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Self-Consistent Green's-Function Approach to the Electron-Gas Problem*

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The electron-gas problem is investigated by means of a self-consistent Green's-function formalism with the aim of developing practical approximation schemes for metallic densities. The work is based on the Dyson equation for the single-particle propagator $G[U]$ as a functional of an external potential U. The self-energy functional $\Sigma[U]$, appearing in the Dyson equation, is evaluated by perturbation theory in terms of the exact $G[U]$, thereby leading to a self-consistent problem. A hierarchy of approximations is generated by summing successively larger sets of graphs for $\Sigma[U]$. The Dyson equation is expanded in a functional Taylor series in U and yields a nonlinear integral equation for the $U=0$ propagator as well as linear integral equations for the $U=0$ higher-order Green's functions, with kernels dependent on $\delta\Sigma/\delta U$. In applications of the theory, the emphasis is on calculating the longitudinal dielectric function ϵ in terms of the contracted four-point Green's function. The linear integral equation for the latter is solved after making a low-momentum dominance approximation to the kernel. The result is a general, but approximate, closed-form expression for ϵ which can be used for different choices of Σ. The following five approximations for ϵ, based on different approximations for Σ, are presented: the Hartree-Fock, random-phase, generalized random-phase, second-stage random-phase, and low–high-density approximations. The last approximation is designed to work well at the two extremes of the density spectrum and, hopefully, also at metallic densities. The long-wavelength plasmon dispersion relations obtained from two different versions of the generalized random-phase approximation for ϵ agree closely with the results of Kanazawa *et al.* and of Singwi *et al.*

I. INTRODUCTION

Considerable insight into the physics of a metal can be obtained by studying the so-called electron-gas model of the metal. In this model the zero-temperature conduction electrons are assumed to interact via Coulomb forces only and to move in a uniform, neutralizing background of ions; magnetic and ion-lattice effects are thereby neglected. The properties of the electron gas depend critically on the electron density $n=N/\Omega$, where N is the number of electrons in a given volume Ω. Instead of n, it is customary to use the dimensionless parameter $r_s=r_0/a_0$, where $r_0=(\frac{4}{3}\pi n)^{-1/3}$ and $a_0=1/me^2$ is the Bohr radius.[1] At very high electron densities ($r_s\ll 1$, the weak-coupling limit) the properties of the electron gas are well accounted for in the random-phase approximation (RPA).[2] At low densities ($r_s\gg 1$, the strong-coupling limit), on the other hand, the electron gas supposedly solidifies into a Wigner crystal.[3] In this case the model can be solved by means of the strong-coupling approximation in which the electrons are allowed to execute small vibrations about their fixed lattice sites.[4] In the metallic density regime ($r_s\sim 2$ to 6) neither of the two approximation schemes is satisfactory; here one faces a difficult intermediate-coupling problem in which the average kinetic and potential energies per electron are comparable. The standard method of getting answers in this regime is to interpolate between the high- and the low-density values of physical quantities of interest.[3,5] Clearly, this method cannot be considered fundamental, and a "first-principles" approach would be desirable. In particular, the interpolation procedure cannot answer the interesting and important question about the existence of a phase transition in the electron gas which is conjectured to occur at $r_s\sim 5$.[6] A first-principles treatment of the electron-gas problem at metallic densities is of great interest not only because of its applicability to real metals but also from a more general standpoint, mainly because one expects that any insight gained in the electron-gas problem would be useful in treating other many-body systems with intermediate coupling strengths.

The electron-gas problem would in principle be solved if one had determined all the electron Green's functions. In practice, it is neither feasible nor necessary to know all of them, since they contain much more information than one could ever use. At present, the single-particle and the two-particle Green's functions suffice to interpret the experimental data, although perhaps in a not too distant future the solid-state experimental techniques will be refined to the point where it will be important to have some theoretical information on higher electron correlations deducible from the higher-order Green's functions. For this reason, it seems worthwhile to formulate a theory which is sufficiently general to allow one to calculate efficiently the higher-order Green's functions, if and when necessary.[7]

Despite many attempts, there has been little progress made in devising approximation schemes, valid at metallic densities, for calculating Green's functions or other related quantities. An exception is the recent work of Singwi *et al.*[8] which, however, is restricted to computing the longitudinal dielectric function ϵ (with apparently quite good results). As discussed in the last paragraph, one would like to have a more general theory available which could be used to calculate the full two-particle Green's function (of which the dielectric function is a special case) and also the higher-order Green's functions. It is the purpose of this paper to attempt the formulation of such a theory. No *numerical* calculations will be reported here, since our principal aim in this paper is to erect a theoretical framework for such calculations on the basis of a sequence of progressively more accurate approximations for determining the Green's functions. Inasmuch as most of the work on the electron-gas problem reported in the literature has been aimed toward producing a physically acceptable dielectric function ϵ, we shall also emphasize the calculation of ϵ in Sec. III in order to be able to compare with the work of other authors. Nevertheless, our formulation is completely general, as will be evident from what follows.

The basic ideas of our approach are as follows. The central object of study is the two-point Green's function or the single-particle propagator G as a functional of a weak external potential U. Once G has been determined, the higher-order Green's functions may in principle be obtained from it by functional differentiation with respect to U. The single-particle propagator $G[U]$ satisfies the Dyson equation

$$G[U]^{-1}=K+U-\Sigma[U], \tag{1.1}$$

where K is the kinetic-energy term and Σ is the self-energy functional. If one calculates Σ by perturbation theory in terms of the exact propagator $G[U]$, thereby ignoring all electron self-energy corrections, then (1.1) effectively becomes a self-consistent nonlinear equation for $G[U]$. A hierarchy of approximations for $G[U]$ is generated by choosing progressively larger sets of graphs contributing to Σ.

Once a particular approximation for Σ has been decided upon, all the Green's functions can be obtained from the solution of the approximate version of (1.1). In practice, it is convenient to expand (1.1) in a functional Taylor series in U. This leads to an infinite set of integral equations for the $U=0$ Green's functions. With the exception of the equation for the two-point Green's function, all the integral equations are linear and contain kernels which depend only on the lower-order Green's functions. Thus the integral equations may be solved one by one starting with the equation for the two-point Green's function.

The contents of the paper are as follows. In Sec. II we discuss the Green's functions for an electron-gas system subject to an external potential and present the momentum-space Feynman rules for computing them. We then sketch the derivation of integral equations satisfied by the various Green's functions and show how the dielectric function can be computed in terms of the four-point Green's function. In Sec. III we apply the results of Sec. II to compute the dielectric function $\epsilon(p)$ in various approximations of increasing complexity. We first briefly review the Hartree-Fock and the random-phase approximations in order to indicate how they fit into our hierarchy of approximations. We then proceed to discuss the generalized RPA (GRPA) and, upon making further approximations, exhibit two closed expressions for $\epsilon(p)$ which contain exchange corrections to the usual RPA result. The long-wavelength plasmon dispersion relations derived from each of the two expressions for $\epsilon(p)$ are compared with those of other authors and are found to agree closely. Section III is concluded with a discussion of the second-stage random-phase and the high–low-density approximations, the latter being specifically designed to work well at the high and the low ends of the density spectrum and, hopefully, also at the intermediate densities. A general discussion of our results is given in Sec. IV. The $U=0$ Hartree-Fock version of the Dyson equation for the single-particle propagator is investigated in the Appendix.

II. BASIC FORMALISM

A. Lagrangian Density

In the presence of an external spin-dependent potential, the electron gas is described by the Lagrangian density

$$\mathcal{L}(x)=\psi_\alpha(x)^\dagger K_x\psi_\alpha(x)+\int d^4x'\ \psi_\alpha(x)^\dagger U_{\alpha\alpha'}(x,x')\psi_{\alpha'}(x')$$
$$-\tfrac{1}{2}\int d^4x'\ \psi_\alpha(x)^\dagger\psi_{\alpha'}(x')^\dagger V(x-x')\psi_{\alpha'}(x')\psi_\alpha(x). \tag{2.1}$$

Here $\psi_\alpha(x)$ and $\psi_\alpha(x)^\dagger$ are, respectively, the destruction and creation operators of an electron of spin $\alpha=\pm$ at the space-time point $x=(x_0,\mathbf{x})$,

$$K_x=i(\partial/\partial x_0)+(2m)^{-1}\nabla^2+\mu, \tag{2.2}$$

$$V(x)=\delta(x_0)e^2/|\mathbf{x}|, \tag{2.3}$$

μ is the chemical potential, and U is the external potential. In (2.1) and elsewhere repeated spin indices are to be summed. The external potential introduces space-time inhomogeneities into the electron-gas system, so that the four-momentum is not conserved. This inconvenience is more than offset by the ease with which various quantities may be computed once the single-particle propagator is known as a functional of U.

B. Green's Functions

In this subsection we define the general n-particle Green's function and collect a number of results which will be used in the rest of the paper. The functional approach to many-body problems used here has been developed principally by Martin and Schwinger[9] some ten years ago on the basis of the variational (or functional) derivative techniques of Schwinger.[10] Subsequently, this formalism has been elaborated upon by Baym and Kadanoff[11] and others.[12] Most of the results we need can be found in the literature just referred to; for this reason, we shall content ourselves with the barest outline of their derivation.

Let $|0\rangle$ be the exact ground state of an N-electron system subject to the external potential U. The general

n-particle or $2n$-point Green's function is defined as

$$G_{\alpha_1\cdots\alpha_n;\beta_1\cdots\beta_n}(x_1\cdots x_n;\, y_1\cdots y_n \mid U)\equiv(-i)^n \times\langle 0\mid T\psi_{\alpha_1}(x_1)\cdots\psi_{\alpha_n}(x_n)\psi_{\beta_n}(y_n)^\dagger\cdots\psi_{\beta_1}(y_1)^\dagger\mid 0\rangle, \tag{2.4}$$

where T is the usual time-ordering operator. The Green's functions may be calculated by functional differentiation of a certain Green's functional[9] $F[U]$, according to the formula

$$G_{\alpha_1\cdots\alpha_n;\beta_1\cdots\beta_n}(x_1\cdots x_n;\, y_1\cdots y_n \mid U) =\{D_{\alpha_1\beta_1}(x_1y_1)\cdots D_{\alpha_n\beta_n}(x_ny_n)F[U]\}/F[U], \tag{2.5}$$

where the operator

$$D_{\alpha\beta}(x,y)\equiv\delta/\delta U_{\beta\alpha}(y,x) \tag{2.6}$$

satisfies

$$D_{\alpha\beta}(x,y)U_{\alpha'\beta'}(x',y')=\delta_{\alpha\beta'}\delta_{\alpha'\beta}\delta(x-y')\delta(x'-y). \tag{2.7}$$

In the usual perturbation expansion of the Green's function defined by (2.5), the denominator $F[U]$ serves to cancel out the contributions of disconnected graphs, so that G, as defined, is given in terms of connected graphs only.

It is somewhat simpler to compute the single-particle propagator $G_{\alpha;\beta}$ than the functional F, since the various perturbation terms for $G_{\alpha;\beta}$ are not weighted by the factors n^{-1} (n is the order of perturbation) as are those for F. For this reason, we shall direct our efforts toward calculating $G_{\alpha;\beta}$. Next, we discuss how the higher-order Green's functions may be expressed in terms of $G_{\alpha;\beta}$ and its functional derivatives.

Omitting space-time and functional arguments, we find from (2.5) that

$$G_{\alpha_1\alpha_2;\beta_1\beta_2}=G_{\alpha_1;\beta_1}G_{\alpha_2;\beta_2}+\tilde{G}_{\alpha_1\alpha_2;\beta_1\beta_2}, \tag{2.8}$$

where

$$\tilde{G}_{\alpha_1\alpha_2;\beta_1\beta_2}\equiv D_{\alpha_2\beta_2}G_{\alpha_1;\beta_1}. \tag{2.9}$$

Equation (2.8) is a slight generalization of Eq. (5–11) of Kadanoff and Baym[12] in that our four-point Green's function $G_{\alpha_1\alpha_2;\beta_1\beta_2}$ has all arguments distinct in contrast to their $G_2(12,12^+;U)$ having the second and the fourth arguments the same (apart from an infinitesimal). Expressions for higher-order Green's functions can be derived in analogy with (2.8). We quote here only the expression for the six-point function,

$$G_{\alpha_1\alpha_2\alpha_3;\beta_1\beta_2\beta_3}=G_{\alpha_1;\beta_1}G_{\alpha_2;\beta_2}G_{\alpha_3;\beta_3} +G_{\alpha_1;\beta_1}\tilde{G}_{\alpha_2\alpha_3;\beta_2\beta_3}+G_{\alpha_2;\beta_2}\tilde{G}_{\alpha_3\alpha_1;\beta_3\beta_1} +G_{\alpha_3;\beta_3}\tilde{G}_{\alpha_1\alpha_2;\beta_1\beta_2}+\tilde{G}_{\alpha_1\alpha_2\alpha_3;\beta_1\beta_2\beta_3}, \tag{2.10}$$

where the last term is a double functional derivative of $G_{\alpha_1;\beta_1}$.

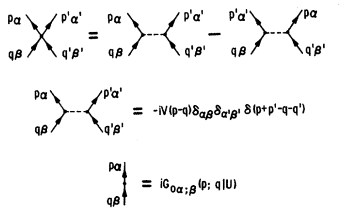

FIG. 1. Feynman rules for an electron-gas system with an external potential $U_{\alpha\beta}(x,y)$. The usual factor of -1 is to be supplied for each closed electron loop, and integrations over internal four-momenta are to be performed.

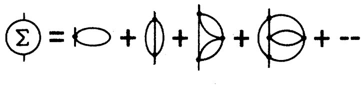

FIG. 2. Graphs contributing to the electron self-energy functional Σ.

C. Single-Particle Propagator

It is convenient to go over to the momentum space, using

$$\psi_\alpha(x)=\int_p \exp(-ip\cdot x)\psi_\alpha(p),\quad\text{etc.}, \tag{2.11}$$

where $p\cdot x=p_0x_0-\mathbf{p}\cdot\mathbf{x}$ and

$$\int_p=(2\pi)^{-4}\int d^4p. \tag{2.12}$$

We also write

$$D_{\alpha\beta}(p,q)=\int d^4x\int d^4y\exp[-i(p\cdot x-q\cdot y)]D_{\alpha\beta}(x,y), \tag{2.13}$$

$$U_{\alpha\beta}(p,q)=\int d^4x\int d^4y\exp[+i(p\cdot x-q\cdot y)]U_{\alpha\beta}(x,y), \tag{2.14}$$

so that

$$D_{\alpha\beta}(p,q)U_{\alpha'\beta'}(p',q')=\delta_{\alpha\beta'}(p-q')\delta_{\beta\alpha'}(q-p'), \tag{2.15}$$

where

$$\delta_{\alpha\beta}(p)=\delta_{\alpha\beta}(2\pi)^4\delta^4(p)\equiv\delta_{\alpha\beta}\delta(p). \tag{2.16}$$

The Feynman rules for the perturbation theory based on the Lagrangian density (2.1) are given in Fig. 1 with

$$G_0(p;q\mid U)^{-1}=K(p)\delta(p-q)+U(p,q), \tag{2.17}$$

$$K(p)=p_0-\mathcal{E}_0(p)+\mu, \tag{2.18}$$

$$\mathcal{E}_0(p)=p^2/2m, \tag{2.19}$$

$$V(p)=4\pi e^2/\mathbf{p}^2\quad\text{if}\quad\mathbf{p}\neq\mathbf{0};\qquad =0\quad\text{if}\quad\mathbf{p}=\mathbf{0}. \tag{2.20}$$

The exact single-particle propagator G is given as the solution of the Dyson equation

$$G(p;q\mid U)^{-1}=G_0(p;q\mid U)^{-1}-\Sigma(p;q\mid U). \tag{2.21}$$

Here Σ is the usual proper self-energy functional. In computing Σ only skeleton graphs of the type shown in Fig. 2 will be retained in which each electron line contributes iG.[13] No electron self-energy corrections should then be used, since they are already accounted for when one does perturbation theory in terms of the exact propagator G. With an appropriate approximate expression for Σ as a functional of G, (2.21) becomes a self-consistent equation determining G.

D. Integral Equations for Green's Functions

We now use (2.21) to derive equations satisfied by the various Green's functions in the absence of an external potential. In the limit $U\rightarrow 0$ the electron-gas system becomes spatially and temporally homogeneous and is described by a spin-independent Hamiltonian. Hence we expect to have

$$G_{\alpha;\beta}(p;q\mid 0)\equiv G(p)\delta_{\alpha\beta}(p-q), \qquad (2.22)$$

and similarly for the other two-point functions. Taking $U=0$ in (2.21), we obtain

$$G(p)^{-1}=K(p)-\Sigma(p), \qquad (2.23)$$

which is the usual form of the Dyson equation without external potentials. Next, taking the U derivative of (2.21) at $U=0$, using

$$DG^{-1}=-G^{-1}(DG)G^{-1}, \qquad (2.24)$$

and simplifying, we find

$$\tilde{G}_{\alpha\alpha';\beta\beta'}(pp';qq')=G(p)G(q)[\tilde{\Sigma}_{\alpha\alpha';\beta\beta'}(pp';qq') \\ -\delta_{\alpha\beta'}(p-q')\delta_{\alpha'\beta}(p'-q)], \qquad (2.25)$$

where $\tilde{\Sigma}=D\Sigma=\delta\Sigma/\delta U$ follows the definition (2.9) of $\tilde{G}$, and where the lack of the argument U signifies $U=0$. It is worth remarking that the δ-function term in (2.25) arises from the U term in the definition (2.17) of G_0^{-1}. From the symbolic identities

$$\tilde{\Sigma}\equiv\delta\Sigma/\delta U=(\delta\Sigma/\delta G)(\delta G/\delta U)\equiv(\delta\Sigma/\delta G)\tilde{G} \qquad (2.26)$$

we see that $\tilde{\Sigma}$ is linear in $\tilde{G}$, so that (2.25) is a *linear* (integral) equation for $\tilde{G}$.

By a procedure used above one can derive linear integral equations for the higher-order Green's functions. One of the attractive features of our scheme, we believe, is that the kernel of the integral equation for the n-particle Green's function involves only the lower-order (1 to $n-1$) Green's functions. This statement is illustrated by the integral equation (2.25) for the two-particle Green's function. It is evident from (2.25) and (2.26) that its kernel involves only $G(p)$, which has presumably been determined by solving (2.23).

E. Dielectric Function

Let us now establish the relation between the longitudinal dielectric function ϵ and the four-point Green's function $G_{\alpha\alpha';\beta\beta'}$. It is convenient to introduce the time-ordered polarization function[14]

$$P_t(p)=-i\int dx\exp(ip\cdot x)\langle 0\mid T\rho(x)\rho(0)\mid 0\rangle, \qquad (2.27)$$

where

$$\rho(x)=\psi_\alpha(x+\eta)^\dagger\psi_\alpha(x) \qquad (2.28)$$

is the density operator with $\eta=(\eta_0,\mathbf{0})$, $\eta_0\rightarrow 0^+$. Substituting (2.28) into (2.27) and using (2.11) and (2.4), we find

$$P_t(p)=i\int_{qrs}\exp[i(q+s)\cdot\eta]G_{\alpha\beta;\alpha\beta}(p+q,r;q,s). \qquad (2.29)$$

The dielectric function is defined by[15]

$$\epsilon(p)^{-1}=1+V(p)P_r(p), \qquad (2.30)$$

where $P_r(p)$ is the *retarded commutator* polarization function, whose definition involves a commutator of two density operators. The precise definition of P_r is of no concern to us. It suffices to note here the relation[16]

$$P_t(p)=P_r(p) \qquad (p_0>0), \qquad (2.31)$$

which enables us to compute $\epsilon(p)$ (for $p_0>0$) once $P_t(p)$ has been found from (2.29),

$$\epsilon(p)^{-1}=1+V(p)P_t(p) \qquad (p_0>0). \qquad (2.32)$$

As one sees from (2.29), in order to calculate the polarization function P_t it is sufficient to determine the *contracted* four-point Green's function

$$g(p;q)\equiv\frac{1}{2}\int_{p'q'}\exp(iq'\cdot\eta)G_{\alpha\beta;\alpha\beta}(pp';qq'), \qquad (2.33)$$

in terms of which

$$P_t(p)=2i\int_q\exp(iq\cdot\eta)g(p+q;q). \qquad (2.34)$$

Using (2.8) and (2.22) in (2.33) and (2.34), we find

$$P_t(p)=-in^2\delta(p)+2i\int_q\exp(iq\cdot\eta)\tilde{g}(p+q;q), \qquad (2.35)$$

where $\tilde{g}$ is defined in analogy with g. In (2.35) n is the electron density arising from the normalization integral

$$-2i\int_q\exp(iq\cdot\eta)G(q)=n. \qquad (2.36)$$

One notes that the $\delta(p)$-proportional term in (2.35), due to the direct noninteraction part of $G_{\alpha\beta;\alpha\beta}$, does not contribute to $\epsilon(p)$, since it is multiplied by $V(p)$, which vanishes for $p=0$. This term will henceforth be omitted from P_t without further comment. In the sequel we shall not bother to keep track of factors such as $\exp(ip\cdot\eta)$, replacing them everywhere by unity and remembering to restore them appropriately when ambiguities arise as to the path of integration in the complex energy-parameter plane.

Our next task is to derive an integral equation for the contracted Green's function $\tilde{g}$. Rather than doing this directly, we shall first derive an integral equation satisfied by the full four-point Green's function, and shall then obtain a related equation for $\tilde{g}$. In this manner, we shall be able to obtain a clear physical interpretation of the kernel appearing in the integral equation for $\tilde{g}$. Our starting point is (2.25), which we rewrite, using (2.8), as follows:

$$G_{\alpha\alpha';\beta\beta'}(pp';qq')=G(p)G(p')$$
$$\times[\delta_{\alpha\beta}(p-q)\delta_{\alpha'\beta'}(p'-q')-\delta_{\alpha\beta'}(p-q')\delta_{\alpha'\beta}(p'-q)]$$
$$-\delta(p+p'-q-q')G(p)G(p')\Gamma_{\alpha\alpha';\beta\beta'}(pp';qq')G(q)G(q'). \tag{2.37}$$

Here Γ, the vertex part,[17] is related to $\tilde{\Sigma}$ by

$$\delta(p+p'-q-q')\Gamma_{\alpha\alpha';\beta\beta'}(pp';qq')$$
$$=-G(p')^{-1}\tilde{\Sigma}_{\alpha\alpha';\beta\beta'}(pp';qq')G(q')^{-1}. \tag{2.38}$$

From (2.37) we see that Γ inherits the well-known antisymmetry properties of $G_{\alpha\alpha';\beta\beta'}$, namely,

$$G_{\alpha\alpha';\beta\beta'}=-G_{\alpha\alpha';\beta'\beta}=-G_{\alpha'\alpha;\beta\beta'}, \tag{2.39}$$

with the associated four-momentum changes not explicitly shown. Equation (2.37) is illustrated in Fig. 3(a). To relate Γ to $\tilde{G}$ we use the detailed form of (2.26),

$$\tilde{\Sigma}_{\alpha\alpha';\beta\beta'}(pp';qq')$$
$$=\int_{rs}\left.\frac{\delta\Sigma_{\alpha;\beta}(p;q\mid U)}{\delta G_{\gamma;\delta}(r;s\mid U)}\right|_{U=0}\tilde{G}_{\gamma\alpha';\delta\beta'}(rp';sq'). \tag{2.40}$$

We abbreviate the functional derivative by writing

$$\left.\frac{\delta\Sigma_{\alpha;\beta}(p;q|U)}{\delta G_{\gamma;\delta}(r;s|U)}\right|_{U=0}\equiv\delta(p+s-q-r)I_{\alpha\delta;\beta\gamma}(ps;qr). \tag{2.41}$$

The reason for the particular momentum δ function is explained graphically in Fig. 4. Substituting (2.41) and (2.8) into (2.40), letting $r\rightarrow r+p$, and then using (2.37), we find

$$\tilde{\Sigma}_{\alpha\alpha';\beta\beta'}(pp';qq')$$
$$=-G(p')G(q')\delta(p+p'-q-q')\Big[I_{\alpha\alpha';\beta\beta'}(pp';qq')$$
$$+\int_r I_{\alpha\delta;\beta\gamma}(pq+r;qp+r)G(p+r)G(q+r)\Gamma_{\gamma\alpha';\delta\beta'}$$
$$\times(p+rp';q+rq')\Big]. \tag{2.42}$$

Substituting this expression for $\tilde{\Sigma}$ into (2.38) and simplifying, we find

$$\Gamma_{\alpha\alpha';\beta\beta'}(pp';qq')=I_{\alpha\alpha';\beta\beta'}(pp';qq')$$
$$+\int_r I_{\alpha\delta;\beta\gamma}(pq+r;qp+r)G(p+r)G(q+r)\Gamma_{\gamma\alpha';\delta\beta'}$$
$$\times(p+rp';q+rq'). \tag{2.43}$$

This is just the Bethe-Salpeter equation for Γ with I the irreducible kernel, as illustrated in Fig. 3(b). Note that the interaction term in (2.43) involves the exchange of a particle-hole pair. The two intermediate lines are therefore inequivalent. For this reason, there is no factor of $\frac{1}{2}$ in front of the integral, as there would be in the case of two equivalent intermediate lines.[18]

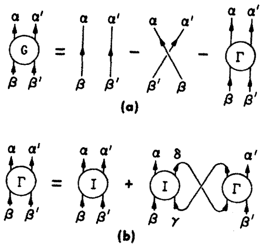

FIG. 3. (a) Graphical form of Eq. (2.37) with four-momenta suppressed. The long straight lines represent the exact single-particle propagators $G(p)$, $G(p')$, etc. The short stubs on G are for clarity only. (b) Graphical form of the Bethe-Salpeter equation (2.43).

Equation (2.43) will not be needed in this paper. It has been derived here for the sake of completeness in order to indicate how one might go about determining the full two-particle Green's function and also in order to exhibit the role of I as an irreducible kernel.

We are now ready to derive an integral equation for $\tilde{g}$. From (2.33), (2.37), and (2.8) we get

$$\tilde{g}(p;q)=-G(p)G(q)\Bigg[1+\frac{1}{2}\int_{p'q'}G(p')G(q')$$
$$\times\Gamma_{\alpha\beta;\alpha\beta}(pp';qq')\delta(p+p'-q-q')\Bigg], \tag{2.44}$$

while from (2.38), (2.40), and (2.41) it follows that the second term in brackets above is just

$$-\frac{1}{2}\int_{p'q'r}I_{\alpha\delta;\alpha\gamma}(pq+r;qp+r)\tilde{G}_{\gamma\beta;\delta\beta}(p+rp';q+rq'). \tag{2.45}$$

Now $I_{\alpha\delta;\alpha\gamma}$ is proportional to $\delta_{\gamma\delta}$,

$$I_{\alpha\delta;\alpha\gamma}(pq+r;qp+r)\equiv L(p;q\mid r)\delta_{\gamma\delta}. \tag{2.46}$$

Putting (2.44)–(2.46) together, we find the desired integral equation for $\tilde{g}$,

$$\tilde{g}(p;q)+G(p)G(q)$$
$$=G(p)G(q)\int_r L(p;q\mid r)\tilde{g}(p+r;q+r). \tag{2.47}$$

The kernel L of this integral equation is just the spin-contracted irreducible kernel I of the Bethe-Salpeter equation, according to (2.46).

Letting $p\rightarrow p+q$ in (2.47), multiplying it by $2i$, and integrating over q, we obtain, using (2.35),

$$P_t(p)=\chi(p)+2i$$
$$\times\int_{qr}G(p+q)G(q)L(p+q;q\mid r)\tilde{g}(p+q+r;q+r); \tag{2.48}$$

here

$$\chi(p)\equiv-2i\int_q G(p+q)G(q). \tag{2.49}$$

Thus P_t can be calculated from (2.48) once (2.47) has been solved for $\tilde{g}$. In general, it is a rather arduous task to find solutions to (2.47). For this reason it is worthwhile to look at a simple approximation which obviates

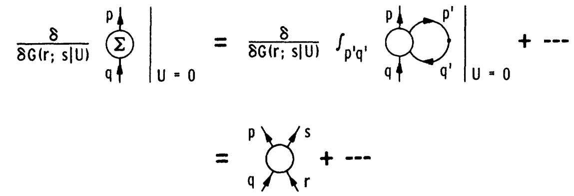

FIG. 4. Functional derivative of Σ with respect to G at $U=0$. A typical term in $\delta\Sigma/\delta G$ is shown in which the internal electron line contributes $iG(q';\,p'\,|\,U)$. The four-point graphs on the bottom are proportional to $\delta(p+s-q-r)$ by the four-momentum conservation which is valid when $U=0$.

the necessity of solving (2.47). We first rewrite (2.48) as

$$P_t(p)=\chi(p)+2i\int_r M(p+r;r)\tilde{g}(p+r;r), \qquad (2.50)$$

where

$$M(p+r;r)=\int_q G(p+q)G(q)L(p+q;q\,|\,r-q). \qquad (2.51)$$

Let us suppose that under appropriate circumstances the r dependence of M may be ignored,

$$M(p+r;r)\simeq M(p;0)\equiv M(p). \qquad (2.52)$$

Then the second term in (2.50) is proportional to P_t and hence (2.48) can immediately be solved:

$$P_t(p)\simeq\chi(p)/[1-M(p)]. \qquad (2.53)$$

Had we included the $-in^2\delta(p)$ term in the definition (2.35) of P_t, we would have found precisely the same term in (2.53), without any renormalization. The approximate formula (2.53) for P_t will be used in Sec. III. The approximation (2.52), henceforth referred to as the low-momentum dominance approximation (LMDA), is expected to be substantially better than the alternative, more naive approximation of neglecting the r dependence of the kernel L in (2.48). The reason for this expectation is that M is an *integrated* quantity whose r dependence is likely to be smoother than that of L. Using (2.53) and (2.32), we obtain the following expression for the dielectric function in the LMDA:

$$\epsilon(p)\simeq 1-\frac{V(p)\chi(p)}{1-M(p)+V(p)\chi(p)}. \qquad (2.54)$$

The LMDA will be used several times in the sequel in a slightly different context from (2.52). It is therefore fitting to devote a few lines to an elucidation of the nature of this approximation. Consider the typical expression

$$A\equiv\int_r V(r)G(p+r)G(q+r)X(p+r;q+r), \qquad (2.55)$$

where X is a function satisfying a linear integral equation and VGG is the "kernel." Obviously, it is nonsense to neglect the r dependence of the kernel in (2.55), since $V(r)$ is very strongly dependent on $|\,\mathbf{r}\,|$. A possible application of LMDA consists in neglecting the r dependence of X in (2.55),

$$A\simeq X(p;q)\int_r V(r)G(p+r)G(q+r). \qquad (2.56)$$

Clearly, (2.56) will be a good approximation if X is weakly dependent on its four-vector arguments and especially if the large r contributions to (2.55) are unimportant due to special properties of the kernel. To see how this may happen, let us suppose that it is permissible to neglect the r_0 dependence of X and to approximate G by $G_0=K^{-1}$. Then (2.56) is easily shown to be proportional to

$$\int d^3r\,V(r)$$
$$\times\frac{n_0(p+r)-n_0(q+r)}{p_0-q_0-\mathcal{E}_0(p+r)+\mathcal{E}_0(q+r)+i(p_0-q_0)\delta}X(p+r;q+r), \qquad (2.57)$$

where n_0 is the Fermi-Dirac distribution function. The above numerator vanishes when $|\,\mathbf{p}+\mathbf{r}\,|$ and $|\,\mathbf{q}+\mathbf{r}\,|$ exceed the Fermi momentum. Thus the $|\,\mathbf{r}\,|$ integral is cut off at large $|\,\mathbf{r}\,|$ and the LMDA (2.56) is justified. It is important to note that this happy state of affairs is contingent upon the fact that the kernel VGG in (2.55) represents an interactive propagation of an electron-hole pair. In the case of two electrons, say, one would typically obtain the factor $G(p+r)G(q-r)$; this would lead, for large $|\,\mathbf{r}\,|$, to

$$[p_0+q_0-\mathcal{E}_0(p+r)-\mathcal{E}_0(q+r)+2\mu+i(p_0+q_0)\delta]^{-1}\sim r^{-2}$$

instead of the fraction is the integrand of (2.57). Now there is no cutoff for large $|\,\mathbf{r}\,|$. However, we have

$$\int d^3r\,V(r)r^{-2}X\sim\int dr\,r^{-2}X,$$

so that the large-$|\,\mathbf{r}\,|$ contributions of X to the integral are suppressed by the factor r^{-2}. This may or may not be enough to make LMDA a useful approximation.

The above arguments remain essentially the same if the exact G is used in (2.55) instead of G_0, the major change being that the spectral function of G is no longer a δ function as in the case of G_0. The effect of an r_0 dependence of X is somewhat more difficult to assess, although the physical basis for the arguments (electron-hole pair versus two electrons) is expected to remain valid. In any case, known r_0 singularities of X may be subtracted out (and treated exactly) and the LMDA applied to the remaining, more slowly varying function. If the r_0 singularities of X are not known, one still has the recourse to the more difficult self-consistent subtraction of singularities. We shall have no occasion to use these more sophisticated versions of LMDA in this paper.

III. APPLICATIONS

In this section we apply the theory developed so far to derive equations for determining approximate two-point and contracted four-point Green's functions and then, after making additional approximations, to compute the dielectric function $\epsilon(p)$. The different approximations will be labeled according to the form of $\epsilon(p)$ they lead to. We shall first derive the well-known Hartree-Fock and the random-phase approximations for $\epsilon(p)$ in order to illustrate how our formalism works in a familiar context. Then we shall proceed to higher approximations, the last of which will be specifically tailored to the metallic density regime.

A. Hartree-Fock Approximation

The simplest approximation to Σ is zero,

$$\Sigma \simeq 0. \tag{3.1}$$

Then (2.23) gives

$$G(p) \simeq G_0(p)$$
$$\equiv K(p)^{-1} = [p_0 - \epsilon_0(p) + \mu + ip_0\delta]^{-1}, \tag{3.2}$$

where $ip_0\delta$ ($\delta > 0$ and infinitesimal) takes care of the boundary conditions in the usual way. By (2.41) $L \equiv 0$, so that (2.48) yields

$$P_t(p) \simeq \chi_0(p), \tag{3.3}$$

where, according to (2.49) and (3.2),

$$\chi_0(p) = 2\int \frac{d^3q}{(2\pi)^3} \frac{n_0(q) - n_0(p+q)}{p_0 + \mathcal{E}_0(q) - \mathcal{E}_0(p+q) + ip_0\delta}, \tag{3.4}$$

$$n_0(q) = \theta(p_F - |\mathbf{q}|), \tag{3.5}$$

$$p_F = (2m\mu)^{1/2} = \text{Fermi momentum}. \tag{3.6}$$

Of course, χ_0 is just the familiar density-density response function (if $p_0 > 0$) for a noninteracting electron gas. Substituting (3.3) into (2.32), we obtain

$$\epsilon(p) \simeq [1 + V(p)\chi_0(p)]^{-1}$$
$$\equiv \epsilon_{\mathrm{HFA}}(p), \tag{3.7}$$

the Hartree-Fock expression for the dielectric function.[19]

B. RPA

The Hartree approximation to Σ

$$\Sigma \simeq \Sigma_{\mathrm{HA}} \tag{3.8}$$

amounts to keeping the contribution of the graph (a) in Fig. 5,

$$\Sigma_{\mathrm{HA}}(p; q \,|\, U) = -iV(p-q) \int_r \mathrm{tr}\, G(p+r; q+r \,|\, U). \tag{3.9}$$

In the limit $U \to 0$, G in (3.9) is proportional to $\delta(p-q)$, so that Σ_{HA} vanishes. Thus $G(p) \simeq G_0(p)$, where G_0 is given by (3.2). The first derivative of Σ_{HA} is, however, nonzero at $U=0$ and yields, according to (2.41), the r-independent kernel

$$L_{\mathrm{HA}}(p; q \,|\, r) = -2iV(p-q). \tag{3.10}$$

With this form of L, (2.53) is an *exact* consequence of (2.48). From (2.51) and (3.10) we find

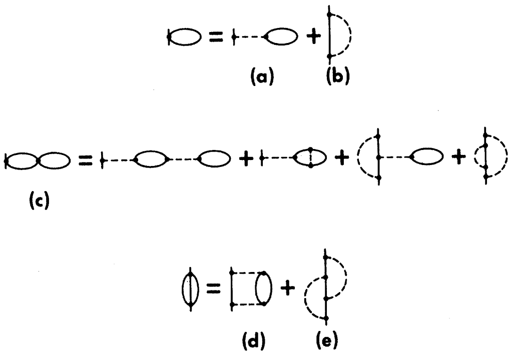

FIG. 5. First- and second-order graphs contributing to Σ and their decomposition: (a) Hartree, (b) exchange, (c) Hartree-Fock with electron self-energy correction, (d) polarization, and (e) exchange polarization.

$$M_{\mathrm{HA}}(p) = V(p)\chi_0(p). \tag{3.11}$$

Substituting (3.11) into (2.54) (remembering to let $\chi \to \chi_0$, since $G \simeq G_0$ in the present approximation), we find[20]

$$\epsilon(p) \simeq 1 - V(p)\chi_0(p)$$
$$\equiv \epsilon_{\mathrm{RPA}}(p). \tag{3.12}$$

Thus the Hartree approximation for $\Sigma[U]$ leads to the RPA dielectric function. This of course is expected in view of the known equivalence of the random-phase and the time-dependent (due to the external potential U, in the present instance) Hartree approximations.[21] Similarly, the Hartree-Fock approximation for Σ is expected to yield a dielectric function in the GRPA, as we next discuss.

C. GRPA

Figures 5(a) and 5(b) lead to the Hartree-Fock approximation for Σ

$$\Sigma_{\mathrm{HFA}}(p; q \,|\, U) = -iV(p-q) \int_r \mathrm{tr}\, G(p+r; q+r \,|\, U)$$
$$+ i\int_r V(r) G(p+r; q+r \,|\, U). \tag{3.13}$$

The second, exchange, term in (3.13) survives the $U \to 0$ limit and, by (2.23), yields the following nonlinear integral equation for the single-particle propagator:

$$G(p) = \left[K(p) - i\int_r V(r) G(p+r)\right]^{-1}. \tag{3.14}$$

Instead of (3.10) we now get an r-dependent kernel,

$$L_{\mathrm{HFA}}(p; q \,|\, r) = -2iV(p-q) + iV(r). \tag{3.15}$$

Substituting (3.15) into (2.48) and rearranging, we find

$$P_{t,\mathrm{HFA}}(p)=\epsilon_{\mathrm{RPA}}(p)^{-1}\times\left[\chi(p)+2i\int_r \xi(p+r;r)\tilde{g}(p+r;r)\right],\quad(3.16)$$

where ϵ_{RPA} is given by (3.12) with $\chi_0\rightarrow\chi$ [since now G is given by the solution of (3.14)] and

$$\xi(p;q)\equiv i\int_r V(r)G(p+r)G(q+r)=\xi(q;p).\quad(3.17)$$

We emphasize that (3.16) is exact within the present approximation for Σ. Let us now explore some approximate solutions for G and P_t.

Consider first (3.14). In the weak-coupling limit (the high-density case, $r_s\ll 1$), it is reasonable to iterate (3.14) once to get

$$G(p)\simeq K(p)+i\int_r V(r)K(p+r)^{-1}\equiv G_{\mathrm{HFA}}(p),\quad(3.18)$$

the usual Hartree-Fock expression for the propagator. A more general, noniterative way of solving (3.14) is discussed in the Appendix. Let us assume that we are in possession of a solution to (3.14) and proceed to investigate the consequences of (3.16).

As discussed in Sec. II E, in order to determine P_t, we should first solve the integral equation (2.47) with the HF kernel (3.15) and then use (3.16) to calculate P_t. To avoid this difficult task, an approximation scheme was devised in the last section, leading to (2.53) and (2.54), which in the present case amounts to neglecting the r dependence of ξ in (3.16). This approximation scheme (LMDA) will be discussed later in this subsection. First, we wish to explore an alternative approximation which allows us to make contact with previous work in the literature on exchange corrections to the plasma dispersion relation in the high-density case.[22,23] Let us suppose that the ξ-proportional exchange term in (3.16) is small compared to the direct Coulomb term. In that case one may use perturbation theory to compute $\tilde{g}$. Working to first order in the exchange potential, we need $\tilde{g}$ to zero order,

$$\tilde{g}(p+r;r)\simeq\tilde{g}_{\mathrm{RPA}}(p+r;r)=-G(p+r)G(r)/\epsilon_{\mathrm{RPA}}(p),\quad(3.19)$$

as determined from (2.47) by using (3.10) for L. Substituting (3.19) into (3.16), we find

$$P_{t,\mathrm{HFA}''}(p)\simeq\frac{\chi(p)+\eta(p)/\epsilon_{\mathrm{RPA}}(p)}{\epsilon_{\mathrm{RPA}}(p)},\quad(3.20)$$

where the double prime indicates the approximation (3.19), and

$$\eta(p)\equiv-2i\int_r G(p+r)G(r)\xi(p+r;r).\quad(3.21)$$

The dielectric function corresponding to (3.20) is

$$\epsilon(p)\simeq\frac{\epsilon_{\mathrm{RPA}}(p)}{1+V(p)\eta(p)/\epsilon_{\mathrm{RPA}}(p)}\equiv\epsilon_{\mathrm{GRPA}''}(p).\quad(3.22)$$

We refer to (3.22) as the dielectric function in the GRPA with the additional approximation (3.19).

In order to investigate the properties of $\epsilon_{\mathrm{GRPA}''}$, one must know the function $\eta(p)$. Substituting (3.17) into (3.21) and doing the q_0r_0 integrations, we find

$$\eta(p)=-2\int[d^3q/(2\pi)^3]\times\int[d^3r/(2\pi)^3]V(q-r)X(p,q)X(p,r),\quad(3.23)$$

where the function

$$X(p,q)\equiv\int(dq_0/2\pi i)G(p+q)G(q)=\frac{n(q)-n(p+q)}{p_0+\mathcal{E}(q)-\mathcal{E}(p+q)+ip_0\delta}\quad(3.24)$$

also appears in the definition (2.49) of χ:

$$\chi(p)=2\int[d^3q/(2\pi)^3]X(p,q).\quad(3.25)$$

In (3.24) we have written

$$n(q)=\int(dq_0/2\pi i)G(q),\quad(3.26)$$

$$\mathcal{E}(q)=\mathcal{E}_0(q)+i\int_r V(r)G(q+r)=\mathcal{E}_0(q)-\int[d^3r/(2\pi)^3]V(r-q)n(r).\quad(3.27)$$

A complete evaluation of (3.23) by analytical methods does not seem feasible nor is necessary for our purposes. We consider here only the limiting case $|\mathbf{p}|\rightarrow 0$. Moreover, we restrict our attention to the high-density regime, in which case it is reasonable to approximate $n(p)$ in (3.26) by the Fermi-Dirac distribution function (3.5) and $\mathcal{E}(p)$ by its free-electron form $\mathcal{E}_0(p)=\mathbf{p}^2/2m$.

Subject to the above approximations, we now show that in the limit $p\equiv|\mathbf{p}|\rightarrow 0$ (3.22) leads to a plasmon dispersion relation incorporating the well-known exchange corrections. For the high-density case we are considering, it is appropriate to expand (3.22) in powers of r_s (or e^2). Now $\epsilon_{\mathrm{RPA}}=O(1)$ and $V,\eta=O(r_s)$, so that to order r_s^2 the expansion of (3.22) reads[24]

$$\epsilon_{\mathrm{GRPA}''}\simeq\epsilon_{\mathrm{RPA}}(1-V\eta/\epsilon_{\mathrm{RPA}})=1-V(\chi_0+\eta).\quad(3.28)$$

One finds that $-\frac{1}{2}(\chi_0+\eta)$ in this expression is precisely the term in parentheses of Eq. (2.13) of Kanazawa *et al.*,[22] if one makes some changes of variables and if one neglects the self-energy terms $\Sigma^{(1)}$ in the denominator of these authors' expression for χ_0, as they do later in their paper. The result of setting the right-hand side of (3.28) equal to zero is the dispersion relation

$$p_0^2=\omega_{\mathrm{pl}}^2+\tfrac{3}{10}(p_F^2/m^2)(1-m^2\omega_{\mathrm{pl}}^2/4p_F^4)p^2+O(p^4), \qquad (3.29)$$

where

$$\omega_{\mathrm{pl}}=(4\pi ne^2/m)^{1/2}=\text{plasma frequency}. \qquad (3.30)$$

The exchange contribution is the second term in the parentheses of (3.29) with the value $-0.0553r_s$.[25]

The validity of GRPA″ is restricted to low values of $p\equiv|\mathbf{p}|$. This may be seen as follows. Consider (2.52) with $L\rightarrow L_{\mathrm{HFA}}$ and $p\rightarrow p+q$,

$$\tilde{g}(p+q;q)=-G(p+q)G(q)\times\left\{1+i\int_r[2V(p)-V(r-q)]\tilde{g}(p+r;r)\right\}. \qquad (3.31)$$

The derivation of (3.22) was based on the assumption that the exchange term in (3.31) may be treated as small. Apparently, this is not true for *large* p and fixed q, since then $2V(p)\ll V(r-q)$ except when r becomes sufficiently large. But large r values presumably make only a small contribution to the integral in (3.31) in view of the asymptotic behavior

$$\tilde{g}(p+r;r)\sim -G(p+r)G(r)r^{-4}$$

for fixed p and large r. While the above argument is admittedly crude, it nevertheless suggests that the exchange term dominates the high p behavior of (3.31) and hence invalidates GRPA″ for large p.

Let us now briefly turn to the LMDA discussed in Sec. II E. From (2.51) and (3.15) we find

$$M_{\mathrm{HFA}}(p+r;r)=V(p)\chi(p)+\xi(p+r;r), \qquad (3.32)$$

where ξ is given by (3.17), so that

$$\epsilon(p)\simeq 1-V(p)\chi(p)/[1-\xi(p;0)] \equiv \epsilon_{\mathrm{GRPA}'}(p) \qquad (3.33)$$

by (2.52) and (2.54). The dispersion relation now reads

$$\epsilon_{\mathrm{RPA}}(p)-\xi(p;0)=0 \qquad (3.34)$$

and clearly yields exchange corrections to the plasmon frequency for all values of r_s. For small p and taking $G\simeq G_0$, we find

$$\xi(p;0)=\tfrac{1}{2}(p/p_F)^2+O(p^4)$$

with the approximation $p_0\simeq\omega_{\mathrm{pl}}$. Using this in (3.34), we get

$$p_0^2=\omega_{\mathrm{pl}}^2[1+(9/5)(p/p_{FT})^2-(1/2)(p/p_F)^2]+O(p^4), \qquad (3.35)$$

where

$$p_{FT}^2=4me^2/\pi p_F. \qquad (3.36)$$

Our result agrees closely with that of Singwi *et al.*,[8] who, instead of the factor $\frac{1}{2}$ in front of $(p/p_F)^2$, find γ with values from 0.4561 to 0.5986 as r_s ranges from 1 to 20. Thus, at least in this specific instance, the LMDA leads to a GRPA dielectric function with reasonable long-wavelength properties.

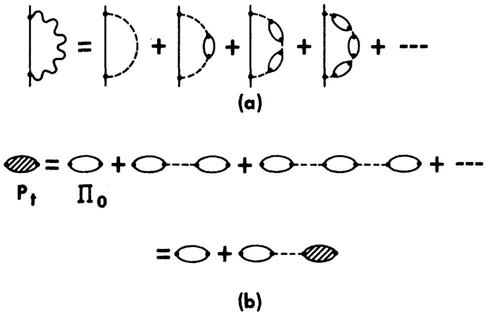

FIG. 6. (a) Screening of the exchange graph, Fig. 5(b), by the addition of an infinite number of ring graphs. (b) Graphical representation of the polarization functional P_t.

D. Second-Stage RPA

To go beyond the HF approximation for Σ, one may consider the second-order graphs shown in Fig. 5. Of these, Fig. 5(c) represents an electron self-energy correction to Figs. 5(a) and 5(b) and hence should be ignored. Of the remaining two graphs, the polarization graph 5(d) dominates the exchange polarization graph 5(c). In fact, the former is divergent in the limit $U\rightarrow 0$, owing to the confluence of two Coulomb potential factors. The divergence is cured in a well-known manner by summing an infinite number of graphs so as to screen out the troublesome Coulomb potentials of Fig. 5(d). The simplest set of graphs which do the job are the ring graphs shown in Fig. 6(a). Ignoring the exchange polarization graph, we take Σ_{HA}, given by (3.9), plus the contributions of the ring graphs as our next approximation for Σ (denoted by Σ_{RPA}):

$$\Sigma_{\mathrm{RPA}}=\Sigma_{\mathrm{HA}}+\Sigma_{\mathrm{RPA}}', \qquad (3.37)$$

$$\Sigma_{\mathrm{RPA}}'(p;q\,|\,U)=i\int_{p'q'}\mathcal{V}(pp';q'q\,|\,U)G(q';p'\,|\,U). \qquad (3.38)$$

Here $\mathcal{V}$ is the effective potential corresponding to the wiggly line of Fig. 6(a). It can be written as

$$\mathcal{V}(pp';qq'\,|\,U)=V(p-q)[\delta(p+p'-q-q')+P_t(p-q;q'-p'\,|\,U)V(q'-p')], \qquad (3.39)$$

where the polarization functional P_t sums the ring graphs of Fig. 6(b) and is given as the solution to

$$P_t(p;q\,|\,U)=\Pi_0(p;q\,|\,U)+\int_r\Pi_0(p;r\,|\,U)V(r)P_t(r;q\,|\,U), \qquad (3.40)$$

with

$$\Pi_0(p;q\mid U)$$
$$=-i\int_{p'q'}\mathrm{tr}G(q';p'\mid U)G(p+p';q+q'\mid U). \quad (3.41)$$

One can show that the definition (3.40) of P_t (with exact Π_0) agrees with (2.37). In the $U=0$ limit, (3.41) reduces to

$$\Pi_0(p)=\chi(p), \quad (3.42)$$

where χ is given by (2.49). Similarly, (3.40) leads to

$$P_t(p)=\Pi_0(p)[1-V(p)\Pi_0(p)]^{-1}$$
$$\equiv\chi(p)/\epsilon_{\mathrm{RPA}}(p). \quad (3.43)$$

Using this formula and taking $U=0$ in (3.39), we find

$$\mathcal{V}(pp';qq'\mid 0)=V_{\mathrm{RPA}}(p-q)\delta(p+p'-q-q'), \quad (3.44)$$

where

$$V_{\mathrm{RPA}}(p)=V(p)/\epsilon_{\mathrm{RPA}}(p) \quad (3.45)$$

is the RPA-screened Coulomb potential.

The $U=0$ limit of (3.37) is now easily found to be

$$\Sigma_{\mathrm{RPA}}(p)=i\int_r V_{\mathrm{RPA}}(r)G(p+r). \quad (3.46)$$

Comparing this result with the $U=0$ limit of (3.15),

$$\Sigma_{\mathrm{HFA}}(p)=i\int_r V(r)G(p+r), \quad (3.47)$$

we see that Σ_{RPA} is just the Hartree-Fock expression for Σ with the bare Coulomb potential replaced by the RPA-screened one.

In order to compute the kernel L defined by (2.41) we need the functional derivative of P_t. Writing (3.40) in an operator form and solving for P_t, we have

$$P_t=(1-\Pi_0V)^{-1}\Pi_0.$$

Making use of a formula analogous to (2.33) and writing $\mathfrak{D}\equiv\delta/\delta G$, we find

$$\mathfrak{D}P_t=P_t\Pi_0^{-1}(\mathfrak{D}\Pi_0)\Pi_0^{-1}P_t.$$

At $U=0$ this explicitly reads

$$\left.\frac{\delta P_t(p;q\mid U)}{\delta G_{\gamma;\delta}(r;s\mid U)}\right|_{U=0}$$
$$=-i\delta_{\gamma\delta}(p+s-q-r)\epsilon_{\mathrm{RPA}}(p)^{-1}\epsilon_{\mathrm{RPA}}(q)^{-1}$$
$$\times[G(r-p)+G(r+q)]. \quad (3.48)$$

With the help of this result the kernel L is now easily found from (3.37) and (3.38),

$$L_{\mathrm{RPA}}(p;q\mid r)=-2iV(p-q)+iV_{\mathrm{RFA}}(r)$$
$$+2\int_s V_{\mathrm{RPA}}(p-s)V_{\mathrm{RPA}}(q-s)G(s)$$
$$\times[G(r+s)+G(r-s+p+q)]. \quad (3.49)$$

Comparing this expression with (3.15), we see that the exchange part of the Coulomb potential is screened in L_{RPA} and that L_{RPA} has an additional term due to the U dependence of the screened Coulomb interaction.

From (2.56), (2.57), and (3.49), we obtain

$$M_{\mathrm{RPA}}(p)=V(p)\chi(p)+\xi_{\mathrm{RPA}}(p;0)+M_{\mathrm{RPA}'}(p),$$

where ξ_{RPA} is given by (3.17) with $V\rightarrow V_{\mathrm{RPA}}$ and

$$M_{\mathrm{RPA}'}(p)=2\int_{qr}V_{\mathrm{RPA}}(r)V_{\mathrm{RPA}}(p+r)$$
$$\times G(q)G(p+q)G(p+q+r)[G(-r)+G(p+r)]. \quad (3.50)$$

The dielectric function, by (2.54), is then

$$\epsilon(p)\simeq 1-V(p)\chi(p)/[1-\xi_{\mathrm{RPA}}(p;0)-M_{\mathrm{RPA}'}(p)]$$
$$\equiv\epsilon_{2\mathrm{RPA}'}(p), \quad (3.51)$$

where the prime in 2RPA′ is supposed to remind one of LMDA used to derive (2.54). We shall not attempt to explore the properties of $\epsilon_{2\mathrm{RPA}'}(p)$, since to do so would require a considerable amount of numerical computation in view of the complicated nature of the functions involved in (3.51). Instead, we immediately proceed to our next, and last, approximation, making use of the results obtained in this subsection.

E. High-Low-Density Approximation

In devising the last approximation for Σ to be considered in this paper, we shall attempt to take into account those graphs which can be expected to provide a reasonable description of the electron gas at metallic densities. Suppose we are able to identify and perform the summation of two sets of graphs, one of which is important at high densities and the other at low densities. Having obtained a correct description of the two extremes of the density spectrum, we may hope that intermediate densities are also reasonably well taken care of, especially if we can find and include additional graphs which "interpolate" between the high- and the low-density sets of graphs.

In order to explore the above ideas, we must first identify the important graphs at high and low densities.

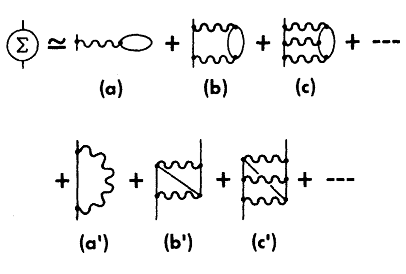

FIG. 7. Graphs dominant at low densities for fermion many-body systems with finite-range interactions. Here $(a, b, c, \ldots)$ and $(a', b', c', \ldots)$ are, respectively, the direct and exchange graphs.

It is a well-known fact that the ring graphs, of the type shown in Fig. 6(a), are dominant at high densities.[26] On the other hand, for fermion many-body systems with finite-range interactions, graphs with the fewest possible hole lines are known to dominate at low densities.[27] Those graphs are shown in Fig. 7. Now there is evidence that electron-electron interactions in metals are quite effectively screened.[28] The screening of the Coulomb interaction is also well understood from the theoretical point of view (RPA), at least for the high-density electron gas. Thus there is good reason to believe that effective electron-electron interactions are of finite range well into the metallic density regime and perhaps beyond.[29] As the analysis of Galitskii[27] shows, the graphs of Fig. 7 are dominant at low densities provided the ratio of the range of the potential to the mean interparticle distance is small (gas approximation). In the present case, the criterion of dominance is $\lambda_{sc}/r_0 \ll 1$, where λ_{sc} is the screening length or the range of the effective interaction. Now the RPA result for λ_{sc} is $p_{FT}^{-1}=(0.82p_F)^{-1}r_s^{-1/2}$, so that $\lambda_{sc}/r_0 \sim r_s^{-1/2}$. We see that indeed $\lambda_{sc}/r_0 \ll 1$ for large r_s corresponding to low densities. Of course, the above estimates are based on the RPA expression for λ_{sc}, which is not expected to be strictly valid as one goes to lower densities. Nevertheless, the corrections to these estimates are not expected to be dramatic, and hence there are some grounds to believe that the contributions of Fig. 7 may be important for a reasonably accurate description of the electron-gas system at the lower densities.

It should be realized that the graphs of Fig. 7 are more general than the low-density graphs considered by Galitskii[27] in that each of the latter contain only a single hole propagator, whereas the former, depending on the signs of the various energy parameters, contain both electron and hole propagators in various combinations. Moreover, the graphs of Fig. 7 are to be computed, at least in principle, using the propagators determined by the $U=0$ Dyson's equation, rather than in terms of $G_0=K^{-1}$, as in ordinary perturbation theory. Thus, in effect, we are summing a much larger class of ordinary perturbation graphs than does Galitskii. These extra graphs may be thought of as the "interpolating graphs" mentioned at the end of the first paragraph.

We shall take the wiggly line in Fig. 7 to represent the RPA-screened U-dependent potential (3.39), although more complicated expressions for $\mathcal{V}$ could be used to take into account exchange corrections, etc. The graphs (a) and (b) of Fig. 7 must be modified to avoid overcounting. The first graph should be replaced by the Hartree graph (a) of Fig. 5, while the second should be omitted altogether, since its components are already included in the expansion of graph (a′) of Fig. 7. For computational purposes, however, it is convenient to add and subtract graph (b) and to rewrite the graphical expansion of Fig. 7 in the form given in Fig. 8(a), where K is a sum of ladder graphs, as shown. We now see that the first two terms in the expansion of Σ in the present approximation are just those contributing to Σ_{RPA} discussed in the last subsection. Denoting the approximate Σ by Σ_E (Sec. III E), we have

$$\Sigma_E=\Sigma_{\mathrm{RPA}}+\Sigma_E{}', \tag{3.52}$$

$$\Sigma_E{}'=\Sigma_{\mathrm{pol}}+\Sigma_{Kd}+\Sigma_{Ke}, \tag{3.53}$$

where the last three terms are the respective contributions of the RPA-screened polarization, the direct ladder, and the exchange ladder graphs of Fig. 7. Explicitly, we have

$$\Sigma_{x\alpha;\beta}(p;q\mid U)=i\int_{p'q'}\mathcal{S}_{x\alpha\alpha';\beta\beta'}(pp';qq'\mid U)G_{\beta';\alpha'}(q';p'\mid U), \tag{3.54}$$

where

$$\mathcal{S}_{\mathrm{pol}\;\alpha\alpha';\beta\beta'}(pp';qq'\mid U)=i\delta_{\alpha\beta'}\delta_{\alpha'\beta}\int_{r_1\cdots r_4}\mathcal{V}(pr_4;q'r_1\mid U)\mathcal{V}(p'r_2;qr_3\mid U)\times\mathrm{tr}[G(r_1;r_2\mid U)G(r_3;r_4\mid U)], \tag{3.55}$$

$$\mathcal{S}_{Kd\alpha\alpha';\beta\beta'}(pp';qq'\mid U)=\delta_{\alpha\beta}\delta_{\alpha'\beta'}\mathcal{V}(pp';qq'\mid U)-K_{\alpha\alpha';\beta\beta'}(pp';qq'\mid U), \tag{3.56}$$

$$\mathcal{S}_{Ke\alpha\alpha';\beta\beta'}(pp';qq'\mid U)=-\delta_{\alpha\beta'}\delta_{\alpha'\beta}\mathcal{V}(pp';q'q\mid U)+K_{\alpha\alpha';\beta'\beta}(pp';q'q\mid U). \tag{3.57}$$

The kernel K satisfies the integral equation

$$K_{\alpha\alpha';\beta\beta'}(pp';qq'\mid U)=\delta_{\alpha\beta}\delta_{\alpha'\beta'}\mathcal{V}(pp';qq'\mid U)+i\int_{rr'ss'}\mathcal{V}(pp';rr'\mid U)G_{\alpha;\delta}(r;s\mid U)\times G_{\alpha';\delta'}(r';s'\mid U)K_{\delta\delta';\beta\beta'}(ss';qq'\mid U). \tag{3.58}$$

Putting $U=0$ in this equation and writing

$$K_{\alpha\alpha';\beta\beta'}(pp';qq'\mid 0)=\delta_{\alpha\beta}\delta_{\alpha'\beta'}K(pp';q)\delta(p+p'-q-q'), \tag{3.59}$$

we find

$$K(pp';q)=V_{\mathrm{RPA}}(p-q)+i\int_r V_{\mathrm{RPA}}(r)G(p+r)G(p'-r)K(p+rp'-r;q). \tag{3.60}$$

Making the LMDA (see Sec. II E) in (3.60), we obtain an approximate expression for K

$$K(pp';q)\simeq[1-\zeta_{\mathrm{RPA}}(p;p')]^{-1}V_{\mathrm{RPA}}(p-q), \tag{3.61}$$

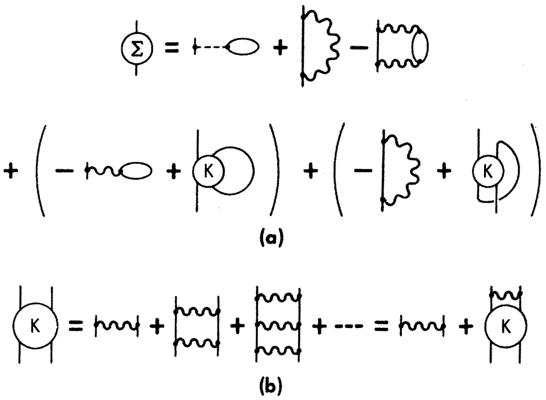

FIG. 8. (a) Graphs contributing to the approximate electron self-energy functional Σ_E. (b) Graphs contributing to the K functional and the graphical integral equation satisfied by K.

where

$$\zeta_{\mathrm{RPA}}(p;p')=i\int_r V_{\mathrm{RPA}}(r)G(p+r)G(p'-r). \quad (3.62)$$

Next, we take the G derivative of (3.58) and find

$$\begin{aligned}\bar{K}_{\alpha\alpha'\alpha'';\beta\beta'\beta''}&(pp'p'';qq'q'')\\ &\equiv[\delta K_{\alpha\alpha';\beta\beta'}(pp';qq'\mid U)/\delta G_{\beta'';\alpha''}(q'';p''\mid U)]_{U=0}\\ &=I_{\alpha\alpha'\alpha'';\beta\beta'\beta''}(pp'p'';qq'q'')\\ &\quad+i\int_r V_{\mathrm{RPA}}(r)G(p+r)G(p'-r)\\ &\quad\times\bar{K}_{\alpha\alpha'\alpha'';\beta\beta'\beta''}(p+rp'-rp'';qq'q''), \end{aligned}\quad (3.63)$$

where

$$\begin{aligned}I_{\alpha\alpha'\alpha'';\beta\beta'\beta''}&(pp'p'';qq'q'')\\ &=\delta(p+p'+p''-q-q'-q'')\\ &\times\{-i\delta_{\alpha\beta}\delta_{\alpha'\beta'}\delta_{\alpha''\beta''}V_{\mathrm{RPA}}(p-q)V_{\mathrm{RPA}}(p'-q')\\ &\times[G(p''+p-q)+G(p''+p'-q')]\\ &+\delta_{\alpha\beta}\delta_{\alpha'\beta'}\delta_{\alpha''\beta''}\int_s V_{\mathrm{RPA}}(p-q-s)V_{\mathrm{RPA}}(p'-q'+s)\\ &\times[G(p''+p-q-s)+G(p''+p'-q'+s)]\\ &\times G(q+s)G(q'-s)K(q+sq'-s;q)\\ &+i\delta_{\alpha\beta''}\delta_{\beta\alpha''}\delta_{\alpha'\beta'}V_{\mathrm{RPA}}(p-q'')\\ &\times G(p+p'-q'')K(p''p+p'-q'';q)\\ &+i\delta_{\alpha\beta}\delta_{\alpha'\beta''}\delta_{\beta'\alpha''}V_{\mathrm{RPA}}(p'-q'')\\ &\times G(p+p'+q'')K(p+p'-q''p'';q)\}. \end{aligned}\quad (3.64)$$

Again making the LMDA, this time in (3.63), we find

$$\begin{aligned}\bar{K}_{\alpha\alpha'\alpha'';\beta\beta'\beta''}&(pp'p'';qq'q'')\\ &\simeq[1-\zeta_{\mathrm{RPA}}(p;p')]^{-1}I_{\alpha\alpha'\alpha'';\beta\beta'\beta''}(pp'p'';qq'q''). \end{aligned}\quad (3.65)$$

Having determined K and its G derivative at $U=0$, we can now proceed to compute Σ.

Letting $U=0$ in (3.52) and using (3.61), we get

$$\begin{aligned}\Sigma_E(p)\simeq i\int_r &V_{\mathrm{RPA}}(r)\\ &\times[1-V_{\mathrm{RPA}}(r)\chi(r)+\bar{\zeta}_{\mathrm{RPA}}(p;p+r)]G(p+r), \end{aligned}\quad (3.66)$$

where

$$\bar{\zeta}=\zeta(1-\zeta)^{-1}. \quad (3.67)$$

The three terms in (3.66), in the order written, represent, respectively, the RPA, the RPA-screened polarization (with the correct minus sign), and the exchange ladder contributions. The direct ladder graphs do not contribute to Σ_E, at least in the LMDA for $K(pp';q)$, by virtue of $V_{\mathrm{RPA}}(0)$ vanishing.

The computation of the kernel L is quite tedious. We look at each piece of Σ_E' separately, starting with Σ_{Kd}. Applying (2.41) to (3.56) and using (3.39), (3.48), (3.65), (3.64), and (3.61), we find, after some labor,

$$\begin{aligned}L_{Kd}(p;q\mid r)\simeq&-2iV_{\mathrm{RPA}}(p-q)\bar{\zeta}_{\mathrm{RPA}}(p;q+r)\\ &-i\int_s J_{Kd}(pqrs)G(s), \end{aligned}\quad (3.68)$$

where

$$\begin{aligned}J_{Kd}(pqrs)=&[1-\zeta_{\mathrm{RPA}}(p;s)]^{-1}\{2i[1-\zeta_{\mathrm{RPA}}(s-r;q+r)]^{-1}\\ &\times[V_{\mathrm{RPA}}(r)^2+V_{\mathrm{RPA}}(s-p-r)V_{\mathrm{RPA}}(s-q-r)]G(s-r)\\ &+4\int_t[1-\zeta_{\mathrm{RPA}}(s-t;q+t)]^{-1}V_{\mathrm{RPA}}(t)^2V_{\mathrm{RPA}}(p-q-t)\\ &\times[G(r+p-t)+G(r+q+t)]G(s-t)G(q+t)\}. \end{aligned}\quad (3.69)$$

The function J_{Kd} owes its origin to the G derivative of K. The exchange ladder graphs, after similar calculations, lead to

$$\begin{aligned}L_{Ke}(p;q\mid r)\simeq& iV_{\mathrm{RPA}}(r)\bar{\zeta}_{\mathrm{RPA}}(p;q+r)\\ &+i\int_s J_{Ke}(pqrs)G(s), \end{aligned}\quad (3.70)$$

with

$$\begin{aligned}J_{Ke}(pqrs)=&[1-\zeta_{\mathrm{RPA}}(p;s)]^{-1}\\ &\times\{-2i\zeta_{\mathrm{RPA}}(p;s)V_{\mathrm{RPA}}(p-s)V_{\mathrm{RPA}}(q-s)\\ &\times[G(r+s)+G(p+q+r-s)]\\ &+i[1-\zeta_{\mathrm{RPA}}(s-r;q+r)]^{-1}V_{\mathrm{RPA}}(r)\\ &\times[V_{\mathrm{RPA}}(r+p-s)+V_{\mathrm{RPA}}(r+q-s)]G(s-r)\\ &+2\int_t[1-\zeta_{\mathrm{RPA}}(s-t;q+t)]^{-1}V_{\mathrm{RPA}}(t)V_{\mathrm{RPA}}(p-s+t)\\ &\times V_{\mathrm{RPA}}(q-s+t)[G(r+s-t)+G(r+p+q-s+t)]\\ &\times G(s-t)G(q+t)\}. \end{aligned}\quad (3.71)$$

The first term in the curly brackets of (3.71), having no counterpart in (3.69), can be traced back essentially to $\delta\mathcal{V}/\delta G$, where $\mathcal{V}$ is the one in (3.57). This term is proportional to $V_{\mathrm{RPA}}(0)$ in the case of the direct ladder graphs and hence vanishes. We emphasize that the LMDA has been used to obtain the formulas (3.68) and (3.71) for L_{Kd} and L_{Ke}. This approximation is of course not necessary to compute L_{pol}, which reads

$$L_{\mathrm{pol}}(p;q\,|\,r)=-iV_{\mathrm{RPA}}(r)^2\chi(r)+i\int_s J_{\mathrm{pol}}(pqrs)G(s)\,, \tag{3.72}$$

where

$$\begin{aligned}J_{\mathrm{pol}}(pqrs)&=2iV_{\mathrm{RPA}}(p-s)\,V_{\mathrm{RPA}}(q-s)\\&\quad\times[1+V_{\mathrm{RPA}}(p-s)\chi(p-s)+V_{\mathrm{RPA}}(q-s)\chi(q-s)]\\&\quad\times[G(r+s)+G(r-s+p+q)].\end{aligned} \tag{3.73}$$

The first term on the right-hand side of (3.72) is due to the U dependence of the direct electron propagator in the screened polarization graph [the third graph in the expansion of Σ in Fig. 8(a)]; the last term in (3.72) comes from the U dependence of the electron loop and the screened Coulomb interaction of the same graph.

To partially check the algebra, let us expand the various terms of L_E in powers of the bare Coulomb potential V and compare the results with those of a direct calculation of L_E to *second order* in V. The relevant graphs are (a)–(e) of Fig. 5. By direct calculation, their contributions to $O(V^2)$ are

$$L_a(p;q\,|\,r)=-2iV(p-q),\qquad L_b(p;q\,|\,r)=iV(r),$$

$$L_d(p;q\,|\,r)=iV(r)^2\chi(r)+2\int_s V(p-s)V(q-s)G(s+r)[G(s)+G(p+q-s)],$$

$$\begin{aligned}L_e(p;q\,|\,r)=-\int_s\{&V(r)[V(r-s+p)+V(r-s+q)]\\&\times G(s)\,G(r-s)+V(p-s)\,V(p+r-s)\\&\times G(s)\,G(r-s+p+q)\}.\end{aligned}$$

The different L_x are given to $O(V^2)$ as

$$L_{\mathrm{RPA}}=L_a+L_b+L_d,\qquad L_{\mathrm{pol}}=-L_d,$$

$$L_{Kd}=L_d,\qquad L_{Ke}=L_e.$$

Expanding (3.49), (3.72), (3.68), and (3.70) in powers of V, we find expressions for L_{RPA} and L_{pol} which are identical to those given above. The results for L_{Kd} and L_{Ke} are different in that

$$2\int_s V(p-s)V(q-s)G(s+r)G(p+q-s)\rightarrow 2\int_s V(p-q)V(q-s)G(s+r)G(p+q-s) \tag{3.74}$$

for $L_{Kd}=L_d$ and

$$\begin{aligned}-\int_s V(p-s)V(p+r-s)G(s)G(r-s+p+q)&\equiv-\int_s V(s)V(r-s)G(s+p)G(r-s+q)\\&\rightarrow-\int_s V(s)V(r)G(s+p)G(r-s+q)\end{aligned} \tag{3.75}$$

for $L_{Ke}=L_e$. The reason for these discrepancies is that (3.68) and (3.70) are *approximate* expressions arrived at by making the LMDA. In fact, the significance of LMDA can clearly be seen in the approximations associated with the replacements (3.74) and (3.75). In (3.74) the replacement $V(p-s)\rightarrow V(p-q)$ is suggested by the fact that $V(q-s)$ is large for $s\simeq q$. Similarly, in (3.75) the dominance of $V(s)$ at $s\simeq 0$ suggests letting $V(r-s)\rightarrow V(r)$.

The complete expression for L_E is the sum of (3.49), (3.72), (3.68), and (3.70). Given L_E, we may proceed to calculate the dielectric function ϵ in the now familiar way using the LMDA. We shall refer to ϵ so obtained as the dielectric function in the high–low-density approximation ϵ_{HLDA}. We shall not bother to write down ϵ_{HLDA} explicitly, since its form is quite complicated. It seems that further approximations must be made to the kernel L_E before a numerical exploration of the dielectric function can profitably be undertaken. We hope to investigate these matters in the future.

To conclude this section, we shall briefly discuss the relation of our scheme of treating the metallic density regime of the electron gas and contrast it with the interpolation procedures used by various authors. First of all, it must be realized that our scheme is much more comprehensive in that we have developed a formalism for calculating the various *full* Green's functions, although in this paper the emphasis has been on the dielectric function. In contrast, Wigner[3] and others[5] were mainly interested in computing quantities such as the correlation energy, specific heat, spin susceptibility, etc. In such a case, it is by far simpler to use *ad hoc* interpolation procedures for these quantities or for the dielectric function (or some function related to it) from which the latter may be calculated. These interpolation procedures are clearly insufficient for a deeper understanding of the physics of the electron gas. In particular, they are totally inadequate when one wishes to study the behavior of the electron gas as a function of the electron density. Inasmuch as the methods of this section for calculating the dielectric function go far beyond the RPA, it is expected that they may enable one to penetrate deeper into the low-density regime than has hitherto been possible. Whether or not these methods will suffice to treat the important question of phase transitions is at present unclear and is being investigated.

IV. DISCUSSION

In this paper we have attempted to develop practical approximation schemes for calculating the various electron Green's functions. Our approach has been general, although in applications we have concentrated on computing the longitudinal dielectric function ϵ from which most of the physically interesting quantities may be obtained. We have determined ϵ in a number of approximations by selecting and summing successively larger sets of graphs for the self-energy functional Σ. In obtaining closed-form solutions for ϵ, an essential use was made of the LMDA which allowed us to avoid solving linear integral equations for the various contracted four-point Green's functions. The domain of validity of LMDA is at present not clear and remains to be explored. Some optimism for LMDA may be generated by the observation that $\epsilon_{\text{GRPA}'}$, whose derivation required making the LMDA, led to a plasmon dispersion relation in good agreement with that obtained by Singwi *et al.*[8]

It is difficult to judge the quality of the various approximate expressions for ϵ obtained in this paper without making some numerical calculations. These we hope to undertake in a sequel to this paper, at least for the simpler forms of ϵ; an exploration of ϵ_{HLDA} should perhaps be deferred until the validity of LMDA is understood in simpler contexts. Although the expressions obtained for the various approximate ϵ's are rather complicated, especially for ϵ_{HLDA}, nevertheless they are in the form of quadratures and should therefore be susceptible to direct numerical analysis, perhaps after some further simplifying approximations.

The problem of self-consistency merits some discussion. In this paper self-consistency was achieved by requiring that the self-energy functional Σ, needed to obtain the exact single-particle propagator G, be computed by perturbation theory in terms of G itself. The result of this requirement was a self-consistent nonlinear Dyson equation for G. More sophisticated calculational schemes come to mind in which higher-order Green's functions or their contractions are also treated self-consistently. For example, we may imagine the following procedure. All bare Coulomb interactions are replaced by screened ones according to the prescription $V\rightarrow V_{\text{sc}}=V/\epsilon$, where ϵ is the *exact* dielectric function. Taking the usual care to avoid overcounting of graphs, one computes an approximate Σ in terms of V_{sc} and the exact propagator G. Then ϵ is calculated in the manner explained earlier in this paper. As a result, one obtains a self-consistent set of equations for G and ϵ. It is clear that in this scheme the electron screening effects are taken into account more satisfactorily (self-consistently) than before. The price one pays for this is a considerably more complicated set of equations one has to solve.

Although in this paper we have concentrated on the case of an electron gas without externally imposed fields, it is quite straightforward to account for these fields in our formalism. All one has to do is to take everywhere the limit $U\rightarrow U_{\text{ext}}$ instead of $U\rightarrow 0$. The problem of solving equations for the various Green's functions is, of course, by far more difficult when $U_{\text{ext}}\neq 0$.

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APPENDIX

We first wish to explore the possibility of self-consistently solving the $U=0$ Dyson's equation in the HFA,

$$G(p)^{-1}=K(p)-i\int_r V(r)G(p+r). \qquad (3.14)$$

Then we shall make a few comments regarding the general case.

Let $r\rightarrow r-p$ in (3.14) above and put

$$\delta\mathcal{E}(p)=i\int_r V(r-p)G(r). \qquad (\text{A1})$$

Since V is independent of $(r-p)_0$, $\delta\mathcal{E}(p)$ can depend only on $|\mathbf{p}|$ if we also take into account the rotational symmetry. Hence, using (2.18), we have

$$G(p)=[p_0+\mu-\mathcal{E}_1(p)+ip_0\delta]^{-1}, \qquad (\text{A2})$$

where

$$\mathcal{E}_1(p)=\mathcal{E}_0(p)+\delta\mathcal{E}(p) \qquad (\text{A3})$$

is the quasiparticle energy. Substituting (A2) into (A1), remembering to restore the factor $\exp(ir_0\eta)$ in the integrand, and performing the r_0 integration, we find

$$\delta\mathcal{E}(p)=-\int[d^3r/(2\pi)^3]V(r-p)n(r), \qquad (\text{A4})$$

where

$$n(r)=\theta[\mu-\mathcal{E}_1(r)] \qquad (\text{A5})$$

is the electron distribution function. Performing the angular integrations in (A4) and substituting the result into (A3), we find the following equation for $\mathcal{E}_1$:

$$\mathcal{E}_1(p)=\frac{p^2}{2m}-\frac{e^2}{\pi p}\int_0^\infty dr\, r\ln\left|\frac{p+r}{p-r}\right|\,\theta(\mu-\mathcal{E}_1(r)). \qquad (\text{A6})$$

The appearance of $\mathcal{E}_1$ in the argument of a step function makes (A6) rather formidable. Actually, the equation can be solved fairly easily, at least for high densities, as we shall now show.

Let us introduce

$$p_F=(3\pi^2n)^{1/3}, \qquad (\text{A7})$$

the *free-electron* Fermi momentum, and write

$$x=p/p_F, \qquad y=r/p_F,$$

$$\lambda(x)=2m\mathcal{E}_1(p_Fx)/p_F^2, \qquad \lambda_0=2m\mu/p_F^2. \qquad (\text{A8})$$

Then (3.18) can be put into the dimensionless form

$$\lambda(x)=x^2-\frac{\kappa r_s}{x}\int_0^\infty dy\, y\ln\left|\frac{x+y}{x-y}\right|\theta(\lambda_0-\lambda(y)),\qquad\text{(A9)}$$

where

$$\kappa=(2/\pi)(4/9\pi)^{1/3}\simeq 0.332.\qquad\text{(A10)}$$

The distribution function

$$\begin{aligned}\nu(x)&\equiv n(p_0x)\\&=\theta(\lambda_0-\lambda(x))\end{aligned}\qquad\text{(A11)}$$

evidently depends on the shape of $\lambda(x)$. If $\lambda(x)$ is monotonically increasing, as in the free-electron case, then $\nu(x)$ will be unity for $0\leq x<x_0$ and zero for $x\geq x_0$, where $\lambda(x_0)=\lambda_0$. If, however, $\lambda(x)$ is *not* monotonic but does exhibit local minima and maxima, then $\nu(x)$ may be nonzero for a number of disjoint intervals on the real x axis, as illustrated, for a typical $\lambda(x)$, in Fig. 9. For large x, $\lambda(x)$ must still increase monotonically for otherwise the integral in (A9) would not exist. In fact, it is easy to see that $\lambda(x)\sim x^2$ for $x\rightarrow\infty$. For small enough x, the integral in (A9) starts out as a positive constant times x, regardless of the shape of $\lambda(y)$ in $\theta(\lambda_0-\lambda(y))$. It follows that $\lambda(x)<0$ for sufficiently low x and that electron states close to $\mathbf{p}=\mathbf{0}$ are necessarily populated at all densities, even though the interval from $p=0$ to the nearest cutoff momentum (at which ν becomes zero) may be arbitrarily small. It should be clear that whatever be the shape of $\lambda(x)$, $\nu(x)$ may be specified, for a given fixed value of λ_0, by the numbers $\alpha_i\equiv\alpha_i(\lambda_0)$ and $\beta_i\equiv\beta_i(\lambda_0)$, $i=1,\ldots,N$, where α_i and β_i, respectively, indicate the discontinuities $0\rightarrow1$ and $1\rightarrow0$ in $\nu(x)$. These numbers are subject to the inequalities

$$0=\alpha_1<\beta_1<\alpha_2<\beta_2<\cdots<\alpha_N<\beta_N<\infty.\qquad\text{(A12)}$$

With the above specification of $\nu(x)$ we can do the integral in (A9) and find

$$\lambda(x)=x^2-\kappa r_s F(x),\qquad\text{(A13)}$$

where

$$F(x)=\sum_{i=1}^{N}[f(x,\beta_i)-f(x,\alpha_i)]\qquad\text{(A14)}$$

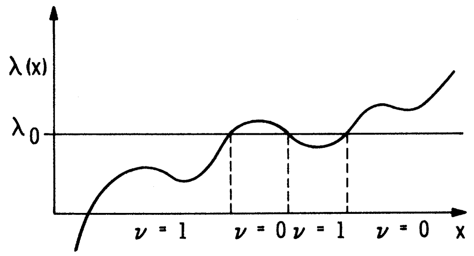

FIG. 9. Plot of a hypothetical function $\lambda(x)$ showing regions of zero and unity values of the distribution function $\nu(x)$.

and

$$f(x,\alpha)\equiv\alpha+(1/2x)(\alpha^2-x^2)\ln|(x+\alpha)/(x-\alpha)|.\qquad\text{(A15)}$$

The function f has the special values

$$\begin{aligned}&f(x,0)=0,&&f(0,\alpha)=2\alpha,\\&f(\alpha,\alpha)=\alpha,&&f(\infty,\alpha)=0,\end{aligned}\qquad\text{(A16)}$$

and the monotonic property

$$f(x,\beta)\geq f(x,\alpha)\quad\text{for}\quad\beta\geq\alpha.\qquad\text{(A17)}$$

In view of (A12), $F(x)>0$ for all finite x. However, neither $F(x)$ nor $\lambda(x)$ is monotonic, in contrast to f. To see this, we examine

$$\lambda'(x)=2x+\kappa r_s\sum_{i=1}^{N}\left(\frac{\beta_i^2+x^2}{2x^2}\ln\left|\frac{x+\beta_i}{x-\beta_i}\right|-\frac{\beta_i-\alpha_i}{x}-\frac{\alpha_i^2+x^2}{2x^2}\ln\left|\frac{x+\alpha_i}{x-\alpha_i}\right|\right).\qquad\text{(A18)}$$

Consider an x such that $\alpha_i<x<\beta_i$ for some arbitrary but fixed value of $i>1$. It is clear that $\lambda'(x)\rightarrow-\infty$ as $x\rightarrow\alpha_i$ and $\lambda'(x)\rightarrow+\infty$ as $x\rightarrow\beta_i$. Thus λ' vanishes somewhere in each interval (α_i,β_i), $i>1$; in the interval $(\alpha_i=0,\beta_i)$ there is easily seen to be no zero of λ'. A similar reasoning establishes zeros of λ' in the intervals (β_i,α_{i+1}) for $i=1,\ldots,N-1$. The conclusion is that $\lambda(x)$ has $2(N-1)$ local extrema, $N-1$ of them maxima and $N-1$ minima by virtue of the fact that $\lambda<0$ for $x\rightarrow0$ and $\lambda\rightarrow+\infty$ as $x\rightarrow+\infty$. Evidently, $\lambda(x)$ will be a solution of (A9) if the equation $\lambda_0=\lambda(x)$, with $\lambda(x)$ computed by (A13), has precisely $2N-1$ zeros located at $\beta_1,\alpha_2,\beta_2,\ldots,\alpha_N,\beta_N$. Thus the α_i and β_i are subject to a self-consistency condition arising from matching the input with the output for given values of λ_0 and r_s. We shall examine this self-consistency condition only for $N=1$, leaving open the question for $N>1$.

The normalization condition

$$n=2\int[d^3p/(2\pi)^3]n(p)\qquad\text{(A19)}$$

can easily be shown to be equivalent to

$$1=\sum_{i=1}^{N}(\beta_i^3-\alpha_i^3).\qquad\text{(A20)}$$

Consider now the $N=1$ case for which only $\beta_1\equiv\beta>0$. From (A20) we immediately conclude that $\beta=1$. Equation (A13) then reads

$$\lambda(x)=x^2-\kappa r_s f(x,1).\qquad\text{(A21)}$$

The self-consistency condition is obviously

$$\lambda_0=\lambda(\beta),\qquad\text{(A22)}$$

requiring that the jump in the calculated $\lambda(x)$ should occur precisely at $x=\beta$, as initially assumed. But $\beta=1$, so that using (A21) and $f(1,1)=1$, we get

$$\lambda_0=1-\kappa r_s.\qquad\text{(A23)}$$

If r_s is small, as in the high-density case, then $\lambda_0 \simeq 1$ and hence, by (A8), we find

$$p_F \simeq (2m\mu)^{1/2},$$

the well-known expression for the free-electron Fermi momentum in terms of the chemical potential μ. In the general case, the connection between p_F and μ is given by

$$p_F = (1-\kappa r_s)^{-1}(2m\mu)^{1/2}. \tag{A24}$$

Obviously, the solution breaks down when $r_s > 1/\kappa \simeq 3$, leading to a nonpositive chemical potential, according to (A23). Physically this means that for densities such that $r_s \gtrsim 3$ the $N=1$ solution is unstable and the electron gas chooses a different solution, one with $N>1$. We leave open the interesting question whether self-consistent solutions can be found for $N>1$.

In summary, we have shown the existence of a self-consistent solution to (3.14) valid up to $r_s \simeq 3$. For larger r_s this solution implies a negative chemical potential $\mu = \partial E_0(N)/\partial N$, where $E_0(N)$ is the ground-state energy, and N is the number of electrons in the system. But $\mu < 0$ means that adding a particle to the system lowers its energy or that the solution corresponds to an unstable "ground" state. For $r_s > 3$, one must then search for solutions corresponding to a true ground state such that $\mu > 0$; this we have not done. It is interesting to note that the simple relation $p_F = (2m\mu)^{1/2}$ is valid only in the high-density limit.

In the general case, the Coulomb potential in (3.14) is replaced by a frequency- and G-dependent effective potential, so that instead of (A6) one is faced with a much more difficult nonlinear equation. Yet the qualitative features of the Hartree-Fock case are expected to persist even in the more accurate versions of the Dyson equation. In particular, the likely existence of several different solutions, valid for different ranges of densities, is presumably a general feature and a consequence of the nonlinearity of the Dyson equation.

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[1] Here m and e are the electronic mass and charge. We use units such that $\hbar = 1$.

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[13] Expansions of Σ in terms of G are discussed in Ref. 12, for example.

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[17] Note that Γ is here defined with the four-momentum-conserving δ function factored out; this is by no means the universal practice. Further note that Γ is just the connected part of G with the external single-particle propagators removed. For a discussion of Γ see, for example, J. M. Luttinger, in *Many-Body Theory,* edited by R. Kubo (Benjamin, New York, 1966), p. 86 ff.

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