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Franz Mohling and Charles Ray Smith

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MICROSCOPIC THEORY OF A MULTICOMPONENT SYSTEM OF CHARGED AND NEUTRAL PARTICLES

I. GENERAL QUANTUM STATISTICAL FORMULATION

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November 12, 1969

ABSTRACT

Recent contributions to the Lee-Yang-Mohling theory of single-component quantum fluids have enabled us to develop a new theory of the quantum statistics for a multicomponent nonrelativistic system of charged and neutral particles in thermal equilibrium. With the emphasis as much as possible on the physical content of the theory, this paper presents the new formulation of quantum statistics with explicit rules for calculating the grand potential and particle and photon momentum distributions. The present formalism not only simplifies and corrects an earlier version, but also it has made possible clear and systematic procedures for removing many divergencies that occur in the many-body theory of fully ionized gases.

I. INTRODUCTION

Recently, Mohling, RamaRao and Sheal developed a simple and appealing new master-graph formulation of the quantum statistical theory of a real quantum fluid in thermal equilibrium. The derivation given in MRS applied to a single-component system with short-range interactions, and Secs. II-IV of the present paper generalize that theory to apply to a multicomponent system. Our explicit use of the electromagnetic and Coulomb potentials means that our development amounts to a reformulation of the paper by Mohling and Grandy. Here, it should be mentioned that MG contains an oversight in the anlysis of the self-energy problem, and two classes of photon self-energy structures were accidentally omitted. Hence, in Sec. IV, the necessary amendments to MG are made so that the missing self-energy structures [called (0,2) and (2,0) structures] can be included. It turns out that (0,2) and (2,0) structures have a critical bearing on the calculations given in the following paper. In MRS the existence of (0,2) and (2,0)structures is tantamount to high quantum mechanical degeneracy in Bose fluids (which occurs at extremely low temperatures); it is interesting to note that these structures are important (for photons) in ionized gases at all temperatures.

It seems characteristic of any many-body theory to be plagued by divergencies and spurious results, and the present formalism is not without such features. In the present case our understanding of quantum electrodynamics allows us to take cognizance of prospective troublesome features of the theory. Thus, from the beginning we address ourselves

to the tasks of mass-renormalization, of cancelling the infrared divergence and of summing the so-called Coulomb ring diagrams, whereby we impose upon our theory the constraint that such problems are to be solvable in principle and in practice. Some of these problems can be treated by means of a very powerful counterterm technique used recently by Tuttle in the study of uncharged quantum fluids, and Sec. V presents the counterterm technique as it relates to the other topics in this paper.

An application of the theory given in the following paper will then make explicit use of most of the features of the present development, particularly as discussed in Sec. V.

In the next section we present some background material which is important for our subsequent discussion.

II. PRELIMINARY DISCUSSION

The investigations described herein apply to a volume Ω of charged and neutral particles (with no internal states) in thermal equilibrium--periodic boundary conditions are employed, and eventually the infinite-volume limit will be imposed. The system is considered to be multicomponent, and the constituent particles are labeled by Greek letters $\alpha, \beta, \eta, \cdots$ (the symbol γ is reserved exclusively for photons). All particles are treated as point particles with mass, charge and spin (where applicable), but spin-dependent interactions are not considered. For most of the subsequent analysis it is not necessary to specify the constituents of the system; however, we assume always that photons, electrons and heavy ions are present. We complete the definition of our nonrelativistic system by the specification of the Hamiltonian. In standard notation, the N-particle Hamiltonian is

$$H = H_{rad} + \sum_{i=1}^{N} \frac{1}{2M_{i}(0)} \left(p_{i} - \frac{eZ_{i}}{c} A_{i} \right)^{2} + \frac{1}{2} \sum_{\substack{i,j=1\\i \neq j}}^{N} \frac{Z_{i}Z_{j}e^{2}}{r_{i,j}}$$
(2.1)

$$= H_{0} + V_{1\gamma} + V_{1\gamma}^{\dagger} + V_{2\gamma} + V_{2\gamma}^{\dagger} + V_{2}$$

$$= H_{0} + V_{\gamma} + V_{2} = H_{0} + V . \qquad (2.2)$$

In Eq.(1.1) the label i runs over all particle labels (except photons) and all particles of each type. Since photons (and later, quasiparticles) are continually annihilated and created, it is desirable to remove the dependence of the Hamiltonian on particle number by the use of Fockspace methods. (This also means that the grand canonical ensemble will be employed.) Thus, using the number representation (corresponding to the single-particle momentum representation) we write

$$H_0 = \sum_{\alpha} \sum_{\underline{k}^{\alpha}} w^{(0)}(\underline{k}^{\alpha}) a^{\dagger}(\underline{k}^{\alpha}) a(\underline{k}^{\alpha}) \qquad (2.3)$$

$$V_{1\gamma} = \sum_{\substack{\alpha \\ \alpha \neq \gamma}} \sum_{\substack{k_1, k_2, k_3, \gamma \\ (2.4)}} a^{\dagger}(\underline{k_1}^{\alpha}) \langle \underline{k_1}^{\alpha} | V_{1\gamma} | \underline{k_2}^{\alpha} \underline{k_3}^{\gamma} \rangle \ a(\underline{k_2}^{\alpha}) \ a(\underline{k_3}^{\gamma})$$

$$v_{2\gamma} = \sum_{\substack{\alpha \\ \alpha \neq \gamma}} \sum_{\substack{k_1^{\alpha}, k_2^{\alpha}, k_3^{\gamma}, k_4^{\gamma}}}$$

(2.5)

$$v_{2} = \frac{1}{2} \sum_{\substack{\alpha \beta \\ \alpha \neq \gamma \\ \beta \neq \gamma}} \sum_{\substack{k_{1}^{\alpha}, k_{2}^{\beta}, k_{3}^{\alpha}, k_{4}^{\beta} \\ \beta \neq \gamma}} a^{\dagger}(\underline{k_{1}}^{\alpha}) a^{\dagger}(\underline{k_{2}}^{\beta})$$

$$\chi \langle \underline{k}_{1} \overset{\alpha}{\sim}_{2}^{k} | \underline{v}_{2} | \underline{k}_{3} \overset{\alpha}{\approx}_{\underline{\mu}}^{\beta} \rangle \ a(\underline{k}_{\underline{\mu}}^{\beta}) \ a(\underline{k}_{3}^{\alpha}) , \qquad (2.6)$$

where the notation k^{α} includes spin degrees of freedom with each momentum state. In Eq.(2.3) the sum is over all particles and photons, and the (undressed) free-particle energy-momentum relations are

$$w^{(0)}(k^{\alpha}) = \frac{\hbar^2(k^{\alpha})^2}{2M_{\alpha}(0)}$$
 for particles,

=
$$\hbar ck$$
 for photons $(\alpha = \gamma)$.

In Eq.(2.6) if α and β are charged particles then V_2 is understood to be the Coulomb potential; otherwise, V_2 is assumed to be a short-range potential.⁵

We next introduce the interaction picture by means of the operator

$$W(\beta) = e \qquad e \qquad (2.8)$$

where β is (κT)⁻¹, κ is the Boltzmann constant and T is the absolute temperature; then, we express the grand partition function in terms of this operator and apply to the resulting mathematical expressions the Ursell expansion. If we apply Lee and Yang's analysis⁶ of the combinatorial problem we arrive readily at expansions in terms of the so-called primary graphs. In the primary graphs the line factors (or, equivalently, the 1-vertex functions) are

$$\beta[g_{\alpha} - w^{(0)}(k_{\alpha})]$$

$$\epsilon_{\alpha} e \qquad (2.9)$$

where ϵ_{α} = +1 if α symbolizes a Boson and ϵ_{α} = -1 if α symbolizes a Fermion. A partial summation over 1-vertices leads to the replacement of the line factor in Eq.(2.9) by the new line factor $\epsilon_{\alpha}v_{\alpha}(k)$, where

$$v_{\alpha}(\underline{k}) = \{\exp \beta[w_{\alpha}^{(0)}(\underline{k}) - g_{\alpha}] - \epsilon_{\alpha}\}^{-1}$$
 (2.10)

is the free-particle momentum distribution, and the associated graphs are called contracted graphs. In Eqs. (2.9) and (2.10) g_{α} is the partial thermodynamic (or chemical) potential for α -type particles, and $g_{\gamma} = 0$. If now Eqs. (2.3)-(2.6) are introduced explicitly into the formalism then a new expansion, known as the linked-pair expansion, can be derived. Finally, the very complicated analysis in MG, of the self-energy structures in the linked-pair expansion, leads to the master-graph formulation of quantum statistics.

The developments discussed in the preceding paragraph all involve the free-particle momentum distribution in an intimate way. It is well appreciated that the true momentum distribution for interacting particles may deviate considerably from the free-particle momentum distribution. Hence, in place of the theory in which one must correct the free-particle momentum distribution, Lee and Yang expended considerable effort to introduce a theory in terms of new line factors which were related more closely to the true momentum distribution. Because practical calculations with the resulting theory were difficult and cumbersome, the Lee and Yang analysis was still unsatisfactory—Mohling's formalism also did not eliminate this unattractive feature.

Mohling, RamaRao, and Shea¹ realized that the way to avoid the undesirable features of the free-particle momentum distribution is to avoid this distribution from the beginning--that is, do not sum over the 1-vertices in the primary graphs. If then the primary graphs, with the line factor given by Eq.(2.9), are used as a basis for the linked-pair expansion, several very desirable features arise: the analysis of the self-energy problem is enormously simplified, and the ensuing integral equations for the new line factors are not only simplified but also reduced in number. Of course, the point can be made that the 1-vertices, being self-energy structures (of a very simple type), might best be included in the summation of all self-energy structures--this is indeed the case. Because the ensuing MRS formalism is both clear and straightforward, it is susceptible to much more penetrating analyses than were the other theories. In particular Tuttle³ has developed a counterterm (or a Hartree-Fock) technique which affords a new and simple

scheme for analytically continuing the theory when it is necessary to change the region of convergence. Moreover, the counterterm technique can be adapted easily to various renormalization programs. This technique can be applied readily to the present formalism for fully-ionized gases, in which we must develop specialized schemes for mass renormalization, for cancelling the electromagnetic infrared divergence and for solving the one-particle self-energy problem (see the following paper).

III. PRIMARY LINKED-PAIR (μ, ν) GRAPHS

In this and the next section we discuss the modifications of MRS necessary to adapt that theory to apply to a system of charged as well as neutral particles; also, we indicate the revisions of MG brought about by the developments in MRS. The discussion will be qualitative, since most technical detail can be filled in with the aid of MRS and MG. Also, in the interest of keeping this paper to a reasonable length, we do do not include the generalizations of the diagrammatic rules for primary graphs given in MRS. This is especially appropriate since our generalized master graphs of Sec. V embrace all of the diagrams given in MRS and MG, and these graphs are the only ones used in practice.

The linked-pair graphs using line factors based on the statistical factor in Eq. (2.9) rather than the free-particle momentum distribution in Eq. (2.10) are called primary linked-pair (μ,ν) graphs. A primary linked-pair (μ,ν) graph is defined to be a graphical structure consisting of P cluster vertices and P_x x-vertices [corresponding to the statistical factor in Eq. (2.9)] which are entirely interconnected by m internal wiggly lines; attached to the entire structure are μ outgoing external solid lines and ν incoming external solid lines. The self-energy analysis (in the next section) is greatly simplified if we define primary linked-pair (μ,ν) graphs to have no line factors; thus, the statistical factor in Eq. (2.9) is to be associated with the x-vertex. Photon lines representing strictly zero momentum are to be excluded from diagrams, since such photons correspond to vacuum interactions (and the sum of all such contributions can be shown to be zero). The rules for interconnecting the P + P_{\times}

vertices and for associating with the graph the appropriate mathematical expression can be generalized from the corresponding rules in MRS.

It is in order, here, to point out that a major error in MG originates in the assumption that $\mu=\nu$ for photon lines. This assumption implies (incorrectly) that diagrams containing structures with only two incoming or only two outgoing photon lines cannot occur. Moreover, the self-energy analysis in MG is incomplete since such (0,2) and (2,0) self-energy structures have not been summed.

In applications of quantum statistics one is interested in thermodynamic functions, momentum distributions, pair-correlation functions and so forth. In this paper we concern ourselves only with techniques for calculating thermodynamic functions and momentum distributions (defined below). Thermodynamic functions can be calculated directly from the grand potential by partial differentiation. For example, if f is the grand potential and Ω is the volume of the system, then the pressure $\mathcal P$, the average particle number $\langle N_{\mathcal Q} \rangle$, the particle density ρ , the average energy $\langle E \rangle$ and the average entropy $\langle S \rangle$ can be calculated as follows:

$$\mathcal{P} = \beta^{-1} \partial(\Omega f)/\partial\Omega = \beta^{-1} f , \qquad (3.1)$$

$$\langle N_{\alpha} \rangle = \beta^{-1} \, \partial(\Omega f) / \partial g_{\alpha} \quad , \tag{3.2}$$

$$\rho = \langle N \rangle / \Omega = \sum_{\alpha} \langle N_{\alpha} \rangle / \Omega = \beta^{-1} \sum_{\alpha} \partial f / \partial g_{\alpha} , \qquad (3.3)$$

$$\langle E \rangle = G - \partial(\Omega f)/\partial \beta , \qquad (3.4)$$

$$\langle s \rangle = \partial(\beta^{-1}\Omega f)/\partial T$$
 , (3.5)

where $G = \sum_{\alpha} \langle N_{\alpha} \rangle_{g_{\alpha}}$ is the Gibbs potential. Thus, as far as these thermodynamic quantities are concerned, we need concentrate only on the calculation of the grand potential.

The basic definition of the grand potential is

$$\Omega f(\beta, g_{\alpha}, \Omega) = \ln Tr\{exp[\beta(G - H)]\}$$
 (3.6)

where H is the Hamiltonian in Eq. (2.2) and Tr indicates the trace in Fock space. The momentum distribution $\langle n_{\alpha}(\underline{k}) \rangle$ (which is the average number of α -type particles with momentum \underline{k}) is defined by

$$\langle n_{\alpha}(\underline{k}) \rangle = \text{Tr}\{a^{\dagger}(\underline{k}^{\alpha}) \ a(\underline{k}^{\alpha}) \ \exp(-\Omega f) \ \exp[\beta(G - H)]\}$$

$$= -\beta^{-1}[\delta/\delta \ w(\underline{k}^{\alpha})]\Omega f|_{V} . \qquad (3.8)$$

In terms of primary linked-pair (u,v) graphs the grand potential is given by

$$\Omega f(\beta, g_{\alpha}, \Omega) =$$
 all different primary linked-pair (0,0) graphs

and the momentum distribution for α-type particles is given by

$$\langle n_{\alpha}(\underline{k}) \rangle = e^{\beta \left[g_{\alpha}^{=w_{\alpha}}(0)(\underline{k})\right]} \left\{ 1 + \epsilon_{\alpha} \right\} \left[\text{all different primary} \\ \text{linked-pair (1,1) graphs} \right]_{\underline{k}^{\alpha}} \right\},$$
(3.10)

where in Eq. (3.10) the momentum k^{α} is the momentum preassigned to the external solid lines. One notes that the expression in Eq. (3.10) for the momentum distribution for real systems differs significantly from the free-particle momentum distribution due to contributions from the expression in the brackets. By performing the temperature integrals associated with the x-vertices and then summing over all possible x-vertices, one can show that Eqs. (3.9) and (3.10) reproduce the linked-pair expansion of Ml and its generalization in MG.

The primary linked-pair expansion or the linked-pair expansion is neither the logical completion of nor the most powerful form of the Lee-Yang formulation of quantum statistics. In particular, the Lee-Yang program needed to be extended so as to include a self-energy analysis. Such a self-energy analysis of the theory was formulated by Mohling (M2), the result being the viable master-graph formulation of

quantum statistics. The original analysis of the self-energy problem by Mohling (M2 and MG) was, unfortunately, extremely complicated. Thus, it is important that, in the next section, we generalize the simpler self-energy analysis of MRS to multicomponent systems with charged particles.

IV. ANALYSIS OF THE SELF-ENERGY STRUCTURES

In this section we generalize MRS to a multicomponent system of charged and neutral particles and formally sum all self-energy and improper structures. It is our purpose to improve the incomplete and complicated self-energy analysis in MG, as regards (0,2) and (2,0) photon.self-energy structures. Our presentation is qualitative and only a minimal amount of formal detail is given; however, we attempt to provide a sound basis for the comprehension of the generalized master graph theory which evolves from the self-energy analysis.

which can be removed from a diagram by cutting one or two internal lines are called self-energy structures. Self-energy structures are always linked-pair (1,1), (0,2) or (2,0) graphs, where we emphasize again that (0,2) and (2,0) structures have only photon external lines. In linked-pair (μ,ν) graphs it is possible to sum all self-energy structures and to relegate the effect of the summation of these structures to line factors. We accomplish this summation procedure formally by eliminating all improper graphical structures.

An improper linked-pair (μ,ν) graph is one which can be separated into two graphs by cutting one internal line, where one of the two subgraphs is itself a (1,1), (0,2), or (2,0) structure. A proper graph is a graph which is not improper. We now perform a summation which will

result in proper graphs with no self-energy parts (such graphs are

called irreducible graphs).

In primary linked pair (u.v) graphs, graphical structures

Except for a wiggly line the most primitive self-energy structure contains precisely one x-vertex and two external lines--chains of these structures are also self-energy structures. We include x-vertices in our program of summing self-energy structures. More generally, there occur (μ, ν) self-energy structures with μ outgoing and ν incoming lines such that $\mu + \nu = 2$.

Conservation of momentum requires that the external lines of (1,1) structures have the same momentum and that the external lines of (0,2) or (2,0) (photon) structures have momenta equal in magnitude and oppositely directed.

The fruition of our program of summation of all self-energy structures, or improper parts, will be primary master (μ, ν) graphs [and generalized master (μ, ν) graphs in the next section] which contain line factors instead of self-energy parts. While primary master (μ, ν) graphs can be set in one-to-one correspondence, for $(\mu, \nu) = (1, 1)$, with the master graphs defined in MG, it will become clear subsequently that the new treatment of the self-energy problem involves integral equations for these graphs which are simpler and fewer in number.

We begin our analysis by introducing the quantity $L_{\mu,\nu}(t_2,t_1,k^{\alpha})$ which is defined

$$L_{\mu,\nu}(t_2,t_1,k^{\alpha}) = \begin{bmatrix} \text{all different primary} \\ \text{linked-pair } (\mu,\nu) \text{ L-graphs} \\ k^{\alpha} \end{bmatrix}$$

In Eq. (4.1) the term primary linked pair (μ, ν) L-graph has been introduced, and, since the term L-graph will be used in other contexts,

we give here the definition of a general (μ, ν) L-graph. Corresponding to any given (μ, ν) graphs, $(\mu, \nu) \not= (0, 0)$, we define a (μ, ν) L-graph to be a graph with the same structure and rules as the given (μ, ν) graph with the following exceptions:

- (a) the external lines will be treated diagrammatically like wiggly, instead of solid, internal lines with pregiven momenta;
- (b) a temperature label $t(t \le \beta)$ is assigned to the head end of each outgoing external line (if any); and
- (c) the integration over the temperature label of any vertex to which is attached an incoming external line (if any) is not performed.

On the right-hand side of Eq. (4.1), whenever (0,2) L-graphs have both external lines attached to the same vertex then a factor of $\delta(t_2-t_1)$ is to be included in the corresponding term.

Now, we define the line factor $G_{\mu,\nu}(t_2,t_1,k^{\alpha})$ in terms of $L_{\mu,\nu}(t_2,t_1,k^{\alpha})$ by the equation

$$G_{\mu,\nu}(t_2,t_1,k^{\alpha}) = \delta(t_2^{(-)}-t_1) \delta_{\mu,\nu} + \epsilon_{\alpha}L_{\mu,\nu}(t_2,t_1,k^{\alpha}) , \qquad (4.2)$$

where the delta function represents a single internal wiggly line (and the dummy temperature variable is removed in this case) and the presence of the $t_2^{(-)}$ requires $t_2 > t_1$ to prevent the occurrence of those wiggly line loops which are forbidden in primary linked-pair (μ, ν) graphs.

In Eqs. (4.1) and (4.2) k^{α} is the external momentum (for one of the lines and $\pm k^{\alpha}$ for the other), and always $\mu + \nu = 2$.

The summation of all self-energy structures, including the formal elimination of all improper graphs, is most efficiently implemented by means of integral equations whose iterations produce precisely <u>all</u> primary linked-pair (μ, ν) graphs. Hence, we introduce

$$M_{\mu,\nu}(t_2,t_1,k^{\alpha}) = \begin{bmatrix} \text{all different proper primary} \\ \text{linked-pair } (\mu,\nu) \text{ L-graphs} \end{bmatrix}_{k^{\alpha}}.$$
(4.3)

Thus, $M_{\mu,\nu}(t_2,t_1,k^{\alpha})$ represents all possible proper (μ,ν) structures that can occur between two cluster vertices, except for a single internal wiggly line (which is indeed a proper structure), and this structure is taken into account by the delta function term in the definition of $G_{\mu,\nu}(t_2,t_1,k^{\alpha})$ in Eq. (4.2).

Finally, we complete this summation program by stating a set of simple coupled integral equations which interrelate the ${\rm M}_{\mu,\nu}({\rm t}_2,{\rm t}_1,{\rm k}^\alpha) \ \ {\rm and} \ \ {\rm the} \ \ {\rm L}_{\mu,\nu}({\rm t}_2,{\rm t}_1,{\rm k}^\alpha) :$

$$L_{1,1}(t_2,t_1,k^{\alpha}) = \int_{0}^{\beta} ds \left[G_{1,1}(t_2,s,k^{\alpha}) M_{1,1}(s,t_1,k^{\alpha})\right]$$

+
$$\delta_{\alpha, \gamma^{G}_{2, 0}}(t_{2}, s, k^{\alpha}) M_{0, 2}(t_{1}, s, k^{\alpha})]$$

$$L_{0,2}(t_2,t_1,k^{\alpha}) = \delta_{\alpha,\gamma} \int_{0}^{\beta} ds \left[G_{0,2}(t_2,s,k^{\alpha}) M_{1,1}(s,t_1,-k^{\alpha})\right]$$

+
$$G_{1,1}(s,t_2,k^{\alpha}) M_{0,2}(s,t_1,k^{\alpha})]$$
 (4.5)

$$L_{2,0}(t_2,t_1,k^{\alpha}) = \delta_{\alpha,\gamma} \int_{0}^{\beta} ds \left[G_{2,0}(t_2,s,k^{\alpha}) M_{1,1}(t_1,s,-k^{\alpha})\right]$$

+
$$G_{1,1}(t_2,s,k^{\alpha}) M_{2,0}(s,t_1,k^{\alpha})]$$
 (4.6)

For $(\mu, \nu) = (0,2)$ or (2,0) one can show that $G_{\mu,\nu}(t_2, t_1, k^{\alpha}) = G_{\mu,\nu}(t_1, t_2, -k^{\alpha})$ and $M_{\mu,\nu}(t_2, t_1, k^{\alpha}) = M_{\mu,\nu}(t_1, t_2, -k^{\alpha})$.

The preceding summation program is most succinctly expressed in graphical form by the identification of the $G_{\mu,\nu}(t_2,t_1,k^{\alpha})$ as line factors. Then, we achieve the so called master-graph formulation of quantum statistics as follows: first, we define master (μ,ν) L-graphs and

$$K_{\mu,\nu}(t_2,t_1,k^{\alpha}) = \sum_{P=1}^{\infty} \begin{bmatrix} \text{all different Pth-order} \\ \text{master } (\mu,\nu) \text{ L-graphs} \end{bmatrix}_{k}^{\alpha}$$

then, one can verify by iteration that

$$M_{\mu,\nu}(t_{2},t_{1},k^{\alpha}) = \delta_{\mu,\nu} \delta(\beta - t_{1}) \exp[\beta[g_{\alpha} - w_{\alpha}^{(0)}(k)] + K_{\mu,\nu}(t_{2},t_{1},k^{\alpha}), \qquad (4.8)$$

which serves to relate explicitly all proper linked-pair (μ,ν) graphs (including internal self-energy structures) and primary master (μ,ν) graphs. The rules for primary master (μ,ν) graphs and the procedures for calculating physical quantities from primary master (μ,ν) graphs can be generalized from MRS. In fact, the developments in the next section make it superfluous to enumerate further technical aspects of primary master (μ,ν) graphs.

This completes our formal development of the primary master graph theory. The theory, as it now stands, is still fraught with difficulties which probably can be resolved only by renormalization techniques or analytic continuation of the theory. Originally, the Λ -transformation was developed to overcome these difficulties. Unfortunately, the first formulation of the Λ -transformation was not only complicated, but also demanding of ones physical intuition. On the basis of the formulation in MRS it has been possible to greatly simplify and clarify the Λ -transformation. Thus, in the next section we present a reformulation of the preceding theory.

V. THE GENERALIZED MASTER GRAPH THEORY

A very tractable reformulation of the preceding theory is achieved, if one rearranges 11 the Hamiltonian in Eq. (2.2) by the addition and subtraction of one-particle operators (as with the Hartree-Fock method in perturbation theory). 12 As first observed by Tuttle, 3 the introduction of such counterterms into the preceding theory does not affect the form of the theory, except that new vertex functions must be included to take account of the contribution of the counterterms to the interaction term in the Hamiltonian. Tuttle has also shown that the new theory is identical to the so-called A-transformed theory of M2; this feature of the theory is indeed satisfactory, since a simple derivation of the A-transformed theory is now provided and various aspects of the A-transformation are thereby clarified. In this section we give the revised form of the multicomponent theory brought about by the rearrangement of the Hamiltonian; we also discuss at length the selection of the counterterms in the new theory.

We begin our analysis by rearranging the Hamiltonian in Eq. (2.2), with the addition and subtraction of a one-particle operator. Thus, we introduce the operator

$$U \equiv \sum_{\underline{k}} a^{\dagger}(\underline{k}) \ a(\underline{k}) \ u(\underline{k}) + \sum_{\underline{k}} a^{\dagger}(\underline{k}) \ a(\underline{k}) \ S(\underline{k})$$
 (5.1)

$$\equiv \sum_{\alpha} \sum_{\underline{k}}^{\alpha} a^{\dagger}(\underline{k}^{\alpha}) a(\underline{k}^{\alpha}) C(\underline{k}^{\alpha})$$
 (5.2)

and add and subtract it in the Hamiltonian:

$$H = H_O + V$$

$$= H_O + U + V - U$$

$$= H_O' + V - U , \qquad (5.3)$$

where

$$H_0' = \sum_{\alpha} \sum_{\underline{k}}^{\alpha} a^{\dagger}(\underline{k}^{\alpha}) a(\underline{k}^{\alpha}) w'(\underline{k}^{\alpha}) , \qquad (5.4)$$

and

$$w'(\underline{k}^{\alpha}) \equiv w_{\alpha}'(\underline{k}) = w_{\alpha}^{(0)}(\underline{k}) + u_{\alpha}(\underline{k}) + S_{\alpha}(\underline{k}) . \qquad (5.5)$$

It is important to realize that in Eqs. (5.1), (5.2) and (5.4) the sums range over all particle types (including photons). Thus, $u_{\alpha}(\underline{k})$ and $S_{\alpha}(\underline{k})$ depend upon the particle type, and this dependence is displayed by means of a subscript, as in Eq. (5.5). In Eq. (5.1) U consists of two parts: a part $u_{\alpha}(\underline{k})$ (discussed below) and a part $S_{\alpha}(\underline{k})$ which is to be chosen specifically to achieve mass renormalization for charged particles. Thus, we write

$$S_{\alpha}(k) = \left(\frac{h^2 k^2}{2M_{\alpha}}\right) D_{\alpha}, \qquad (5.6)$$

where

$$D_{\alpha} = 1 - M_{\alpha}/M_{\alpha}^{(0)}, \qquad (5.7)$$

and M is the experimentally observed mass (here, α refers to charged particles). With Eqs. (5.6) and (5.7) we see that for charged particles

$$w_{\alpha}^{(0)}(\underline{k}) + S_{\alpha}(\underline{k}) = \frac{\int_{\Omega}^{2} (\underline{k}^{\alpha})^{2}}{2M_{\alpha}},$$
 (5.8)

which is the correct free-particle energy.

The interaction V_{γ} in the Hamiltonian in Eq. (2.2) contains the bare mass $M_{\alpha}^{(0)}$, and thus this portion of the Hamiltonian must also be subjected to mass-renormalization. The mass-renormalization program can be completed if we rewrite V_{γ} as follows [see Eq. (2.1)]:

$$V_{\gamma} = V_{\gamma} \Big|_{M_{\alpha}(0) \to M_{\alpha}(1-D_{\alpha})^{-1}}$$
 (5.9)

with D_{α} given in Eq. (5.7). Thus, the completion of our mass-renormalization program requires the simple replacement in V_{γ} of $M_{\alpha}^{(0)} \to M_{\alpha}^{(1-D_{\alpha})^{-1}}$. Before discussing the formal aspects of the present theory, we wish to make a few comments on the nature of the other counterterm $u_{\alpha}(k)$.

First, it is important to stress that the $u_{\alpha}(k)$ are completely arbitrary: these functions may be discontinuous, temperature dependent, volume dependent and so forth. In particular $u_{\kappa}(k)$ be a sum of terms, each of which has a different physical meaning. Of course, in actual calculations one will try to identify the functions $u_{\kappa}(k)$ and $S_{\kappa}(k)$ with the objectives both to simplify calculations and to facilitate their physical interpretation. Only in the course of definite calculations can mechanisms arise for uniquely identifying and selecting the counterterms $u_{\alpha}(k)$ and $S_{\alpha}(k)$. Thus, the manner in which any arbitrariness of $u_{\alpha}(k)$ and $S_{\alpha}(k)$ can be exploited depends inherently upon the system under consideration. For example, one recognizes that entirely different rearrangements of the Hamiltonian will be useful for the low-temperature degenerate Bose system (for which $D_{\alpha} = 0$) and the high-temperature fully ionized gas. Since this paper concentrates on systems with electromagnetic interactions, it is in order to suggest how counterterms can be used in calculations of the properties of such systems.

First of all, we note that the masses involved in the Hamiltonian in Eq. (2.2) are bare masses; thus, as done above, one introduces counterterms $S_{\chi}(\underline{k})$ which correctly renormalize the mass.

Next, we point out that the theory involves the virtual emission and reabsorption of photons by charged particles (the so-called one-particle problem), and these processes lead to predictions of physical as well as spurious unphysical effects; the unphysical contributions to the theory are to be cancelled by $S_{\alpha}(k)$. With regard to the physical contributions, we point out that the electromagnetic potentials in Eqs. (2.4) and (2.5) are divergent for small photon momenta (a property known as the infrared divergence), and this feature can lead to questions of convergence of the quantum statistical theory; however, the careful summation of infinite series of selected diagrams coupled with the density of states factor usually leads to well-defined physical quantities. It does not appear that the Coulomb problem can be analyzed usefully by means of a procedure based on counterterms. In closing these introductory remarks we suggest another important application of the counterterm technique: if U is selected to contain all of the single-particle properties of V and thus V-U is made small, then one can interpret H_{\circ}^{\bullet} as describing quasiparticles whose small interaction energy is given by V-U-- this situation is also very favorable for the use of perturbation theory. Some of the applications of counterterms alluded to above will be made in the following paper.

If the Hamiltonian in Eq. (5.3) is to be used as the basis of our quantum statistical theory then one must use in place of the interaction representation defined in Eq. (2.8) a modified interaction representation defined by means of the operator

$$\beta H_0' - \beta H$$
 $W'(\beta) = e e \cdots$ (5.10)

Tuttle has shown that the Ursell expansion based on Eq. (5.10) instead of Eq. (2.8) does not significantly affect the MRS approach to the self-energy analysis. While it is straightforward to indicate systematically the modifications of the theory in the preceding section which are incurred by the use of Eqs. (5.3) and (5.10) instead of Eqs. (2.2) and (2.8), it is sufficient to concentrate on the more useful generalized master (μ, ν) graph formulation. Thus, we merely make a few comments on the procedure for arriving at the generalized master-graph theory.

First, we note that the use of Eq. (5.10) instead of Eq. (2.8) means that the single-particle energy $w_Q^{\prime}(\underline{k})$ in Eq. (5.5) appears everywhere in place of $w_Q^{(0)}(\underline{k})$ of Eq. (2.7); this replacement occurs also in the x-vertex in Eq. (2.9). Next, we observe that the interaction term V-U in Eq. (5.3) is now used in place of the interaction V in Eq. (2.2), and this produces another 1-vertex (called a Δ -vertex by Tuttle) which is treated diagrammatically like the x-vertex and can therefore appear along all lines.

In most cases one wishes to sum explicitly over all ways of inserting x-vertices into diagrams. At first sight this program might seem inconsistent with our arguments in Sec. II, where we recommended against this summation, since the resulting theory will depend upon the free-particle momentum distribution. But now, as suggested in the introductory remarks of this section it may be possible to choose

counterterms so that V-U is small and H' corresponds to realistic quasiparticle energies. If U has been thus chosen, then the factors which result from the summation of x-vertices are the quasi-particle momentum distributions $\nu_{\alpha}^{+}(\underline{k})$, where

$$\mathbf{v}_{\alpha}^{\prime}(\mathbf{k}) = \{\exp \beta[\mathbf{w}_{\alpha}^{\prime}(\mathbf{k}) - \mathbf{g}_{\alpha}] - \boldsymbol{\epsilon}_{\alpha}\}^{-1} , \qquad (5.11)$$

and the resulting theory depends upon the $\mathbf{v}_{\alpha}^{\mathbf{r}}(\mathbf{k})$ which are closely related to the true momentum distributions. The $\mathbf{v}_{\alpha}^{\mathbf{r}}(\mathbf{k})$ can be incorporated in a new vertex function for the Δ -vertex and new cluster vertex functions, called generalized vertex functions (see Fig. 1 and Appendix B).

Finally, we apply the self-energy analysis of Sec. IV and note that Δ -vertices are self-energy structures and therefore will be included in the summation of all (1,1) self-energy structures. But now, if we use Eq. (5.11), then all x-vertices will be summed. However, our discussion in Sec. II, as it relates to LY and M2, implies that the summation of 1-vertices before the self-energy analysis is ill-advised, since in M2 the use of contracted graphs (as opposed to primary graphs) led to a very complicated self-energy analysis. However, some of the intricacy of that analysis can be traced to the identification of two kinds of line factors (statistical and dynamical) which appear in several combinations in self-energy structures.

Although the initial simplification (in MRS) of the self-energy analysis was achieved by the use of primary graphs, on the basis of the simplicity and clarity of the new treatment in MRS, it is now realized that the summation of 1-vertices does not necessarily impose complications on any subsequent self-energy analysis. Here, the effects of the summation of x-vertices are relegated to vertex functions (instead of to line factors), and the self-energy analysis of Sec. IV can therefore be adopted.

After the preceding remarks it should be clear that the self-energy analysis for the present contracted linked-pair (μ,ν) graphs will result in a master-graph theory that is diagrammatically similar to the one discussed in Sec. IV. Of course, the self-energy summations now include Δ -vertices and new integral equations as well as mathematical expressions for the diagrammatic symbols are required. The new master graphs, called generalized master (μ,ν) graphs 13 (and defined in Appendix A), follow the same rules as the primary master graphs except generalized master graphs involve generalized cluster vertex functions (given in Appendix B) and new line factors. Thus, it remains for us to present the integral equations for the line factors of the generalized master graph theory; it will be seen that these integral equations provide one very general scheme for selecting counterterms.

The basic line factors for generalized master graphs are defined

$$\mathcal{G}_{\mu,\nu}(t_{2},t_{1},k^{\alpha}) = \delta(t_{2}^{(-)}-t_{1}) \delta_{\mu,\nu} + \epsilon_{\alpha} \mathcal{I}_{\mu,\nu}(t_{2},t_{1},k^{\alpha}) , \qquad (5.12)$$

where $(\mu, \nu) = (1,1), (2,0), (0,2)$, and the quantity $f_{\mu,\nu}(t_2, t_1, k^{\alpha})$ is defined below. Next, we define the functions

$$\mathcal{M}_{\mu,\nu}(t_{2},t_{1},\overset{k}{\sim}) = \epsilon_{\alpha}^{C}(\overset{k}{\sim})[\theta(t_{2}-t_{1}) + \epsilon_{\alpha}^{\nu}(\overset{k}{\sim})]\delta_{\mu,\nu} + \mathcal{K}_{\mu,\nu}(t_{2},t_{1},\overset{k}{\sim}),$$

$$(5.13)$$

where

$$\mathcal{H}_{\mu,\nu}(t_{2},t_{1},k^{\alpha}) \equiv \begin{bmatrix} \text{all different generalized} \\ \text{master } (\mu,\nu) \text{ L-graphs} \end{bmatrix}_{k^{\alpha}}$$
(5.14)

The integral equations for the line factors defined in Eq. (5.12) are now defined on the basis of the following equations:

$$\mathcal{L}_{1,1}(t_{2},t_{1},k^{\alpha}) = \int_{0}^{\beta} ds \left[\mathcal{G}_{1,1}(t_{2},s_{1},k^{\alpha}) \mathcal{M}_{1,1}(s,t_{1},k^{\alpha}) \right]$$

+
$$\delta_{\alpha,\gamma} \mathcal{G}_{2,0}(t_2,s,\underline{k}^{\alpha}) \mathcal{M}_{0,2}(t_1,s,\underline{k}^{\alpha})]$$
,

$$\mathbf{I}_{0,2}(t_2,t_1,\mathbf{k}^{\alpha}) = \delta_{\alpha,\gamma} \int_0^{\beta} ds \left[\mathcal{G}_{0,2}(t_2,s,\mathbf{k}^{\alpha},\overline{\mathcal{M}}_{1,1}(s,t_1,-\mathbf{k}^{\alpha})) \right]$$

+
$$\mathcal{G}_{1,1}(s,t_2,k^{\alpha})$$
 $\mathcal{M}_{0,2}(s,t_1,k^{\alpha})$] , (5.16)

$$\mathbf{I}_{2,0}(\mathbf{t}_2,\mathbf{t}_1,\mathbf{k}^{\alpha}) = \delta_{\alpha,\gamma} \int_0^{\beta} ds \left[\mathbf{g}_{2,0}(\mathbf{t}_2,s,\mathbf{k}^{\alpha}) \mathbf{\overline{M}}_{1,1}(\mathbf{t}_1,s,-\mathbf{k}^{\alpha}) \right]$$

+
$$\mathcal{G}_{1,1}(t_2,s,k^{\alpha}) \mathcal{M}_{2,0}(s,t_1,k^{\alpha})$$
 (5.17)

For subsequent applications it is useful to decouple formally, by means of a partial summation, the integral equation for the line factor $\mathcal{G}_{1,1}(t_2,t_1,k^7)$. This partial summation is based on the following three functions:

$$\overline{\mathcal{G}}(t_2,t_1,-k^{\gamma}) \equiv \delta(t_2^{(-)}-t_1) + \epsilon_{\alpha} \overline{\mathcal{I}}(t_2,t_1,-k^{\gamma}), \quad (5.18)$$

$$\overline{I}(t_2, t_1, -k^{\gamma}) = \int_0^{\beta} ds \, \overline{g}(t_2, s, -k^{\gamma}) \, \overline{\mathcal{M}}_{1,1}(s, t_1, -k^{\gamma}) , \qquad (5.19)$$

$$Q(t_{2},t_{1},k^{\alpha}) = \epsilon_{\alpha}^{c}C_{\alpha}(k)[\theta(t_{2}-t_{1}) + \epsilon_{\alpha}v_{\alpha}(k)] + \mathcal{K}_{1,1}(t_{2},t_{1},k^{\alpha})$$

$$+ \delta_{\alpha,\gamma} \int_{0}^{\beta} ds_{1}ds_{2} \mathcal{K}_{2,0}(t_{2},s_{1},k^{\alpha}) \overline{\mathcal{G}}(s_{2},s_{1},-k^{\alpha}) \mathcal{K}_{0,2}(t_{1},s_{2},k^{\alpha}) .$$

$$(5.20)$$

Now, in terms of the above functions, the line factors become

$$\mathcal{G}_{1,1}(t_{2},t_{1},k^{\alpha}) = \delta(t_{2}^{(-)}-t_{1}) + \epsilon_{\alpha} \int_{0}^{\beta} ds \, \mathcal{G}_{1,1}(t_{2},s,k^{\alpha}) \, Q(s,t_{1},k^{\alpha}) ,$$
(5.21)

$$\mathcal{G}_{0,2}(t_{2},t_{1},\underline{k}^{\gamma}) = \int_{0}^{\beta} ds_{1}ds_{2} \mathcal{K}_{0,2}(s_{2},s_{1},\underline{k}^{\gamma}) \mathcal{G}_{1,1}(s_{2},t_{2},\underline{k}^{\gamma})$$

$$\chi \quad \overline{\mathcal{G}}(s_{1},t_{1},-\underline{k}^{\gamma}) , \qquad (5.22)$$

$$\mathcal{G}_{2,0}(t_{2},t_{1},k^{\gamma}) = \int_{0}^{\beta} ds_{1}ds_{2} \quad \mathcal{G}_{1,1}(t_{2},s_{2},k^{\gamma}) \quad \overline{\mathcal{G}}(t_{1},s_{1},-k^{\gamma})$$

$$\chi \quad \mathcal{K}_{2,0}(s_{2},s_{1},k^{\gamma}) \quad . \tag{5.23}$$

Thus, the integral equation in Eq. (5.21) involves, in a sense, only (1,1) structures owing to the manner in which $Q(t_2,t_1,k^{\alpha})$ in Eq. (5.20) combines (0,2) and (2,0) structures. The general structures of the integral equations in Eqs. (5.20) - (5.23) is provided diagramatically by Figs. 2 and 3.

In Eqs. (5.16) - (5.23) a bar has been introduced to characterize quantities associated with -k lines, and this notation will be used henceforth. It is important to realize that such a notation is necessary, since, for a given function F(k) associated with momentum k, it may be true that

$$\overline{F}(-\underline{k}) \neq F(-\underline{k})$$

In the case of photon lines, the difference between the kernels in Eqs. (5.19) and (5.21) results in two different line factors $\mathcal{G}_{1,1}$ and $\overline{\mathcal{G}}$. For the same reason the counterterms $\overline{u}_{\gamma}(-\underline{k})$ chosen for $-\underline{k}^{\gamma}$ lines must differ from the counterterms $u_{\gamma}(\underline{k})$ chosen for $+\underline{k}^{\gamma}$ lines. For charged particle lines, the present comments are not relevant.

We have deferred until now the presentation of prescriptions for calculating the momentum distribution and thermodynamic functions. Thus, we give next the basic relations between the generalized master-graph formalism and physical quantities. In terms of generalized master (1,1) graphs the momentum distribution, defined in Eq. (3.7), is given by

$$\langle n_{\alpha}(\underline{k}) \rangle = \nu_{\alpha}'(\underline{k}) \int_{0}^{\beta} dt \, \mathcal{G}_{1,1}(\beta,t,\underline{k}^{\alpha}),$$
(5.24)

The grand potential, defined in Eq. (3.6), is given in terms of generalized master (0,0) and (1,1) graphs by the following relation:

$$\Omega f(\beta, g_{\alpha}, \Omega) = \Omega F(\beta, g_{\alpha}, \Omega) + \sum_{\alpha} \epsilon_{\alpha} \sum_{\substack{k = \alpha \\ k}} \ln[1 + \epsilon_{\alpha} v_{\alpha}^{\prime}(k)]$$

+
$$\sum_{\alpha} \sum_{\underline{k}^{\alpha}} \int_{0}^{\beta} dt \left[\mathcal{L}_{1,1}(t;t,t,\underline{k}^{\alpha}) - \mathcal{L}_{1,1}(t,t,\underline{k}^{\alpha}) \right]$$

$$+ \sum_{\alpha} \sum_{\underline{k}^{\alpha}} \epsilon_{\alpha} c_{\alpha}(\underline{k}) \int_{0}^{\beta} dt_{1} dt_{2} [\theta(t_{1} - t_{2}) + \epsilon_{\alpha} v_{\alpha}'(\underline{k})]$$

$$\chi = \mathcal{G}_{1,1}(t_2,t_1,t^{\alpha}) \qquad (5.25)$$

where

$$\Omega F(\beta, g_{\alpha}, \Omega) = \begin{bmatrix} all & different & generalized \\ master & (0,0) & graphs \end{bmatrix}$$
, (5.26)

$$\mathcal{L}_{1,1}(\tau; t_{2}, t_{1}, k^{\alpha}) = \int_{0}^{\tau} ds \, \mathcal{G}_{1,1}(\tau; t_{2}, s, k^{\alpha}) \, Q_{1,1}(\tau; s, t_{1}, k^{\alpha}) , (5.27)$$

$$Q(\tau; t_{2}, t_{1}, k^{\alpha}) = \mathcal{M}_{1,1}(t_{2}, t_{1}, k^{\alpha}) + \delta_{\alpha, \gamma} \int_{0}^{\tau} ds_{1} ds_{2} \, \mathcal{M}_{2,0}(t_{2}, s_{1}, k^{\alpha})$$

$$\chi \, \overline{\mathcal{G}}(\tau; s_{2}, s_{1}, -k^{\alpha}) \, \mathcal{M}_{0,2}(t_{1}, s_{2}, k^{\alpha}) , (5.28)$$

$$\mathcal{G}_{1,1}(\tau; t_2, t_1, k^{\alpha}) = \delta(t_2^{(-)} - t_1) + \epsilon_{\alpha} \mathcal{L}_{1,1}(\tau; t_2, t_1, k^{\alpha}),$$
(5.29)

 $\overline{\mathcal{G}}(\tau; t_2, t_1, -k^{\alpha})$ is defined in analogy with Eqs. (5.18) and (5.19), and τ satisfies the inequality $\beta \geq \tau \geq t_2$ and t_1 . Thermodynamic functions are determined from the grand potential in Eq. (5.25) by means of Eqs. (3.1) - (3.5). Explicit examples of generalized master (μ, ν) graphs, for $\mu + \nu = 2$, are given in the following paper.

The preceding developments mark the end of the presentation of the formal theory, thus fulfilling the goals of this paper. The following paper contains further theoretical developments and the explicit calculation of the photon momentum distribution. Only in the context of a specific application is it reasonable to discuss the choice of counterterms which can be made in such a way that various divergences and spurious quasi-physical effects are cancelled explicitly. However, we can present here a general procedure for choosing a certain class of counterterms. The counterterms are indeed arbitrary, and the following discussion should not be taken to mean that there are no other useful schemes for generating systematically these functions.

We direct attention to Eq. (5.21), the integral equation for the line factor $\mathcal{G}_{1,1}(t_2,t_1,k^{\alpha})$, where the explicit dependence on $Q(t_2,t_1,k^{\alpha})$ of Eq. (5.20) is to be noted. Clearly, the convergence or divergence properties of iterative solutions of this integral

equation depend quite delicately upon $Q(t_2, t_1, k^{\alpha})$. Moreover, $Q(t_2, t_1, k^{\alpha})$ depends, in a particular additive manner, upon the arbitrary functions $C_{\alpha}(k)$. Thus, the choice of $C_{\alpha}(k)$ can affect very strongly the iterative solutions of Eq. (5.21). Indeed, one attempts to choose $C_{\alpha}(k)$ such that

$$\epsilon_{\alpha}^{C}(\underline{k})[\theta(\underline{t}_{2}-\underline{t}_{1})+\epsilon_{\alpha}v_{\alpha}'(\underline{k})]$$
 (5.30)

cancels those contributions to $Q(t_2,t_1,k^{\alpha})$, originating from the second and third terms on the right hand side of Eq. (5.20), which give rise to divergences in Eq. (5.21). Of course, the form of Eq. (5.30) delimits the variety of contributions to $Q(t_2,t_1,k^{\alpha})$ which can be cancelled. 14

Now, we discuss formally a procedure for selecting counterterms which allows us to modify the line factors at an advanced stage of a calculation. From Eq. (5.20) it is clear that the following selection procedure is tenable:

(1). Calculate, in Eq. (5.20),

$$\mathcal{K}_{1,1}(t_{2},t_{1},k^{\alpha}) + \delta_{\alpha,\gamma} \int_{0}^{\beta} ds_{1}ds_{2} \, \mathcal{K}_{2,0}(t_{2},s_{1},k^{\alpha})$$

$$\chi \quad \overline{\mathcal{G}}(s_{2},s_{1},-k^{\alpha}) \, \mathcal{K}_{0,2}(t_{1},s_{2},k^{\alpha})$$
(5.31)

to any desired order.

(2). The quantity $-\epsilon_{\alpha}^{\ C}_{\alpha}(k)$ can be chosen to be any term in Eq. (5.31) which is multiplied by $[\theta(t_2 - t_1) + \epsilon_{\alpha} v_{\alpha}^{\ \prime}(k)]$ and which is otherwise independent of t_1 and t_2 .

The $\overline{u}_{\gamma}(-\underline{k})$, mentioned below Eq. (5.23), can be determined by a similar procedure based on Eq. (5.13) for the $-\underline{k}^{\gamma}$ case. Using this procedure, one can often select counterterms which lead to more convergent iterative solutions for the line factors and which also achieve the correct mass renormalization. After a selection of $C_{\alpha}(\underline{k})$, one must still examine the properties of the integral equations for the line factors to see how the iterative solutions have been affected. The quantities in Eq. (5.31) are actually functionals of the $C_{\alpha}(\underline{k})$; thus, a selection of $C_{\alpha}(\underline{k})$ on the basis of the above procedure leads in general to integral equations for the counterterms.

The above procedure for cancelling contributions to the line factors does not lead to the neglect of any contribution in the theory, since the counterterms reappear elsewhere in the theory. In particular, the counterterms reappear in the Hamiltonian as definite renormalized energies $w'_{\alpha}(k)$ (including alteration of the masses M_{α} , whose system-independent renormalization is well-known in quantum electrodynamics). In the sense that V alone leads to divergences in

the theory (thus, V is large) while V-U gives convergent results (so that V-U is small), one finds already one justification for interpreting the $w_{\alpha}^{\bullet}(k)$ as quasiparticle energies.

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APPENDIX A. RULES FOR GENERALIZED MASTER (μ, ν) GRAPHS

A Pth-order generalized master (μ, ν) graph is defined to be a graphical structure consisting of P cluster vertices (but no l-vertices), defined in Fig. 1 and Appendix B, which are entirely interconnected by m internal solid lines and to which are attached μ outgoing external solid lines and ν incoming external solid lines. Each external solid line carries a single arrow, and each internal solid line carries two arrows -- one at each end. At the head of each arrow there is a dot. If the arrow points toward a vertex this dot is identical with the vertex. Three different types of internal solid lines are possible, depending upon whether the two arrows point in the same direction, point toward each other or point away from each other. A generalized master (μ, ν) graph is irreducible and proper in the sense that the cutting of any one or two of its internal lines must not produce two (or three) disconnected graphs, at least one of which is a (1,1) (0,2) or (2,0) graph. Corresponding to each generalized master (μ, ν) graph there is prescribed an analytic term according to the following rules:

(1) To each external solid line assign a pregiven momentum with a particle label; if $(\mu, \nu) \neq (0, 0)$ the incoming particle (not photon) lines refer to the same set of particles as the outgoing lines. External lines with different momentum labels or directions are treated as distinguishable.

- (2) Two generalized master (μ, ν) graphs are different if their topological structures (including arrow directions, particle-type labels and external lines, but not including the momentum labels of internal arrows and the temperature labels which will be assigned below) are different.
- a different integer i (i=1,2,...,2m) and a corresponding momentum k_i^{α} (the possible choices of α will be fixed by the associated cluster vertices). Assign a different temperature variable t_j to each of the P cluster vertices (encircled dots) and to each of the dots which occur at the head ends of internal arrows that point away from vertices. To each dot of the outgoing external solid lines assign the temperature variable β.
- Assign to the entire graph a factor S⁻¹, where S is the symmetry number. The symmetry number is defined to be the total number of permutations of the 2m integers (assigned to the arrows of the internal lines) which leave the graph topologically unchanged (including the positions of these integers with respect to the arrows).

- (5) Associate with the entire graph the appropriate product of P cluster vertices with the momentum variable assignments of rules (1) and (3). Assign to the graph an overall sign factor $\prod_{\alpha} \epsilon^{\alpha}$, where
 - P_{α} is the parity of the permutation of the bottom row momenta of α -type particles in the vertex functions with respect to the corresponding ones in the top row.
- (6) To each <u>internal</u> solid line with arrow labels i and j assign a line factor and a momentum conserving Kronecker delta as follows:
 - $\delta_{\underline{k}_{i},\underline{k}_{j}} \mathcal{G}_{1,1}(t,s,\underline{k}_{i}^{\alpha})$ when the arrows point in the same direction,
 - $\delta_{\underline{k}_{1},-\underline{k}_{1}} \mathcal{G}_{0,2}(t,s,\underline{k}_{1}^{\gamma}) \delta_{\alpha,\gamma}$ when the arrows point toward each other,
 - $\delta_{\underline{k}_{1},-\underline{k}_{j}} = \delta_{2,0}(t,s,\underline{k}_{1}^{\gamma}) \delta_{\alpha,\gamma}$ when the arrows point away from each other,

where the temperature labels t and s correspond to those assigned by rule (3). In each case, the arrow labeled i points toward the dot labeled t.

(7) Finally, sum over the 2m internal momenta and integrate from 0 to β over the temperature variables t assigned in rule (3).

In one case the rule (5) above needs to be supplemented:

(5a) If two internal lines connect the same two cluster vertices corresponding to pair functions (whose vertices have temperature labels t_3 and t_4) and have for the associated line factor product $\mathcal{G}_{1,1}(t_3,t_1,k_1^{\alpha})$ $\mathcal{G}_{1,1}(t_3,t_2,k_2^{\beta})$,

then we must subtract the wiggly-line double bound correction

$$\delta(t_3 - t_1) \delta(t_3 - t_2) \begin{bmatrix} k_1 & k_2 \\ k_3 & k_4 \end{bmatrix} t_4$$

$$\alpha \beta$$

from the quantity

$$\mathcal{G}_{1,1}(t_3,t_1,k_1^{\alpha}) \mathcal{G}_{1,1}(t_3,t_2,k_2^{\beta}) , \begin{bmatrix} t_1^{t_2} \\ k_1 & k_2 \\ \\ k_3 & k_4 \end{bmatrix} t_4$$

$$\alpha \beta$$

which would be assigned by the above rules.

APPENDIX B. CLUSTER -VERTEX FUNCTIONS FOR GENERALIZED MASTER (μ, ν) GRAPHS

In this appendix we give the explicit expressions for the cluster vertex functions which are involved in the diagrammatic expansions of generalized master (μ,ν) graphs. It should be realized that these vertex functions have evolved directly from the interaction terms in the Hamiltonian.

The generalized cluster-vertex functions are explicitly

$$\begin{array}{c}
\begin{array}{c}
\begin{array}{c}
t_{1}t_{2} \\
\downarrow \\ k_{1} \\
\downarrow \\ k_{2}
\end{array} \\
\stackrel{k_{1}}{\approx} \\
\begin{array}{c}
\downarrow \\ k_{2}
\end{array} \\
\stackrel{k_{2}}{\approx} \\
\begin{array}{c}
\downarrow \\ k_{2}
\end{array} \\
\stackrel{k_{1}}{\approx} \\
\begin{array}{c}
\downarrow \\ k_{2}
\end{array} \\
\stackrel{k_{2}}{\approx} \\
\begin{array}{c}
\downarrow \\ k_{2}
\end{array} \\
\begin{array}{c}
\downarrow \\ \\ k_{2}
\end{array} \\
\begin{array}{c}
\downarrow \\$$

$$\times [\theta(t_{2}-t) + v_{\gamma}'(t_{2})] e^{t[w_{\alpha}'(t_{1})+w_{\gamma}'(t_{2})-w_{\alpha}'(t_{2})-w_{\gamma}'(t_{2})} \times \delta(t_{1}+t_{2}), (t_{3}+t_{4})^{\delta} t_{1},t_{3}$$

$$\times \quad e^{t[w_{\alpha}^{\prime}(\underbrace{k}_{\downarrow_{\downarrow}})-w_{\alpha}^{\prime}(\underbrace{k}_{\downarrow})-w_{\gamma}^{\prime}(\underbrace{k}_{2})-w_{\gamma}^{\prime}(\underbrace{k}_{3})]} \delta_{\underbrace{k}_{\downarrow}}, \quad (\underbrace{k}_{\downarrow}+\underbrace{k}_{2}+\underbrace{k}_{3})\delta_{\underbrace{m}_{\downarrow},\underbrace{m}_{\downarrow}}$$

(B.3)

$$\times \left[\theta(t_2 - t) + \nu_{\gamma}'(k_2)\right] \left[\theta(t_3 - t) + \nu_{\gamma}'(k_3)\right] e^{t\left[w_{\alpha}'(k_1) + w_{\gamma}'(k_2) + w_{\gamma}'(k_3) - w_{\alpha}'(k_4)\right]}$$

$$\times$$
 $\delta_{\underline{k}_{4}},(\underline{k}_{1}+\underline{k}_{2}+\underline{k}_{3})\delta_{\underline{m}_{1},\underline{m}_{4}}$

(B.4)

$$= e^{t[w_{\alpha}'(k_{3})-w_{\alpha}'(k_{1})-w_{\gamma}'(k_{2})]} \delta_{k_{3},(k_{1}+k_{2})\delta_{m_{1},m_{3}}}$$

$$(B.5)$$

$$\times \left[\theta(t_2-t) + \nu_{\gamma}'(k_2)\right] e^{t\left[w_{\alpha}'(k_1) + w_{\gamma}'(k_2) - w_{\alpha}'(k_3)\right]} \delta_{k_3}, (k_1+k_2)^{\delta_{m_1}, m_3}$$

(B.6)

$$\mathbf{x} \begin{bmatrix} \mathbf{k}_{1} & \mathbf{k}_{2} \\ \mathbf{k}_{3} & \mathbf{k}_{4} \end{bmatrix}_{t} = \theta(\mathbf{t}_{2} - \mathbf{t}) + [\theta(\mathbf{t}_{2} - \mathbf{t}_{1}) + \epsilon_{\beta} \mathbf{v}_{\beta}^{\dagger}(\mathbf{k}_{2})]$$

In Eqs. (B.2) - (B.6) $\alpha_0 = e^2(hc)^{-1}$ is the fine structure constant, and the Kronecker deltas conserve momentum and spin (m_i) is the spin projection); the photon polarization vector is represented by \hat{e}_i .

The symbol used in Eq. (B.1) is defined by

$$\begin{pmatrix} k_1 & k_2 \\ k_3 & k_4 & t \end{pmatrix} = - \left[\langle k_1, k_2 | V_c(t) | k_3, k_4 \rangle \right]$$

$$+ \epsilon_{\alpha} \langle k_1, k_2 | V_c(t) | k_4, k_3 \rangle \qquad \text{for } \alpha = \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_4, k_3 \rangle \qquad \text{for } \alpha \neq \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_3, k_4 \rangle \qquad \text{for } \alpha \neq \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_3, k_4 \rangle \qquad \text{for } \alpha \neq \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_3, k_4 \rangle \qquad \text{for } \alpha \neq \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_3, k_4 \rangle \qquad \text{for } \alpha \neq \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_4, k_5 \rangle \qquad \text{for } \alpha \neq \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_4, k_5 \rangle \qquad \text{for } \alpha \neq \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_4, k_5 \rangle \qquad \text{for } \alpha \neq \beta$$

$$= - \epsilon_{\alpha} \epsilon_{\beta} \langle k_1, k_2 | V_c(t) | k_4, k_5 \rangle \qquad \text{for } \alpha \neq \beta$$

In Eqs. (B.1) and (B.8) α and β are both charged particles and

$$< \underbrace{k_{1}^{\alpha}, k_{2}^{\beta} | v_{c}(t) | k_{3}^{\alpha}, k_{4}^{\beta}} > = \frac{\frac{4\pi Z_{\alpha} Z_{\beta} e^{2}}{\Omega q^{2}}$$

$$\text{χ exp $t[w_{\alpha}^{(0)}(k_{1}) + w_{\beta}^{(0)}(k_{2}) - w_{\alpha}^{(0)}(k_{3}) - w_{\beta}^{(0)}(k_{4})] $}$$

where V_c corresponds to the Coulomb interaction between two particles, one of charge $Z_{\alpha}e$ and the other of charge $Z_{\beta}e$; $q=k_3-k_1$ is the momentum transfer.

In Eq. (B.7) the primed bracket symbol (excluding hard-core potentials) is

$$\begin{bmatrix}
k_1 & k_2 \\
k_3 & k_4
\end{bmatrix}_{t} = \exp t[-u_{\alpha}(k_3) - u_{\beta}(k_4)] \left\{ \exp t[u_{\alpha}(k_1) + u_{\beta}(k_2)] \\
\alpha \beta
\end{bmatrix}$$

$$\alpha \beta$$

$$+ \left[-u_{\alpha}(\underline{k}_{1})-u_{\beta}(\underline{k}_{2})\right] \int_{\underline{t}_{1}}^{\underline{t}_{2}} ds \exp s\left[u_{\alpha}(\underline{k}_{1}) + u_{\beta}(\underline{k}_{2})\right]$$

$$\times \begin{bmatrix} \underline{k}_{1} & \underline{k}_{2} \\ \underline{k}_{3} & \underline{k}_{4} \end{bmatrix}, \quad (B.10)$$

where

$$\begin{bmatrix}
k_{1} & k_{2} \\
k_{3} & k_{4}
\end{bmatrix}_{t} = \langle k_{1}, k_{2} | R(t_{1}, t) | k_{3}, k_{4} \rangle$$

$$\alpha \beta + \epsilon_{\alpha} \langle k_{1}, k_{2} | R(t_{1}, t) | k_{4}, k_{3} \rangle \quad \text{for } \alpha = \beta$$

$$= \epsilon_{\alpha} \epsilon_{\beta} \langle k_{1}^{\alpha}, k_{2}^{\beta} | R(t_{1}, t) | k_{3}^{\alpha}, k_{4}^{\beta} \rangle \quad \text{for } \alpha \neq \beta$$
(B.11)

In Eq. (B.11) the operator $R(t_1,t)$ is defined

$$R(t_1,t) = -\frac{\partial}{\partial t} \exp [t_1 H_0^{(2)}] \exp [-(t_1-t)H^{(2)}] \exp [-tH_0^{(2)}],$$
(B.12)

where the superscript on $H_0^{(2)}$ and $H^{(2)}$ means "two-particle"--compare Eq. (2.1) with N=2. The operator $R(t_1,t)$ is discussed in detail in MI, and its matrix elements (called pair functions) will not be analyzed here. It is worth observing that the pair function represents the effective interaction for short-range forces and, being expressible in terms of wave functions or reaction matrices, is well-behaved even when a hard-core interaction is present. In Eq. (B.11) neither α nor β can be a photon, and the operator $R(t_1,t)$ is defined only for non-electromagnetic interactions.

REFERENCES AND FOOTNOTES

- * IRL Faculty Fellow supported jointly by Associated Western

 Universities, Inc. and the U. S. Atomic Energy Commission.
- 1. F. Mohling, I. RamaRao and D. W. J. Shea, Phys. Rev. (to be published); hereafter referred to as MRS.
- 2. F. Mohling and W. T. Grandy, Jr., J. Math. Phys. 6, 348 (1965); hereafter referred to as MG.
- 3. E. R. Tuttle (to be submitted to Physical Review); hereafter referred to as Tuttle.
- 4. The notation $M_{\underline{i}}^{(0)}$ is used for the bare mass of the \underline{i} th particle. Omission of the superscript zero means that the dressed or renormalized mass is to be used.
- 5. In this paper we concentrate on systems containing charged particles; thus, we do not discuss degenerate Bose systems (which are discussed quite adequately in MRS), nor do we discuss the short-range interaction, since this case is treated in Ml (see Footnote 7) and MRS. Moreover, it seems unrealistic to include the possibility of Bose-Einstein condensation in a fully ionized gas. For the sake of completeness, the pair function is included in/the definitions of the generalized vertex; however, explicit rules to prevent the occurrence of forbidden wiggly-line double bonds are not given here (see MRS).
- 6. T. D. Lee and C. N. Yang, Phys. Rev. 117, 22 (1960); hereafter referred to as LY. Lee and Yang use the Heisenberg picture, while we use the interaction picture.

- 7. F. Mohling, Phys. Rev. 122, 1043 (1961); hereafter referred to as Mi.
- 8. F. Mohling, Phys. Rev. 122, 1062 (1961); hereafter referred to as M2.
- 9. It is precisely the (0,2) and (2,0) self-energy structures (whose external lines are always photon lines) which are omitted in MG.
- 10. F. Mohling, I. RamaRao and D. W. J. Shea, Phys. Rev. (to be published).
- 11. The simplest rearrangements of the Hamiltonian seem to be: (1) addition and subtraction of one-particle operators, and (2) transformation of the creation and annihilation operators by means of a Bogoliubov transformation. These two rearrangements are, in general, not equivalent.
- 12. Here, the counterterm is introduced into the Hamiltonian in the same manner as the effective one-body potential in Hartree-Fock theory. We refrain from applying the terminology "Hartree-Fock technique" to our counterterm technique, since this would suggest that we are using only a self-consistent, effective-field theory.
- 13. Generalized master graphs include all graphs in MRS, Tuttle and MG. Generalized master graphs are equivalent to the one-component transformed master graphs of Tuttle. If the counterterm is equated to zero, then the master-graph formulation of MG results (but now with the correct self-energy analysis). If the $\nu_{\alpha}^{\bullet}(\mathbf{k})$ are

- expanded in terms of exp $\{\beta[g_{\alpha} w_{\alpha}^{*}(k)]\}$, then the primed primary master graphs result (see Tuttle); if next the counterterm is equated to zero then one obtains primary master graphs (see MRS).
- 14. It is reasonable to inquire whether there will arise terms in $Q(t_2,t_1,k^{\alpha})$ of a form which can be cancelled by the counterterm in Eq. (5.30). The general answer to this question is not known, but explicit calculations show that such terms usually occur and that their cancellation by counterterms eliminates most (if not all) divergences in the theory.
- 15. In essence, this procedure regroups terms in the integral equations for the line factors in such a way that an analytic continuation of the line factors is achieved. In this process of analytic continuation, single-particle energies $\mathbf{w}_{\alpha}(\mathbf{k})$ are renormalized to quasiparticle energies $\mathbf{w}_{\alpha}(\mathbf{k})$.

FIGURE CAPTIONS

- Fig. 1. Symbols for the cluster vertices. The corresponding generalized cluster vertex functions are given explictly in Appendix B.
- Fig. 2. Diagrammatic representation of Eqs. (5.20) and (5.21). The graphical symbol for $\mathcal{G}_{1,1}(t_2,t_1,k^{\alpha})$ is also defined.
- Fig. 3. Diagrammatic representation of Eqs. (5.22) and (5.23). The graphical symbols for $G_{0,2}(t_2,t_1,k^{\alpha})$ and $G_{2,0}(t_2,t_1,k^{\alpha})$ are also defined.

$$k_{2}^{\gamma}$$

$$k_{3}^{\alpha}$$

$$k_{3}^{\gamma}$$

$$k_{3}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{1}^{\gamma}$$

$$k_{2}^{\gamma}$$

$$k_{3}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{3}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{2}^{\gamma}$$

$$k_{1}^{\alpha}$$

$$k_{3}^{\gamma}$$

$$k_{1}^{\gamma}$$

$$k_{3}^{\gamma}$$

$$k_{1}^{\gamma}$$

$$k_{2}^{\gamma}$$

$$k_{3}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\alpha}$$

$$k_{4}^{\alpha}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{4}^{\gamma}$$

$$k_{5}^{\gamma}$$

$$k_{6}^{\gamma}$$

$$k_{7}^{\gamma}$$

$$\begin{array}{c}
\uparrow_{1} \\
k_{3}^{\alpha} \\
\downarrow_{k_{1}} \\
\downarrow_{k_{1}} \\
\downarrow_{k_{2}} \\
\downarrow_{k_{1}} \\
\downarrow_{k_{1}} \\
\downarrow_{k_{1}} \\
\downarrow_{k_{2}} \\
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\downarrow_{k_{1}} \\
\downarrow_{k_{1}} \\
\downarrow_{k_{2}} \\
\downarrow_{k_{1}} \\
\downarrow_$$

XBL 701-123

Fig. 1

$$Q(t_{2},t_{1},k^{\alpha}) = Q = \epsilon_{\alpha} C_{\alpha}(k) \left[\theta(t_{2}-t_{1}) + \epsilon_{\alpha} \nu_{\alpha}^{1}(k)\right] + \left[\zeta_{1,1}\right]_{t_{1}}^{t_{2}}$$

$$+ \delta_{\alpha,\gamma} \qquad k^{\alpha} \qquad k^{\alpha}$$

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Fig. 2

$$\mathcal{G}_{0,2}(t_2,t_1,k^{\gamma}) \equiv k^{\gamma}$$

$$= \underbrace{\begin{array}{c} S_2 \\ S_2 \\ K^{\gamma}-k \end{array}}_{t_2} \underbrace{\begin{array}{c} K_{0,2} \\ S_1 \\ K^{\gamma}-k \end{array}}_{-k^{\gamma}} \underbrace{\begin{array}{c} G_{1,1} \\ G_{1,1} \end{array}}_{-k^{\gamma}} \underbrace{\begin{array}$$

$$G_{2,0}(t_2,t_1,k^{\gamma}) \equiv k^{\gamma}$$

$$G_{1,1}(s_2,t_1,k^{\gamma}) \equiv k^{\gamma}$$

$$G_{2,0}(t_2,t_1,k^{\gamma}) \equiv k^{\gamma}$$

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Fig. 3

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