only irreducible cluster with one basis point consists of just this point only. However, this result may also be written in the form of the series (5.1). We thus obtain an alternative derivation of the identity I (4.34) mentioned in I.

The reduction from (5.1) to (5.4) was derived in case of a diagonal distri-

bution function. It can be used for the calculation of the pair distribution function, which is sufficient for calculating the expectation value of the potential energy in case of two-body forces. However, for the calculation of the expectation value of the kinetic energy, the non-diagonal distribution function $g_1(\boldsymbol{r}, \boldsymbol{r}')$ is needed. Although in this case, a similar reduction occurs, we shall use the expression (5.1), to calculate a non-diagonal distribution function. In a third paper, we shall give explicit results for the distribution functions and the expectation value of the energy. In the same paper, we shall give the extension to (mixtures of) particles with spin (and isobaric spin).

It can finally be mentioned that it was also proposed by Jastrow [4]) to use cluster expansions for the case of interacting bosons, using a wave function of the form I(2.4), but without Slater determinant. The cluster expansions are then much easier than for fermions and closely analogous to the usual treatment in classical statistical mechanics. It was checked in some cases that a similar reduction as from (5.1) to (5.2) for fermions, holds also for bosons (taking as b's, terms corresponding to irreducible graphs with basis- and R-connections only) and it can be conjectured that such a reduction will hold generally for bosons and even for a mixed gas of bosons and fermions in the ground state.

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CHAPTER III

EXPRESSIENS FOR THE DISTRIBUTION FUNCTIONS AND THE ENERGY; APPLICATION TO NUCLEAR MATTER; EXPANSIONS AT LOW TEMPERATURE

Synopsis

The cluster developments for Jastrow wave functions, formulated in two previous chapters, are extended to particles with spin. Explicit results are given for the distribution functions and the energy, including the case of fermion mixtures. A discussion is given of the application of the method to nuclear matter. The splitting in a "statistical" part and a "dynamical" part can also be made for a Bose or Fermi gas at low temperature. It leads to the introduction of more detailed cluster integrals. In the fugacity expansion of the pressure and the density, they can be rearranged, roughly to increasing powers of (δ/λ) (δ, range of the forces; λ, the De Broglie wave length).

§ 1. *Introduction.* In two preceding chapters[1) 2)] (hereafter referred to as I and II) we derived cluster expansions for the ground state of interacting fermions, specified by a Jastrow wave function. The fermions were assumed to be particles without spin coordinate. The extension to real fermions can easily be made in the simple case of a Jastrow wave function, with spin dependent one-particle wave functions and a *spin independent* dynamical correlation factor, F. This extension will be made in section 2. In the same section, we shall give the explicit results for the distribution functions and the energy in case of a system, containing "spinless" fermions, fermions (with spin) and a mixture of fermions (nuclear matter), respectively. A comparison is made with the work of Iwamoto and Yamada [3)]. In section 3, a discussion of the method is given, in case it is applied to nuclear matter. In the appendix, finally, the method is applied to an imperfect Bose or Fermi gas *at low temperature*. In the evaluation of the grand partition function of such a system, the splitting in a "dynamical" part and a "statistical" part, offers the possibility to introduce more detailed cluster integrals. In the fugacity expansion of the pressure and the density, at low temperature, these cluster integrals can be ordered, roughly, to increasing powers of (δ/λ) (δ, range of the interaction; λ, the De Broglie wave length).

§ 2. *Explicit results for the distribution functions and the energy.*

a. Spinless fermions. Using the graph representation (cf. Fig. 1), introduced in § 2 of II, the terms of the cluster development can easily be written down. The first terms of the normalized pair distribution function (cf. I (2.4), I (2.12), I (2.13), I (3.25) for definitions and notations), write

$$\begin{aligned} g_2(r_{12}) = {} & n^2 R_{2,2}(r_{12})\, L_2(\boldsymbol{r}^2) + n^3 \int R_{2,3}(\boldsymbol{r}^2;\, \boldsymbol{r}_3)\, L_3(\boldsymbol{r}^3)\, \mathrm{d}\boldsymbol{r}_3 + \\ & + n^3 R_{2,2}(r_{12}) \int [R_{0,2}(r_{13})(l_{12}l_{23}l_{31} + l_{13}l_{32}l_{21} - l_{11}l_{23}l_{32}) + \\ & + R_{0,2}(r_{23})(l_{12}l_{23}l_{31} + l_{13}l_{32}l_{21} - l_{22}l_{13}l_{31})]\, \mathrm{d}\boldsymbol{r}_3 + \\ & + \tfrac{1}{2} n^4 R_{2,2}(r_{12}) \int R_{0,2}(r_{34})(l_{14}l_{41}l_{23}l_{32} + l_{13}l_{31}l_{24}l_{42} - \\ & - l_{14}l_{43}l_{32}l_{21} - l_{13}l_{34}l_{42}l_{21} - l_{12}l_{24}l_{43}l_{31} - l_{12}l_{23}l_{34}l_{41} - \\ & - l_{14}l_{42}l_{23}l_{31} - l_{13}l_{32}l_{24}l_{41})\, \mathrm{d}\boldsymbol{r}_3\, \mathrm{d}\boldsymbol{r}_4 + \\ & + \tfrac{1}{2} n^4 \int R_{2,4}(\boldsymbol{r}^2;\, \boldsymbol{r}_3,\, \boldsymbol{r}_4) L_4(\boldsymbol{r}^4)\, \mathrm{d}\boldsymbol{r}_3\, \mathrm{d}\boldsymbol{r}_4 + \ldots\ldots\ldots \quad (2.1) \end{aligned}$$

In the derivation of (2.1), we have applied the result (5.4) of II, where we proved that the graph representation of a diagonal distribution function contains only irreducible graphs.

The non-diagonal 1-distribution function, $g_1(\boldsymbol{r}_1,\, \boldsymbol{r}_1')$, which is needed in the evaluation of the kinetic energy, is given by (cf. I (2.14), I (4.33); point 1 in the graph corresponds to the coordinates $\boldsymbol{r}_1$ and $\boldsymbol{r}_1'$)

$$\begin{aligned} & g_1(\boldsymbol{r}_1, \boldsymbol{r}_1') = n l_{11} + n^2 \int R_{1,2}(\boldsymbol{r}_1, \boldsymbol{r}_1';\, \boldsymbol{r}_2)(l_{11}l_{22} - l_{12}l_{21})\, \mathrm{d}\boldsymbol{r}_2 + \\ & + \tfrac{1}{2} n^3 \int R_{0,2}(r_{23})(-l_{12}l_{21}l_{33} - l_{13}l_{31}l_{22} + l_{12}l_{23}l_{31} + l_{13}l_{32}l_{21})\, \mathrm{d}\boldsymbol{r}_2\, \mathrm{d}\boldsymbol{r}_3 + \ldots \quad (2.2) \end{aligned}$$

The function l_{ij}, in (2.1) and (2.2), is defined according to (I (3.4) and I (4.33))

$$l_{ij} = N^{-1} \sum_{\lambda=1}^{N} \mathrm{e}^{i\boldsymbol{k}\lambda \cdot (\boldsymbol{r}_i - \boldsymbol{r}_j')}. \quad (2.3)$$

If j corresponds to a non-basis coordinate, over which coordinate is integrated, one has $\boldsymbol{r}_j = \boldsymbol{r}_j'$. The same holds for a basis coordinate in case of a diagonal distribution function (cf. (2.1)). A cycle of one point contributes with a factor l_{ii}. Only in case of plane waves, spinless particles and $\boldsymbol{r}_i = \boldsymbol{r}_i'$, one has $l_{ii} = 1$ (cf. (2.3)).

The energy per particle, E, for a system of N particles and a hamiltonian

Fig. 1. Examples of graphs corresponding to terms of $b_{k,l}$ with $k = 2$ and $k = 1$, respectively. A double line represents a basis-connection, a single line represents an R-connection; a dotted line represents an l-connection, forming cycles of all possible orders; a cycle of one point, which corresponds to a l_{ii}-factor, is not indicated in the figure; in case $k = 1$ we have used the symbol * to distinguish the basis point, $(\boldsymbol{r}_1,\, \boldsymbol{r}_1')$, from the non-basis points.

(admitting k-body forces to some order in k)

$$H = \sum_i -\frac{\hbar^2}{2m}\Delta_i + \sum_k \sum_{(\boldsymbol{r}^k)} V^{(k)}(\boldsymbol{r}^k), \tag{2.4}$$

can be expressed in the distribution functions g_k, normalized according to I (2.13), as

$$E = N^{-1}\int\left[-\frac{\hbar^2}{2m}\Delta_{\boldsymbol{r}_1} g_1(\boldsymbol{r}_1, \boldsymbol{r}_1')\right]_{\boldsymbol{r}_1=\boldsymbol{r}_1'} \mathrm{d}\boldsymbol{r}_1 + \\ + \sum_{k\geqslant 2} (N(k)!)^{-1}\int V^{(k)}(\boldsymbol{r}^k) g_k(\boldsymbol{r}^k)\,\mathrm{d}\boldsymbol{r}^k. \tag{2.5}$$

In case of short range interactions and a large number N, the energy E, for the state specified by the Jastrow wave function I (2.4), is obtained by inserting the cluster developments for g_k, derived in I and II. The result is a cluster development for $E(n, \alpha)$, which is a function of the density, n, and the parameters α, specifying the dynamical correlation factor, F, in I (2.4). $E(n, \alpha)$ may be used in a variational principle, by varying α at constant density, n, in order to find the best approximate wave function for the ground state. One should note, however, that *the choice of functions* $F(\boldsymbol{r}^N, \alpha)$ *is limited* to such functions for which I (4.26) is satisfied. ($b_{0,s}$ in I (4.26) may not be replaced by $(b_{0,s})_{id.}$). The necessity of a restriction on F (besides the normalization property I (2.6)), in order to get a finite result for E_{min} was already pointed out by Emery [4]). If we may restrict ourselves to $s = 2$, this (sufficient) condition is

$$-\tfrac{1}{4} < 2b_{0,2}(n, \alpha) = N^{-1} n^2 \int R_{0,2}(r_{12})(l_{11}l_{22} - l_{12}l_{21})\,\mathrm{d}\boldsymbol{r}^2 < 1. \tag{2.6}$$

We can use the order of magnitude extimate I (4.13), in order to arrange the various terms of the cluster developments.

In case F is given by I (2.8) one can derive expressions in terms of f-, h- and l-functions (cf. I (3.25); and the definition of $b_{k,l}$ in terms of graphs, to be given in § 2*d* of this section, in case only one type of particles occurs.) The energy E, in case of two-body forces specified by a potential $V(r)$ (which may have a hard core), can now be written as

$$E(n, \alpha) = \frac{3\hbar^2}{10m} k_F{}^2 - n\frac{\hbar^2}{2m}\int\Big[f^*(r)(f''(r) + \frac{2}{r}f'(r))(1 - l^2(r)) - \\ - 2f^*(r)f'(r)l(r)l'(r)\Big]\,\mathrm{d}\boldsymbol{r} + \frac{n}{2}\int f^*(r)f(r)\,V(r)(1 - l^2(r))\,\mathrm{d}\boldsymbol{r} + \ldots \tag{2.7}$$

The dash and double dash in (2.7) indicate the first and second derivatives with respect to r, respectively. The function $l(r)$ in the two integrands of (2.7) may be replaced by I (3.5):

$$l(r) = 3\,[\sin(k_F r) - (k_F r)\cos(k_F r)](k_F r)^{-3}, \text{ with } k_F = (6\pi^2)^{\frac{1}{3}} n^{\frac{1}{3}}. \tag{2.8}$$

§ 2b. *Particles with spin.* The normalized wave function for the ground state of N non-interacting fermions (with spin), is given by

$$\Phi_0(x^N,n) = (\Omega^N N!)^{-\frac{1}{2}} \text{ Det } (\varphi_\lambda(x_j)), \tag{2.9}$$

where x_j abbreviates the place coordinate $\boldsymbol{r}_j$ and spin coordinate ξ_j; $j = 1,2, \ldots, N$. The one-particle wave functions $\varphi_\lambda(x)$ ($\lambda = 1,2, \ldots, N$ and $\lambda = (\mu, \nu)$) are

$$\varphi_\lambda(x) = e^{i\boldsymbol{k}_\mu \cdot \boldsymbol{r}} \chi_\nu(\xi), \text{ with } \langle \varphi_{\lambda'} | \varphi_\lambda \rangle = \Omega \delta_{\lambda'\lambda}. \tag{2.10}$$

The possible values of $\boldsymbol{k}_\mu (\mu = 1,2, \ldots, N/2)$ are given by I (2.2) and lie within the Fermi sphere, which has now the radius $k_F = (6\pi^2)^{\frac{1}{3}}(n/2)^{\frac{1}{3}}$; $\nu = +$ and $-$ correspond to spin up, χ_+, and spin down, χ_-, respectively.

We shall limit ourselves to wave functions for the ground state of the interacting fermions, which are of the form

$$\Phi(x^N, n) = F(\boldsymbol{r}^N, n)\, \Phi_0(x^N, n), \tag{2.11}$$

where the dynamical correlation factor $F(\boldsymbol{r}^N,n)$ is a function of the place coordinates only. The derivation in I then remains unchanged, if we replace l_{ij} everywhere by its generalization

$$\begin{aligned} l_{ij} = l(x_i, x_j') &= N^{-1} \textstyle\sum_{\lambda=1}^{N} \varphi_\lambda(x_i)\, \varphi_\lambda^*(x_j') = \\ &= \tfrac{1}{2}[\chi_+(\xi_i)\chi_+^*(\xi_j') + \chi_-(\xi_i)\chi_-^*(\xi_j')]\, (N/2)^{-1} \textstyle\sum_{\mu=1}^{(N/2)} e^{i\boldsymbol{k}_\mu \cdot (\boldsymbol{r}_i - \boldsymbol{r}_j')}. \end{aligned} \tag{2.12}$$

This replacement must also be carried out for l_{ii}, which is now no longer equal to 1.

The reduction in case of diagonal distribution functions, formulated in II, remains also valid, as one has again ($x_j = x_j'$)

$$\textstyle\sum_{\xi_j} \int l_{ij} l_{jk}\, \mathrm{d}\boldsymbol{r}_j = n^{-1} l_{ik}. \tag{2.13}$$

The results for $g_2(x_1, x_2)$ and $g_1(x_1, x_1')$ can again be written as (2.1) and (2.2), if we use (2.12) instead of (2.3) and replace $\mathrm{d}\boldsymbol{r}$ by $\mathrm{d}x = \sum_\xi \mathrm{d}\boldsymbol{r}$. The same holds for the condition I (4.26). Using these results for an $F(\boldsymbol{r}^N)$-factor specified by I (2.8) and a spin dependent two-body potential

$$V_{12} = V_S(r_{12})\, P_S^\sigma + V_T(r_{12})\, P_T^\sigma, \tag{2.14}$$

where $P_S^\sigma = \frac{1}{4} - \frac{1}{4}\boldsymbol{\sigma}_1.\boldsymbol{\sigma}_2$ and $P_T^\sigma = \frac{3}{4} + \frac{1}{4}\boldsymbol{\sigma}_1.\boldsymbol{\sigma}_2$ are the singlet and triplet projection operators, respectively ($\boldsymbol{\sigma} = \sigma_x, \sigma_y, \sigma_z$ are the usual spin operators), one finds for the energy per particle, E,

$$\begin{aligned} E = \frac{3\hbar^2}{10m} k_F^2 - \frac{n\hbar^2}{2m} \int \Big[& f^*(r)(f''(r) + \frac{2}{r} f'(r))(1 - \tfrac{1}{2}l^2(r)) - \\ & - f^*(r) f'(r) l(r) l'(r) \Big]\, \mathrm{d}\boldsymbol{r} + \\ + \frac{n}{2} \int & f^*(r) f(r) [\tfrac{3}{4} V_T(r) + \tfrac{1}{4} V_S(r) + l^2(\mathrm{r})(-\tfrac{3}{4} V_T(r) + \tfrac{1}{4} V_S(r))]\, \mathrm{d}\boldsymbol{r} + \ldots \end{aligned} \tag{2.15}$$

The function $l(r)$ in (2.15) is again given by (2.8), but now with a Fermi limit $k_F = (6\pi^2)^{\frac{1}{3}}\,(n/2)^{\frac{1}{3}}$.

§ 2*c*. *Particles with spin and isobaric spin.* In this subsection we generalize the formulation of § 2*b*, by including an isobaric spin variable indicating two types of fermions (so that we have results applicable to nuclear matter). However, we restrict ourselves to equal numbers of fermions of both types and dynamical correlations independent of spin and isobaric spin. In the next subsection (§ 2*d*) we shall treat the more general case of different densities for the different types of fermions and dynamical correlations which depend on the types of the fermions (without the use of the isobaric spin formalism). In the present case Φ_0 ia again given by (2.9), if we introduce

$$\varphi_\lambda(x) = \mathrm{e}^{i\boldsymbol{k}_\mu\cdot\boldsymbol{r}}\chi_\nu(\xi)\pi_\rho(\eta), \text{ with } \langle\varphi_{\lambda'}|\varphi_\lambda\rangle = \Omega\delta_{\lambda'\lambda}, \tag{2.16}$$

where $x_i = (\boldsymbol{r}_i, \xi_i, \eta_i)$, $i = 1,2, \ldots, N$; $\lambda = (\mu, \nu, \rho)$, $\lambda = 1,2, \ldots, N$; and $\rho = +$ and $-$ correspond to the isobaric spin functions $\pi_+(\eta)$, proton, and $\pi_-(\eta)$, neutron, respectively. The allowed values of $\boldsymbol{k}_\mu (\mu = 1,2 \ldots, N/4)$ are now such, that $k_\mu \leqslant k_F = (6\pi^2)^{\frac{1}{3}}(n/4)^{\frac{1}{3}}$. In case of a dynamical correlation factor $F(\boldsymbol{r}^N)$, *independent of* ξ^N *and* η^N, the results of I and II (e.g. (2.1), (2.2), (2.6)) can be generalized in a similar way as in § 2*b*, if we put

$$\begin{aligned} l_{ij} = l(x_i, x_j') &= N^{-1}\textstyle\sum_{\lambda=1}^{N}\varphi_\lambda(x_i)\varphi_\lambda^*(x_j') = \\ &= \tfrac{1}{4}[\chi_+(\xi_i)\pi_+(\eta_i)\chi_+^*(\xi_j')\pi_+^*(\eta_j') + \chi_+(\xi_i)\pi_-(\eta_i)\chi_+^*(\xi_j')\pi_-^*(\eta_j') + \ldots \\ &\qquad \ldots + \ldots]\,(N/4)^{-1}\textstyle\sum_{\mu=1}^{(N/4)}\mathrm{e}^{i\boldsymbol{k}_\mu\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j')}. \end{aligned} \tag{2.17}$$

Applied to the case of an F-factor of the form I (2.8) and a two-body potential

$$V = {}^1V^+(r)P_S{}^\sigma\,P_T{}^\tau + {}^3V^-(r)\,P_T{}^\sigma P_T{}^\tau + {}^1V^-(r)P_S{}^\sigma P_S{}^\tau + {}^3V^+(r)P_T{}^\sigma P_S{}^\tau, \tag{2.18}$$

the result for E takes the form

$$\begin{aligned} E = \frac{3\hbar^2}{10m}k_F{}^2 - \frac{n\hbar^2}{2m}\int\left[f^*(r)\,(f''(r) + \frac{2}{r}f'(r))(1 - \tfrac{1}{4}l^2(r)) - \tfrac{1}{2}f^*(r)f'(r)l(r)l'(r)\right]\mathrm{d}\boldsymbol{r} + \\ + \frac{n}{2}\int f^*(r)\,f(r)\,\tfrac{1}{16}\,[3\,{}^1V^+(r) + 9\,{}^3V^-(r) + {}^1V^-(r) + 3\,{}^3V^+(r) + \\ + (3\,{}^1V^+(r) - 9\,{}^3V^-(r) - {}^1V^-(r) + 3\,{}^3V^+(r))l^2(r)]\,\mathrm{d}\boldsymbol{r} + \ldots \end{aligned} \tag{2.19}$$

In (2.18) we have introduced the isobaric spin projection operators $P_S{}^\tau = \tfrac{1}{4} - \tfrac{1}{4}\boldsymbol{\tau}_1.\boldsymbol{\tau}_2$ and $P_T{}^\tau = \tfrac{3}{4} + \tfrac{1}{4}\boldsymbol{\tau}_1.\boldsymbol{\tau}_2$, where $\boldsymbol{\tau}_i(\tau_{ix}, \tau_{iy}, \tau_{iz})$ is the usual isobaric spin operator of particle i. The function $l(r)$ in (2.19) is given by (2.8) with $k_F = (6\pi^2)^{\frac{1}{3}}\,(n/4)^{\frac{1}{3}}$.

Using a different method, Iwamoto and Yamada derived an expression for E (cf. form (II.8), ..., (II.14) of ref.[3])) in case of a Serber force and an F-factor of the form I (2.8). As far as we have compared this expression for E, it is in agreement with the results derived here (although we could only

derive this expression for E from formula (I.32) of ref.[3]) by omitting the second sum or an equal part of the fourth sum in this formula). The value of $2\,b_{0,2}$ (being the first order term in the condition I(4.26)), for those values of f and n, for which Iwamoto and Yamada found E to be a minimum, is of the order: $-0{,}66 < 2b_{0,2} < -0{,}49$, in disagreement (in this approximation) with our condition (2.6). However, they have made the calculations for a diameter a of the hard core of the potential as large as $a = 0{,}6 \times 10^{-13}$ cm. Recent determinations of the nuclear potential provide a value $a \approx 0{,}4 \times 10^{-13}$ cm. For this value of a, the condition (2.6) is probably satisfied.

Emery ([4]) § 3.) noticed that certain restrictions should be applied to the trial functions $f(r)$. We have only been able to derive our cluster development under the condition I (4.26) (or (2.6) of this paper), which thus seems a natural condition to impose on $f(r)$. (That Iwamoto and Yamada do not find such a condition is only because they suppose from the beginning that a certain type of cluster development will exist.) It should also be required that $n\delta^3$ is sufficiently small (δ, distance over which $f(r)$ differes appreciably from unity) in order to have a reasonable convergence of the cluster expansion. It is plausible that some paradoxal results, indicated by Emery, occurring for certain $f(r)$-functions are eliminated by imposing these conditions on $f(r)$. However, further work on the best choice of $f(r)$, the influence of higher cluster terms and the application to nuclear matter with realistic forces (with a core radius $a \approx 0{,}4 \times 10^{-13}$ cm) remains desirable.

The part of the energy correction which is linear in n, E_1, is obtained from (2.19) by putting $l(r) = 1$ and $l'(r) = 0$. In case of a hard core potential, with diameter a, and a correlation factor

$$f(r) = 1 - (a/r)\, e^{-\alpha(r-a)} \qquad r \geqslant a,$$
$$f(r) = 0 \qquad r \leqslant 0, \tag{2.20}$$

one easily finds

$$E_1 = 4\pi n a(\hbar^2/2m)[2J/(2J+1)]\,[1 + \tfrac{1}{2}\alpha a], \tag{2.21}$$

$$2b_{0,2} = n \int (|f|^2 - 1)[1 - 1/(2J+1)]\, d\boldsymbol{r} =$$
$$= -\,4\pi n a^3[2J/(2J+1)][\tfrac{1}{3} + \tfrac{3}{2}(a\alpha)^{-1} + 2(a\alpha)^{-2}]. \tag{2.22}$$

The cases § 2*a*, § 2*b* and § 2*c* correspond to $J = 0$ ("fermions without spin"), $J = \frac{1}{2}$ and $J = \frac{3}{2}$, respectively. The result derived by Huang and Yang [5]) in this case, is obtained from (2.21) by putting $\alpha = 0$. Although E_1 is a minimum for $\alpha = 0$, one has the difficulty that $2b_{0,2}$ according to (2.22) will violate (2.6) for $\alpha \to 0$. However, for small values of n (i.e. $na^3 \ll 1$) it is easily seen that (2.6) is still satisfied for such small values of α, that the term $\frac{1}{2}\alpha a$ in (2.21) gives only a correction of the order $(na^3)^{\frac{1}{2}} \ll 1$.

§ 2*d*. *Mixture of fermions*. The normalized wave function for a system containing several (possibly more than two) types of non-interacting

fermions, is given by

$$\Phi_0(x^N) = \prod_t \Phi_0^{(t)}(x^{N_t}), \tag{2.23}$$

with $x_i(t) = (\boldsymbol{r}_i(t), \xi_i(t))$, $i = 1,2, \ldots, N_t$ and where the function $\Phi_0^{(t)}(x^{N_t})$ for each type of fermions, characterized by the index t, is given by expressions similar to (2.9) and (2.10). The number of fermions of type t, N_t, may be different for different t. This is expressed by replacing N, n and k_F in (2.9) and (2.10) by N_t, n_t and $k_{F,t} = (6\pi^2)^{\frac{1}{3}}\,(n_t/2)^{\frac{1}{3}}$, respectively.

The Jastrow wave functions for the interacting ground state, which will be studied now, are of the form

$$\Phi(x^N) = F(\boldsymbol{r}^N)\,\Phi_0(x^N), \tag{2.24}$$

where the dynamical correlation factor is a function of the place coordinates only (cf. II (1.2)). The results derived in II, for mixtures of spinless particles, remain valid in the case of fermion mixtures, if we replace the function $l_{ij}^{(t)} = l^{(t)}(\boldsymbol{r}_i, \boldsymbol{r}_j')$ everywhere by its generalization

$$\begin{aligned} l_{ij}^{(t)} &= l^{(t)}(x_i, x_j') = N_t^{-1} \textstyle\sum_{\lambda=1}^{N_t} \varphi_\lambda(x_i)\,\varphi_\lambda^*(x_j') = \\ &= \tfrac{1}{2}[\chi_+(\xi_i)\,\chi_+^*(\xi_j') + \chi_-(\xi_i)\,\chi_-^*(\xi_j')](N_t/2)^{-1} \textstyle\sum_{\mu=1}^{(N/2)} e^{i\boldsymbol{k}_\mu\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j')}. \end{aligned} \tag{2.25}$$

The values of $\boldsymbol{k}_\lambda$ for the type of fermions t lie within the Fermi sphere with radius $k_{F,t} = (6\pi^2)^{\frac{1}{3}}\,(n_t/2)^{\frac{1}{3}}$. The partial densities, n_t, may be different for different values of t. The reduction of the cluster developments for diagonal distribution functions, $g_k(x^k)$, to irreducible graphs remains also valied. A generalization of condition (2.6) (which is a sufficient condition), is now (cf. app. of I)

$$\textstyle\sum_s' s_t b_{0,s} + \sum_s'' 4 s_t\,|b_{0,s}| < (n_t/n) \text{ for each value of } t. \tag{2.26}$$

The first summation in (2.26) is extended over sets $\{s_t\}$ (s_t is the number of particles of the type t), for which $b_{0,s}$ is positive, the second summation over all sets $\{s_t\}$, for which $b_{0,s}$ is negative; $\sum_t s_t \geqslant 2$.

The result of this subsection can be applied to nuclear matter: $t = 1$, a proton; $t = 2$, a neutron. The wave function (2.24) is more general than the one treated in § 2c, because the dynamical correlation factor may depend on the nucleon type, and because n_1 and n_2 may now have different values.

We shall write down some explicit results in case of an F-factor, specified by II (1.3). We abbreviate $f^*(|\boldsymbol{r}_i' - \boldsymbol{r}_j'|)\,f(|\boldsymbol{r}_i - \boldsymbol{r}_j|)$, $f^*(|\boldsymbol{r}_i' - \boldsymbol{r}_j'|)\,f(|\boldsymbol{r}_i - \boldsymbol{r}_j|) - 1$ and $l(x_i, x_j')$ by b_{ij}, h_{ij} and l_{ij}, respectively. One should note that the functions b, and hence h, may be different in the three different cases, corresponding to a proton-proton pair: $b_{ij}^{(11)}$, a neutron-neutron pair: $b_{ij}^{(22)}$, and a proton-neutron pair: $b_{ij}^{(12)}$. It is convenient to use the graph representation, which was formulated in II for mixtures and a general F-factor. In this case, it can be formulated as:

$b_{k,l}(x^k, x^{l-k})$ is the function, corresponding to all connected graphs of l_1 protons and l_2 neutrons, formed with h-connections and l-connections,

the $(k_1 + k_2)$ basis points being mutually connected by b-connections; the $l^{(t)}$-connections should form cycles of *all possible orders* (note, that in general $l_{ij} \neq l_{ji}$ and $l_{ii} \neq 1$); points corresponding to non-basis variables (and for which we put $x = x'$) may not be connected by l-connections only. A point without l-connections contributes with a factor l_{ii} (which factor was equal to 1 for spinless particles and $\boldsymbol{r}_i = \boldsymbol{r}_i'$). In case of a diagonal distribution function, $\boldsymbol{r}^k = \boldsymbol{r}'^k$, only irreducible graphs, $(b_{k,l})_{id.}$, have to be considered.

Using this graph representation and the generalization of formula II (1.5) to non-diagonal distribution functions, one easily finds for the 1-distribution function of a proton

$$g_1^{(1)}(x_1, x_1') = n_1 l_{11}^{(1)} + n_1^2 \int h_{12}^{(11)} (l_{11}^{(1)} l_{22}^{(1)} - l_{12}^{(1)} l_{21}^{(1)}) \, dx_2 +$$
$$+ \frac{n_1^3}{2} \int h_{23}^{(11)} (- 2 l_{12}^{(1)} l_{21}^{(1)} l_{33}^{(1)} + 2 l_{12}^{(1)} l_{23}^{(1)} l_{31}^{(1)}) \, dx_2 \, dx_3 +$$
$$+ n_1 n_2 \int h_{12}^{(12)} l_{11}^{(1)} l_{22}^{(2)} \, dx_2 + n_1^2 n_2$$
$$\int h_{23}^{(12)} (- l_{12}^{(1)} l_{21}^{(1)} l_{33}^{(2)}) \, dx_2 \, dx_3 + \ldots \qquad (2.27)$$

In (2.23) we have abbreviated $\sum_{\xi_i} \int d\boldsymbol{r}_i$ by $\int dx_i$. For a neutron, one finds an expression similar to (2.27). The diagonal pair distribution functions are (cf. II (5.4))

$$g_2^{(11)}(x_1, x_2) = n_1^2 \, |f^{(11)}(r_{12})|^2 \, (l_{11}^{(1)} l_{22}^{(1)} - l_{12}^{(1)} l_{21}^{(1)}) + \ldots \qquad (2.28)$$

$$g_2^{(22)}(x_1, x_2) = n_2^2 \, |f^{(22)}(r_{12})|^2 \, (l_{11}^{(2)} l_{22}^{(2)} - l_{12}^{(2)} l_{21}^{(2)}) + \ldots \qquad (2.29)$$

$$g_2^{(12)}(x_1, x_2) = n_1 n_2 \, |f^{(12)}(r_{12})|^2 \, l_{11}^{(1)} l_{22}^{(2)} + \ldots \qquad (2.30)$$

The energy per particle, E, can be calculated with these expressions, for a hamiltonian with kinetic energy $-(\hbar^2/2m_1)\Delta$, $-(\hbar^2/2m_2)\Delta$ and two-body potentials, which may be different for different nucleon pairs.

§ 3. *Application of the cluster development method to nuclear matter.* In this section we want to discuss the application of the variational method using cluster developments to the nuclear problem. We shall also summarize a number of conclusions concerning this method resulting from our work.

The first purpose of our study was to investigate the consistency of the variational method using cluster developments, in particular for potentials, which have a hard core. Our work leads to the following conclusions:

(1) Wave functions of the Jastrow form I (2.4), I (2.8) are appropriate trial functions for a variational method, in which the $f(r_{ij})$-function represents "dynamical correlations", caused, e.g., by a hard core of a two-body potential.

(2) Expressions for the k-particle distribution function g_k and the energy E can be worked out as cluster developments (see I (4.31) for $g_k(\boldsymbol{r}^k)$ and § 2 for explicit expressions for g_2 and E). The methods, which are used are analogous to the Ursell-Mayer development of statistical mechanics,

but the simultaneous occurrence of dynamical and statistical correlations causes additional complications. The normalization factor (exp $(-\frac{1}{2}Nb)$) of the wave functions is also obtained; I(4.32).

(3) In the derivation of the cluster developments a condition I (4.26) is derived, which is essentially a condition for the f-functions, which should be satisfied if the range δ of the dynamical correlations is sufficiently small in comparison with the average mutual distance.

(4) The methods used provide a systematic way for finding the different terms of the cluster developments, also the higher order terms. The simplifications, which are obtained by introducing irreducible cluster functions are discussed in chapter II.

An attractive feature of the use of Jastrow wave functions in a variational method is that no difficulty occurs at all in the calculation of the energy for a two-body potential with a hard core, whereas an infinite result is found for the energy if simple perturbation theory (Born approximation) is used for the energy calculation.

A disadvantage of a variational method, starting with wave functions containing some parameters, is that no rigorous solutions are obtained, but only approximate solutions. One can never improve on the best approximate wave function contained in the set of wave functions taken as a starting point, so long one stays within the set.

It is therefore desirable to have a further discussion of this initial choice of wave functions. In this respect the work of Gomes, Walecka and Weisskopf [6]) is of importance. These authors discuss some properties of nuclear matter on the basis of the "independent pair model", which can be considered as a certain approximation to the Brueckner theory; they consider the "wounds" in the independent particle wave function caused by the repulsive core of the nuclear two-body potential, and show that these wounds become rather small after a certain "healing distance". It is seen further, e.g. from Fig. 4 and 5 (or 8 and 9) [6]) that the shape of the wounds is very similar for different relative momenta of the two particles. If we now want to make a comparison with the method using Jastrow wave functions, where the dynamical correlations for pairs of particles are expressed by the functions $f(r_{ij})$, it seems that the two approaches show a correspondence in the following way: the Jastrow wave functions specify the state in configuration space, if the following two approximations are made for the dynamical correlations between pairs of particles (the "wounds" in the wave function in the terminology of [6]))

(a) they are taken to be spin independent,

(b) they are taken to be momentum independent.

In view of [6]), this drastic simplification seems still rather satisfactory from a qualitative point of view.

In view of approximation (b) (momentum independent pair correlations)

it would seem reasonable also to use a wave function $\Phi = F\Phi_0$ for finite nuclei, F being the same factor I (2.8) as for infinite nuclear matter and Φ_0 being a shell model wave function (without pair correlations), in the same order of approximation.

The numerical results for the volume energy and density at the equilibrium density of nuclear matter are quite similar, calculated by the method of Gomes, Walecka and Weisskopf [6]) and with the aid of Jastrow wave functions by Emery [4]), Iwamoto and Yamada [3]) (however, a precise comparison would require new calculations, because somewhat different nuclear forces were used). The saturation property is obtained by both methods for a Serber force with hard core potential. The binding energy per nucleon is found as a difference of two large quantities (kinetic and potential energy) and is therefore not easily calculated with high accuracy. The value which is found (about 5 MeV) is substantially lower than the experimental value (about 15 MeV), probably as a result of an averaging out of the tensor force by the approximations which are made.

Summarizing, it may be said that the variational method using cluster developments is a consistent but approximate method for dealing with interacting fermions with e.g. a hard core potential, such as occurs in nuclear matter. The following might be added concerning the method:

(*a*) The result for the first approximation is quite simple and allows a qualitative (to semi-quantitative) understanding of some properties of nuclear matter such as the nuclear saturation property, as discussed along these lines by Iwamoto and Yamada [3]), Emery [4]) and Dabrowski [7]).

(*b*) Further work should show whether the approach making use of Jastrow wave functions (containing the dynamical correlations in a resonable way) provides a good and relatively simple way to obtain a qualitative (to semi-quantitative) understanding of other properties of (finite) nuclei, which depend essentially on such correlations, and where the more precise methods developed by Brueckner (and others) may only be applicable with difficulty or great complication.

Appendix

Cluster expansion for an imperfect Bose or Fermi gas at low temperatures. The cluster development for the k-particle distribution function, g_k, of a Fermi gas in the ground state, was obtained by writing the integrand of g_k, $|\Phi|^2$, as a product of two factors: (1) $|\Phi_0|^2$, being the integrand for non-interacting particles. This part was expanded into permutation cycles, which were graphically represented by means of l-connections, expressing "statistical" correlations with an effective range $k_F^{-1} \approx n^{-\frac{1}{3}}$. (2) $W = |F|^2$, describing the change in the integrand caused by the introduction of short-ranged forces. W was assumed to contain mainly "dynamical" correlations,

with a short range, δ, of the order of the range of the forces. This part was expanded into U-functions, which functions were defined by an Ursell-Mayer development and could be represented by stars. The total integrand of g_k was expanded in B-functions, corresponding to connected graphs containing l-connections as well as U-stars. The order of magnitude of a contribution, corresponding to a certain (complete) graph, could be estimated by comparing the lengths δ and k_F^{-1} (cf. I (4.13)).

Although it is quite a different problem, something analogous can be done in the cluster development of an imperfect Bose or Fermi gas, by writing the "configurational integrand" as a product of two factors: (1) the configurational integrand of such a system at the same temperature, T, but without interactions, (2) the remaining part, which part we shall again call: W. The first factor can be expanded into permutation cycles, which can be represented by l-connections between numbered points (coordinates). They express the statistical correlations between particles without interaction. The range of these correlations is given by the De Broglie wave length, λ, which depends on the temperature. The second factor, W, describing "dynamical" correlations with a range, δ say, is expanded in U-functions by means of an Ursell-Mayer development. The total integrand is expanded in B-functions, represented by connected graphs containing both "statistical' (l) and "dynamical" (U) elements. The splitting of the integrand into two factors, offers the possibility to introduce more detailed cluster integrals, b. In case $\lambda \gg \delta$, they can be rearranged, roughly to increasing powers of (δ/λ), by an order of magnitude estimate, which is similar to I (4.13). It is assumed that δ is not very temperature dependent and is of the order of the range of the forces.

The partition function, Q_N, of N particles (which are assumed to be spinless, for the sake of formal simplicity) with hamiltonian $H^{(N)} = K^{(N)} + V^{(N)}$ ($K^{(N)}$ and $V^{(N)}$: kinetic and potential energy for N particles, $\beta = 1/kT$) is

$$Q_N = \mathrm{Tr}\,[\mathrm{e}^{-\beta H^{(N)}}) = \mathrm{Tr}\,[W_N\,\mathrm{e}^{-\beta K^{(N)}}]. \qquad \text{(A. 1)}$$

The trace is taken over all, orthonormal, properly symmetrized states

$$|\boldsymbol{k}^N(\boldsymbol{r}^N) > = [\Omega^N N!(m!m_2!\ \ldots)]^{-\frac{1}{2}} \sum_P^{(N)} (\pm 1)^P \prod_{i=1}^N \mathrm{e}^{\boldsymbol{k}_{\mu_i}\cdot\boldsymbol{r}_{p_i}}. \qquad \text{(A. 2)}$$

The upper and lower sign refer to bosons and fermions, respectively; $\boldsymbol{k}_\mu = (2\pi/L)\boldsymbol{n}_\mu$ (cf. I (2.2)); m_μ, the number of momenta in the set $\boldsymbol{k}^N$ equal to $\boldsymbol{k}_\mu$ is arbitrary for bosons and 0 or 1 for fermions. If $W(\boldsymbol{r}'^N; \boldsymbol{r}^N)$ is a matrix element of the operator W, defined in (A. 1), in case of coordinate representation, we can write

$$Q_N = (N!\,\Omega^N)^{-1} \iint \mathrm{d}\boldsymbol{r}'^N\,\mathrm{d}\boldsymbol{r}^N\, W_N(\boldsymbol{r}'^N; \boldsymbol{r}^N)\, X_N(\boldsymbol{r}^N; \boldsymbol{r}'^N), \qquad \text{(A. 3)}$$

where we have abbreviated

$$X_N(\boldsymbol{r}^N;\boldsymbol{r}'^N) = A^N \sum_P (\pm 1)^P \prod_{i=1}^N l_{i,Pi}, \tag{A. 4}$$

$$l_{ij} = l(\boldsymbol{r}_i - \boldsymbol{r}_j') = A^{-1} \sum_\mu e^{i\boldsymbol{k}_\mu\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j') - \frac{\hbar^2\beta}{2m}k_\mu^2}. \tag{A. 5}$$

The normalization constant, A, in (A. 5) is such that $l(0) = 1$; putting $A = \Omega\lambda^{-3}$, one has $\lambda = (h^2/2\pi mkT)^{\frac{1}{2}}$, if T is not extremely low. The second factor is expanded in permutation cycles (sign $(\pm 1)^{s-1}$, s number of "points" in the cycle, a point, with number i now represents the coordinates $\boldsymbol{r}_i$ and $\boldsymbol{r}_i'$); W_N is expanded in U-functions, which are defined by an Ursell-Mayer development

$$W_1(\boldsymbol{r}';\boldsymbol{r}) = U_1(\boldsymbol{r}';\boldsymbol{r}) = \delta(\boldsymbol{r}' - \boldsymbol{r});$$

$$W_2(\boldsymbol{r}_1', \boldsymbol{r}_2';\boldsymbol{r}_1, \boldsymbol{r}_2) = U_1(\boldsymbol{r}_1';\boldsymbol{r}_1)\, U_1(\boldsymbol{r}_2';\boldsymbol{r}_2) + U_2(\boldsymbol{r}_1', \boldsymbol{r}_2';\boldsymbol{r}_1, \boldsymbol{r}_2); \ldots \tag{A. 6}$$

We introduce a detailed cluster function:

$B_{l,m,n}(\boldsymbol{r}'^l;\boldsymbol{r}^l)$, the function corresponding to all connected graphs of l points $(\boldsymbol{r}_1', \boldsymbol{r}_1; \ldots)$ formed with l-connections and a number of (unconnected) U_s-stars ($s \geqslant 1$), with the restriction that the number of stars with $s \geqslant 2$ is m and the number of stars with $s = 1$ is n; the l-connections should form cycles.

We put $B_l(\boldsymbol{r}'^l;\boldsymbol{r}^l) = \sum_{m,n} B_{l,m,n}(\boldsymbol{r}'^l;\boldsymbol{r}^l)$. According to the definition of W_N, X_N and B_l we can now expand (cf., e.g., the analogous formula I (3.29))

$$W_N(\boldsymbol{r}'^N;\boldsymbol{r}^N)\, X_N(\boldsymbol{r}^N;\boldsymbol{r}'^N) = A^N S'_{N(l_i)} \prod_i B_{l_i}(\boldsymbol{r}'^{l_i};\boldsymbol{r}^{l_i}) \tag{A. 7}$$

We further introduce the cluster integrals

$$b_{l,m,n} = (\Omega^{-l} A^{l-1}/(l)!) \iint \mathrm{d}\boldsymbol{r}'^l\, \mathrm{d}\boldsymbol{r}^l\, B_{l,m,n}(\boldsymbol{r}'^l;\boldsymbol{r}^l). \tag{A. 8}$$

If we assume that $W_N(\boldsymbol{r}'^N;\boldsymbol{r}^N)$ has, qualitatively, the properties of $\tilde{\delta}(\boldsymbol{r}'^N - \boldsymbol{r}^N) \exp(-\beta V^{(N)}(\boldsymbol{r}^N))$ ($\tilde{\delta}(\boldsymbol{r}'^N - \boldsymbol{r}^N)$: δ-like function of short range cf. form. (7) of ref. [8]), it follows from an order of magnitude extimate, similar to I (4.13) ($m + n - 1$ relations between the momenta $\boldsymbol{k}_\mu$, orthogonality of the plane waves, normalization of (A. 5)), that for a large volume Ω and $\lambda \gg \delta$, $b_{l,m,n} \approx (\delta/\lambda)^{3(l-m-n)}$. Using standard procedures (cf. App. XI [9] and § 4[1]), one finds from (A. 3), (A. 7) and (A. 8) for the partition function, Q_N

$$Q_N = \text{coefficient of } z^N \text{ in } : \exp[A \textstyle\sum_{l,m,n} z^l b_{l,m,n}]. \tag{A. 9}$$

Hence the grand partition function, Q, is immediately found as

$$Q = \sum_{N=0}^{\infty} e^{N\mu/kT} Q_N = \exp(A \textstyle\sum_{l,m,n} z^l\, b_{l,m,n}), \tag{A. 10}$$

where z is the fugacity, $z = \exp(\mu/kT)$ (it should not be confused with the activity, $\lambda^{-3}\exp(\mu/kT)$). Each graph, corresponding to a term of $B_{l,m,n}$,

$m \neq 0$, can be obtained from a graph of $B_{l-n,m,0}$ by extending the $(l-n)$ factors l_{ij} (including $i=j$) with n points: $l_{ij} \to l_{i1}U_1(\boldsymbol{r}_1';\boldsymbol{r}_1)\,l_{1j}$; ..... The integration over these points can be carried out and one finds

$$\Sigma'_{l,n}\, z^l b_{l,m,n} = z^{l'} b^*_{l',m}(z),\ (m \geqslant 1;\ l-n=l' \geqslant 2) \qquad \text{(A. 11)}$$

where $b_{l,m}{}^*$ is defined in the same way as $b_{l,m,0}$, if each l_{ij}-factor (also for $i=j$) is replaced by

$$l_{ij}{}^* = l^*(\boldsymbol{r}_i - \boldsymbol{r}_j';\, z) = A^{-1}\,\Sigma_\mu\, \mathrm{e}^{i\boldsymbol{k}_\mu\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j')} - \frac{\hbar^2}{2m}\beta k_\mu{}^2\,(1 \mp z\ \mathrm{e}^{-\beta\frac{\hbar^2}{2m}k_\mu{}^2})^{-1} =$$

$$(= \Sigma_{s\geqslant 1}\,(\pm z)^{s-1}\, s^{-3/2} \exp\,[-\pi\,|\boldsymbol{r}_i - \boldsymbol{r}_j'|^2/s\lambda^2]). \qquad \text{(A. 12)}$$

The function $l^*(\boldsymbol{r})$ is related to the pair distribution function of non-interacting particles. The same reduction can be carried out for the part which is independent of $V^{(N)}$ ($W=1$, $U_s=0$ for $s \geqslant 2$ if $V^{(N)}=0$)

$$zb_{0,0}{}^* \equiv \Sigma_{l\geqslant 1}\, z^l b_{l,0,l} = A^{-1}\,\Sigma_{s\geqslant 1}\,\Sigma_\mu \pm (\pm z)^s\, s^{-1} \exp\,[-s\hbar^2\beta k_\mu{}^2/2m] =$$

$$(= \Sigma_{s\geqslant 1} \pm (\pm z)^s\, s^{-5/2}). \qquad \text{(A. 13)}$$

According to (A. 11) and (A. 13) the expression (A. 10) for Q reduces to

$$Q = \exp\,\{A[zb^*{}_{0,0} + \Sigma_{l\geqslant 2,m\geqslant 1}\, z^l\, b^*{}_{l,m}(z)]\}. \qquad \text{(A. 14)}$$

Using the relations $\mathrm{e}^{-\beta\omega} = Q$ and $\bar{N} = \rho\Omega = -\beta z(\partial\omega/\partial z)_{\Omega,T}$ (with $\omega = -p\Omega$), we obtain from (A. 14) for the pressure p and density ρ

$$\lambda^3 p/kT = zb^*{}_{0,0}(z) + \Sigma_{l\geqslant 2,m\geqslant 1}\, z^l\, b^*{}_{l,m}(z), \qquad \text{(A. 15)}$$

$$\lambda^3\rho = z\,\frac{\partial}{\partial z}\,[zb^*{}_{0,0}(z) + \Sigma_{l\geqslant 2,m\geqslant 1}\, z^l\, b^*{}_{l,m}(z)]. \qquad \text{(A. 16)}$$

The terms in these series contain higher powers of (δ/λ) if $(l-m)$ increases. Using the graph representation (the same as for $b_{l,m,0}$ but now with (A. 12) instead of (A. 5)), the explicit results for $b^*{}_{l,m}$ can easily be written down; e.g. $l=2$, $m=1$, where it can be reduced to

$$z^2 b^*{}_{2,1}(z) = 2^{-1}\pi^{-3} \int \mathrm{d}\boldsymbol{k} \int \mathrm{d}\boldsymbol{r}\, \frac{1}{\sqrt{2}}\,[\mathrm{e}^{+i\boldsymbol{k}\cdot\boldsymbol{r}} \pm \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}}]^*\, \Theta\, \frac{1}{\sqrt{2}}\,[\mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{r}} \pm \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{r}}], \qquad \text{(A.17)}$$

where we have introduced the relative coordinate $\boldsymbol{r}$, and abbreviated

$$\Theta = (\mathrm{e}^{-\beta H_r}\,\mathrm{e}^{+\beta K_r} - 1)\,\Sigma_{s,t\geqslant 1}\,(\pm z)^{s+t}\,(s+t)^{-3/2} \exp\,[-2st\beta K_r/(s+t)]. \qquad \text{(A. 18)}$$

($H_r = K_r + V(r)$; $K_r = -(\hbar^2/m)\Delta_r$.) We indicate how two results from the literature can be deduced as special cases from the result (A. 15):
(*a*) Putting $s=t=1$ in (A. 18) (permutations only between the two interacting particles) gives the result (8.30) of ref. [10]).

(*b*) The term which is of the first order in V, can be calculated from (A. 17) and (A. 18) by approximating $e^{-\beta Hr} e^{+\beta Kr} - 1 = -\beta V(r)$. Permutations are here taken into account to any order. Using a pseudopotential, $V(r) = 4\pi a(\hbar^2/m)\,\delta(r)\,\partial/\partial r\,(r\ldots)$, for hard spheres with diameter a, this term equals the corresponding term in form. (20) of ref.[11]).

One should be careful in the replacement of summations over $\boldsymbol{k}_\mu$ by integrations over $\boldsymbol{k}$ (cf. the expression between brackets in (A. 12) and (A. 13)). This means that the results which are given and which are of importance for quantum effects at low temperatures, need no longer be valid in the limit $T = 0$; at extremely low temperatures further developments are needed; also the difference between bosons and fermions then becomes still more important.

The classical limit, $T \to \infty$, is formally obtained by putting

$W_N(\boldsymbol{r}'^N; \boldsymbol{r}^N) = \delta(\boldsymbol{r}'^N - \boldsymbol{r}^N) \exp[-\beta V^{(N)}(\boldsymbol{r}^N)]$ and $l_{ij}^* = \delta_{ij}$ ($\lambda \to 0$: $\boldsymbol{r}_i = \boldsymbol{r}_i'$, $s = t = m = 1$ in (A. 5), (A. 12), (A. 13), (A. 15) and (A. 16)).

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SAMENVATTING

Uitgangspunt van dit proefschrift is de grondtoestand, van een fermionengas met wisselwerking van korte dracht (eventueel met afstotende pit), beschreven door een Jastrow-golffunctie. De verandering veroorzaakt door de invoering van de krachten, wordt hierbij weergegeven door een correlatiefactor voor de golffunctie van de ongestoorde grondtoestand. Deze correlatiefactor is een functie van de plaatscoordinaten der deeltjes en van een of meer variatieparameters.

In hoofdstuk I wordt, voor het geval van spinloze fermionen, een clusterontwikkeling afgeleid voor de distributiefuncties. De verkregen resultaten, die gebruikt kunnen worden voor het berekenen van de energie, zijn geldig indien aan een zekere voorwaarde, opgelegd aan de correlatiefactor, is voldaan. Deze voorwaarde beperkt de keuze van Jastrow-golffuncties indien deze worden gebruikt als probeerfuncties in een variatieprincipe.

In hoofdstuk II worden de resultaten van het eerste hoofdstuk, na uitbreiding tot mengsels van spinloze fermionen, vereenvoudigd door de invoering van irreducible clusterfuncties en het gebruik van combinatorische methoden.

De generalisatie tot deeltjes met spin wordt in hoofdstuk II behandeld. Expliciete resultaten voor de distributiefuncties en de energie worden achtereenvolgens gegeven voor fermionen, deeltjes met spin en isobarische spin, mengsels van fermionen. Dit hoofdstuk bevat tevens een bespreking van de toepassing van de methode op kernmaterie. In de appendix wordt de methode tenslotte toegepast op een Bose- of Fermigas bij lage temperatuur. De splitsing in een "statistisch" en een "dynamisch" deel leidt hier tot de fugaciteitsontwikkeling van druk en dichtheid met behulp van meer gedetailleerde clusterintegralen.

Op verzoek van de Faculteit der Wis- en Natuurkunde volgen hier enkele gegevens over mijn studie.

In 1946 legde ik het eindexamen h.b.s.-b af aan de gemeentelijke h.b.s. te Arnhem. In hetzelfde jaar begon ik mijn studie aan de universiteit te Utrecht en behaalde in april 1950 het candidaatsexamen natuur- en wiskunde (*d*). In april 1953 volgde het doctoraalexamen met hoofdvak theoretische natuurkunde en de bijvakken wiskunde en mechanica.

Vanaf september 1953 was ik werkzaam op het Instituut-Lorentz voor theoretische natuurkunde, waar ik onder leiding van Prof. Dr S. R. de Groot en Dr H. A. Tolhoek onderzoek verrichtte op kernfysisch gebied, o.m. over de kernstraling uitgezonden door gerichte atoomkernen.

Het onderzoek op het gebied van de kernmaterie, waarvan de resultaten de inhoud van dit proefschrift vormen, vond plaats in samenwerking met Dr H. A. Tolhoek.