Antiparallel spin correlations in a many-electron system: A new approach

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As a first step towards understanding many-body effects on the properties of conduction electrons in a metal, an often used model is that of an electron gas against a uniform, neutralizing positive background. Most treatments of even this model problem make simplifying assumptions about the correlations between electrons in order to get solvable equations. In particular, the correlations between antiparallel spins are often neglected since they make the many-body equations nonlinear and, therefore, difficult to handle. On the other hand, these correlations may be expected to influence strongly many properties of the system, particularly those that depend on high momentum transfers. This paper attempts to remedy this shortcoming in the application of many-body theory to an electron gas by seeking a variational treatment of the full nonlinear equations and derives expressions for the dielectric function and the paramagnetic spin susceptibility which express a wide range of electrical and magnetic properties of the system. Our results show, on comparison with previous treatments neglecting antiparallel spin correlation, that inclusion of these correlations has the expected effect of enhancing the spin susceptibility and lowering the compressibility of the system. Further, our technique of working consistently with the complete defining equations may find applicability in a wider class of problems; a specific example is the charged-boson system.

I. INTRODUCTION

An electron gas with a uniform neutralizing positive background has been the subject of intense investigation for the past 40 years or so. There are basically two reasons for this; (i) it provides a useful insight into the properties of simple metals and (ii) it is a mathematical model on which many approximation schemes such as Hartree-Fock (HF), random-phase-approximation (RPA), etc., may all be carried out analytically in great detail. Further, a good knowledge of the uniform system is of great value in the development of the density-functional formalism of the inhomogeneous electron system. For a review of these aspects, one may refer to the book by Pines and Nozières.[1] It has become increasingly clear, however, that these approximations fail to include some significant characteristics of the system which strongly influence the mechanical and magnetic properties of the electron gas. The RPA is suitable mainly for low-momentum transfers or, correspondingly, at high densities (higher than those that obtain in metals), where the interaction between electrons is relatively less important than the kinetic energy. The HF approximation and "generalized RPA"[1] include only one type of exchange correlation between the electrons, called the Pauli correlation, which applies to the case of electrons with parallel spins. A particularly significant drawback of all these approximation schemes is that they treat inadequately the correlations between antiparallel spins. These are very important for large-momentum transfers, corresponding to small interelectron separations, since electrons with antiparallel spins can come close together; electrons with parallel spins are, on the other hand, kept apart by the Pauli principle. The antiparallel spin correlation would, therefore, be expected to influence crucially the Coulomb repulsion between electrons at small separations. The neglect of this correlation shows itself in one form through a serious inadequacy of these approximations which has long been recognized, namely, that the pair-distribution function which should be manifestly positive definite, does instead become negative for small interparticle separations over the range of metallic densities. Another feature pointing to the same inadequacy is that the HF approximation and the generalized RPA make identical predictions about the mechanical and magnetic stability of the system whereas one might expect these to be different, since the sum of the parallel and antiparallel density correlations contribute to the former (depending as it does on the over-all density of the system) whereas the difference of these densities is relevant to the spin and magnetic properties of the system.

In recent years, Singwi and his co-workers[2] have addressed themselves to these problems through an *Ansatz* about the structure of the two-particle distribution function in terms of the one-particle functions and have then sought a self-consistent solution for the pair-distribution function. Though this procedure has partially remedied the situation, it has remained an *ad hoc* procedure with as yet no many-body theoretic derivation or justification of the *Ansatz*. Neither has there been any alternative scheme within many-body theory to remedy the defects. The purpose of this paper is to provide such a scheme.

In the many-body scheme, the effects of interaction on the various properties of the electron gas are discussed in terms of the Green's function for the electron propagator and appropriate vertex functions describing the basic interaction between electrons. The properties of interest are given as integrals over these vertex and Green's functions. The RPA and HF approximations result from a scheme which leads to linear integral equations for the vertex functions which are solved to various levels of approximation. Rajagopal and his coworkers[3a] have looked at a more general, so-called "ladder-bubble" scheme which retains consistently all contributions that explicitly involve the potential to the zeroth and first orders, and they have set up more general nonlinear equations for the vertex functions. A linearized version of these equations leads back to the RPA and HF treatments. The antiparallel spin correlations first appear essentially in such a nonlinear way and, it might, therefore, be expected that the ladder-bubble equations will, in fact, carry the crucial elements we are looking for. So far, however, these equations have proved too difficult to handle and all treatments have restricted themselves to linearized versions of them. Even the linearized equations, in their full complexity, can only be handled numerically or by variational procedures that have been developed for this purpose.[3b-3e] There have been successful applications of such variational procedures both in this problem of the electron gas and in the closely related one for the linearized Boltzmann equation for a Fermi liquid.[4] However, the variational methods, even in their most general formulation[5] till very recently, have been restricted to linear equations and have proceeded by guessing a functional and then establishing that it is indeed a variational estimate of the desired quantity. Very recently,[6] a new, unified, and simple method of constructing variational principles (VP's) has been given which applies to linear and nonlinear equations alike. This procedure opens up the way to handling the full nonlinear equations of the ladder-bubble scheme and we show that, indeed, a proper treatment of the ladder-bubble equations gives us results in the right direction regarding the properties of the electron gas discussed above.

The arrangement of this paper is as follows. In brief in Sec. II, we present the general method[6] for constructing VP's in the context of linear integral equations and show that it leads in a direct fashion, with no ingenuity or guessing, to the expressions that have previously been derived in this context. The aim of this purely pedagogical section is to introduce the general method to those unfamiliar with it in a situation uncluttered by the many terms and indices specific to the nonlinear problem that we are ultimately interested in. Also, this material helps motivate certain choices of trial functions that we make later in Sec. III. The main body of the paper starts in Sec. III which develops for the nonlinear-case VP's for the dielectric function and the paramagnetic spin susceptibility, two functions of special physical interest in that they contain information about the electrical and magnetic properties of the system. In Sec. IV, the variational expressions are examined for different starting choices (trial functions) for the vertex functions like, for instance, the solutions of the RPA. These choices lead to expressions for properties like the compressibility and spin susceptibility of the system, expressions which are of the form derived in the HF and generalized RPA schemes. However, whereas these earlier schemes indicated the appearance of singularities in the compressibility and paramagnetic susceptibility (hinting at a phase transition) at a certain value (same for both properties) of the charge density, the singularities now appear shifted and in opposite directions. This might be taken as an effect of the antiparallel spin correlations whose contribution to these properties would be expected to have opposite signs. Another satisfying feature of the variational solutions we present is that working consistently with the Green's function and the vertex functions in the same order of approximation (the ladder-bubble approximation) leads naturally to the occurrence of "renormalization" terms which make all the integrals finite—these renormalizations have previously been derived,[3] with some ingenuity, in the HF approximation.

The procedure we follow of working with the ladder-bubble equations with no commitment to the specific structure of the vertex and Green's functions till the very end (in our choice of trial approximations to them) makes it equally applicable to both statistics. Thus, though the accent throughout the paper and particularly in the evaluation of integrals at the end is on the many-electron system, the main results are equally applicable to a system of bosons where similar nonlinear equations describe the behavior of a charged-boson gas.[7]

II. VARIATIONAL PRINCIPLES FOR INNER PRODUCTS

If we seek a VP for an inner product

$$\chi = (\phi, \psi), \tag{2.1}$$

where ψ obeys an equation

$$\psi = \phi + \Theta\psi, \tag{2.2}$$

with Θ some linear operator and ϕ a known function, we can follow the procedure of Ref. 6 by writing

$$\chi_v = \chi_t - (L_t, \psi_t - \phi - \Theta\psi_t), \quad \chi_t \equiv (\phi, \psi_t), \tag{2.3}$$

where ψ_t is a trial solution of Eq. (2.2) and L_t is a trial approximation to a "Lagrange function" L

which incorporates the defining equation (2.2) as a constraint. The function L is defined through the process of making χ_v in Eq. (2.3) a variational estimate, that is, by setting terms linear in $\delta\psi \equiv \psi_t - \psi$ and $\delta L \equiv L_t - L$ equal to zero. This leads to

$$L = \phi + L\mathcal{O}. \tag{2.4}$$

If $\mathcal{O}$ is symmetric, it follows that

$$L = \psi. \tag{2.5}$$

Though not necessary, a natural trial choice for L_t is then ψ_t and we have the VP from Eq. (2.3):

$$\chi_v = (\phi, \psi_t) + (\psi_t, \phi) - (\psi_t, \psi_t) + (\psi_t, \mathcal{O}\psi_t). \tag{2.6}$$

Such variational functionals have been set up in different ways by Rajagopal and co-workers[3b–3e] for calculating various response functions of the electron gas in a linearized model, by Wilkins and his co-workers[4] for various transport coefficients, and in a general context in Ref. 5.

Thus, the paramagnetic spin susceptibility of an interacting electron system is given by (in units of $e^2/4m^2c^2$)

$$\chi_{zz}(q) \equiv 2i\int \frac{G(k+q)\Gamma_z(k,q)G(k)d^4k}{(2\pi)^4}, \tag{2.7}$$

where $G(k)$ is a one-particle Green's function (assumed known), k and q are four vectors, and $\Gamma_z(k, q)$ is a vertex function satisfying, in the linear approximation,

$$\Gamma_z(k,q) = -1 + i\int \frac{V(\vec{k}-\vec{k}')G(k'+q)\Gamma_z(k',q)G(k')d^4k'}{(2\pi)^4}; \tag{2.8}$$

$V(\vec{k}-\vec{k}')$ is the symmetric momentum-dependent interaction potential. The problem is of the general form presented above and the VP given in Ref. 3 follows:

$$[\chi_{zz}(q)]_v = [\chi_{zz}(q)]_t - \int (2\pi)^{-4}d^4k\, L_t(k,q) \times \left(\Gamma_{zt}(k,q) + 1 - i\int V(k-k')G(k'+q) \times \Gamma_{zt}(k',q)G(k')d^4k'(2\pi)^{-4}\right), \tag{2.9}$$

with L_t a trial approximation to a function given essentially as in Eq. (2.5), that is,

$$L(k,q) = -2iG(k+q)\Gamma_z(k,q)G(k). \tag{2.10}$$

Likewise, the linearized Boltzmann equation of a Fermi liquid at low temperature is of the form[4]

$$X(t) = f(t)Q(t) - \alpha\int_{-\infty}^{\infty} dt' F(t-t')Q(t'), \tag{2.11}$$

where t is an energy variable and $Q(t)$ is related to the deviation from equilibrium of the distribution function. For the thermal conductivity κ,

$$\kappa \equiv \int_{-\infty}^{\infty} dt\, Q(t)X(t), \tag{2.12}$$

the external force term $X(t)$ is $t/\cosh\frac{1}{2}t$, $f(t) = \pi^2 + t^2$ and the kernel $F(t)$, arising from the collision integral, is $\frac{1}{2}t/\sinh\frac{1}{2}t$. α is a ratio of two angular averages of the collision probability. Equations (2.11) and (2.12) are again of the general form, Eqs. (2.1) and (2.2), and the variational expression that follows from Eq. (2.6) is the one considered earlier by Wilkins and his co-workers.[4] It may be mentioned that exact solutions of these transport problems were also found independently by Brooker and Sykes[8] and by Jensen *et al.*[9] and the variational bounds are in excellent agreement with these exact results.

III. NONLINEAR VERTEX EQUATION

A. Definitions and background

The full equations for the vertex functions of a many-electron system are in the form of an infinite hierarchical set of equations. When one retains all contributions from terms that explicitly involve the potential up to the first power, one gets the closed set of equations of the ladder-bubble scheme[3] which are coupled non-linear equations for the Green's function $G(k)$, and the spin-susceptibility and density vertex functions, $\Gamma_z(k, q)$ and $\Gamma(k, q)$, respectively. The equations are

$$\Gamma(k,q) = -1 - 2iV(\vec{q})\int \tilde{\Gamma}(k',q)dk' - i\int V(\vec{k}-\vec{k}')\tilde{\Gamma}(k',q)\Gamma(k,k'-k)dk', \tag{3.1}$$

$$\Gamma_z(k,q) = -1 - i\int V(\vec{k}-\vec{k}')\tilde{\Gamma}_z(k',q)\Gamma(k,k'-k)\,dk', \tag{3.2}$$

$$G^{-1}(k) = k_0 - \frac{\vec{k}^2}{2m} - i\int V(\vec{k}'-\vec{k})G(k')\Gamma(k,k'-k)\,dk'; \tag{3.3}$$

for compactness, we have introduced the following notation which we follow throughout this paper:

$$\tilde{\mathcal{O}}(k,q) \equiv G(k+q)\mathcal{O}(k,q)G(k), \quad dk \equiv d^4k(2\pi)^{-4}.$$

For the charged system of interest to us $V(\vec{q}) = 4\pi e^2/\vec{q}^2$, the Coulomb potential. Note the absence of the "bubble" term in the equation for the spin vertex function, Eq. (3.2).

As is well known, physical quantities of interest such as those that characterize the response of the system to external fields are intimately related to the correlations in the system described by the above vertex functions. Thus, the density-density response function $\chi(q)$, is defined by

$$\chi(q) = 2i\int \tilde{\Gamma}(k,q)dk, \tag{3.4}$$

whereas the spin susceptibility is given in similar fashion by Eq. (2.7). The dielectric function $\epsilon(q)$, another important characteristic of the system, is

defined by

$$\epsilon(q) = [1 + V(q)\chi(q)]^{-1}. \tag{3.5}$$

The familiar approaches to obtaining χ, χ_{zz}, and ϵ have consisted, first of all, in linearizing (and, simultaneously, decoupling) Eqs. (3.1)–(3.3) by replacing $\Gamma(k, k'-k)$ in these equations by -1, the first term in the right-hand side of Eq. (3.1), and then proceeding as if G were a known function everywhere it occurs in Eqs. (3.1) and (3.2). We considered in Sec. II such a procedure for obtaining χ_{zz}. In the simple RPA, one goes further by dropping all together the final terms in the three equations which depend on $V(\vec{k}-\vec{k}')$. A complete solution can then be obtained in the form

$$\Gamma_{\mathrm{RPA}}(k, q) = -[1 + 2V(q)I(q)]^{-1}, \tag{3.6}$$

where $I(q)$ is defined by

$$I(q) \equiv i\int G_0(k+q)G_0(k)\,dk, \quad G_0(k) \equiv (k_0 - \vec{k}^2/2m)^{-1}. \tag{3.7}$$

Note that $\Gamma_{\mathrm{RPA}}(k, q)$ is a function of q alone. As a consequence, we have

$$\chi_{\mathrm{RPA}}(q) = 2I(q)\Gamma_{\mathrm{RPA}}(q), \tag{3.8}$$

$$\epsilon_{\mathrm{RPA}}(q) = 1 + 2V(q)I(q) = -1/\Gamma_{\mathrm{RPA}}(q). \tag{3.9}$$

On the other hand, retention of the linearized terms in Eqs. (3.1)–(3.3) is the content of the HF and generalized RPA models. There are two versions of this, one employing -1 in place of $\Gamma(k, k'-k)$ in these equations and the second which uses instead the RPA value for this function. Because of Eq. (3.9), the second version can be interpreted as differing from the first in that it employs a screened potential, $V(k-k')/\epsilon(k-k')$, in place of the unscreened potential. In either version, note that the Green's function is more complicated than the $G_0(k)$ used in the RPA though it may still be regarded as a known function where it appears in Eqs. (3.1) and (3.2). (We note that the terms RPA and HF have been used in different ways in the literature. Our usage, as indicated by this paragraph, is to have them represent a natural sequence of linearization procedures of the many-body equations. This usage differs from the one in Ref. 1. In particular, our RPA is a much simpler approximation than the RPA of Ref. 1 which corresponds to the next level of sophistication which we call the HF approximation.)

Before seeking VP's for χ, χ_{zz}, and ϵ without making these simplifying approximations of earlier treatments, we note that the vertex function Γ is often cast in an alternative form Λ given by

$$\Lambda(k, q) \equiv \Gamma(k, q)\epsilon(q). \tag{3.10}$$

The corresponding vertex equation is

$$\Lambda(k, q) = -1 - i\int \frac{V(k'-k)}{\epsilon(k'-k)} \times \tilde{\Lambda}(k', q)\Lambda(k, k'-k)\,dk', \tag{3.11}$$

with, correspondingly,

$$G^{-1}(k) = G_0^{-1}(k) - i\int \frac{V(k'-k)}{\epsilon(k'-k)} G(k')\Lambda(k, k'-k)\,dk'. \tag{3.12}$$

The dielectric function is given by an equation of the form

$$\epsilon(q) = 1 - 2iV(\vec{q})\int \tilde{\Lambda}(k', q)\,dk'. \tag{3.13}$$

This is the usual alternative formulation[1] of the dielectric response of a system expressed not with respect to the externally applied potential but with respect to a screened effective potential felt by the particles. Thus, Eqs. (3.11) and (3.12), which are similar to (3.1) and (3.3) except that they involve the screened potential, may be interpreted as representing all contributions that arise from terms up to the first order in the screened potential. We choose in what follows to work with the functions Γ but it is evident that all the steps can be immediately carried over to a description in terms of Λ.

B. Variational principle

The methods of Ref. 6 allow us to construct VP's for χ [once a VP for χ is known, a VP for ϵ follows immediately from Eq. (3.5)] and χ_{zz} even though the defining equations of the system are nonlinear and, in fact, with no more difficulty than in the linear case considered in Sec. II. Though the expressions look longer and more cumbersome now, they are just as simple and natural as those in Eqs. (2.3)–(2.6). The basic philosophy is that we begin by writing a functional in terms of trial functions, Γ_t, Γ_{zt}, and G_t, that will coincide with the quantity of interest when the trial functions are replaced by their exact values and which incorporates the defining equations of the system, Eqs. (3.1)–(3.3), as constraints with the help of Lagrange functions. We therefore, write

$$\chi_v(q) = 2i\int \tilde{\Gamma}_t(k, q)\,dk - \int\int dk\,dq' L_{1t}(k, q, q')\left(\Gamma_t(k, q') + 1 + 2iV(q')\int \tilde{\Gamma}_t(k', q')\,dk' + i\int V(k-k')\tilde{\Gamma}_t(k', q')\Gamma_t(k, k'-k)\,dk'\right) - \int dk L_{2t}(k, q)\left[G_t(k)\left(G_0^{-1}(k) + i\int V(k'-k)G_t(k')\Gamma_t(k, k'-k)\,dk'\right) - 1\right], \tag{3.14}$$

where we have used Eqs. (3.1), (3.3), and (3.4), and

$$[\chi_{zz}(q)]_v = 2i\int \tilde{\Gamma}_{zt}(k,q)\,dk - \int dk\, L_{3t}(k,q)\left(\Gamma_{zt}(k,q) + 1 + i\int V(k-k')\tilde{\Gamma}_{zt}(k',q)\Gamma_t(k,k'-k)\,dk'\right) - \iint dk\,dq' L_{4t}(k,q,q')$$
$$\times\left(\Gamma_t(k,q') + 1 + 2iV(q')\int \tilde{\Gamma}_t(k',q')\,dk' + i\int V(k-k')\tilde{\Gamma}_t(k',q')\Gamma_t(k,k'-k)\,dk'\right)$$
$$- \int dk\, L_{5t}(k,q)\left[G_t(k)\left(G_0^{-1}(k) + i\int V(k'-k)G_t(k')\Gamma_t(k,k'-k)\,dk'\right) - 1\right], \tag{3.15}$$

where we have used Eqs. (2.7) and (3.1)–(3.3). We note that the density-density response function is defined through Γ and G alone, whereas the spin susceptibility requires knowledge of all the three functions Γ_z, Γ, and G. This is easily understood because the spin properties of the system will depend also on the total density (parallel and antiparallel spins) of the system and hence the corresponding vertex function Γ will feature in their description, whereas Γ_z plays no role in quantities such as χ and ϵ. Thus all three defining equations (3.1)–(3.3) have to be incorporated as constraints in writing Eq. (3.15), whereas Eq. (3.2) need not be considered in writing down Eq. (3.14).

The defining equations for the five Lagrange functions follow in a straightforward manner [almost by inspection of Eqs. (3.14) and (3.15)] on setting equal to zero all terms linear in $\delta\Gamma \equiv \Gamma_t - \Gamma$, $\delta\Gamma_z \equiv \Gamma_{zt} - \Gamma_z$, and $\delta G \equiv G_t - G$ in Eqs. (3.14) and (3.15). Some fairly routine steps of interchanging variables of integration and simple algebra leads to

$$L_1(k,q,q') = 2iG(k+q')\,G(k)\,\delta(q-q') + A(k,q,q';L_1,L_2), \tag{3.16}$$

$$L_2(k,q) = 2i[\tilde{\Gamma}(k-q,q) + \tilde{\Gamma}(k,q)] + B(k,q;L_2,L_1), \tag{3.17}$$

$$L_3(k,q) = 2iG(k+q)G(k) - i\int V(k'-k)\,G(k+q)\,G(k)\,L_3(k',q)\,\Gamma(k',k-k')\,dk', \tag{3.18}$$

$$L_4(k,q,q') = -iL_3(k,q)\,V(q')\tilde{\Gamma}_z(k+q',q) + A(k,q,q';L_4,L_5), \tag{3.19}$$

$$L_5(k,q) = 2i[\tilde{\Gamma}_z(k-q,q) + \tilde{\Gamma}_z(k,q)] + B(k,q;L_5,L_4)$$
$$- i\int dk' L_3(k',q)[V(k'-k+q)\,\tilde{\Gamma}_z(k-q,q)\Gamma(k',k-k'-q) + V(k'-k)\,\tilde{\Gamma}_z(k,q)\,\Gamma(k',k-k')]. \tag{3.20}$$

We have defined the functions

$$A(k,q,q';L_i,L_j) = -2iV(q')\,G(k+q')\,G(k)\int L_i(k',q,q')\,dk' - i\int V(k'-k)\,G(k+q')\,G(k)L_i(k',q,q')\Gamma(k',k-k')\,dk'$$
$$- i\int V(q')\,\tilde{\Gamma}(k+q',k'-k)\,L_i(k,q,k'-k)\,d(k'-k) - iL_j(k,q)\,G(k)\,G(k+q')\,V(q'),$$

$$B(k,q;L_i,L_j) = -\int L_i(k',q)\,V(k-k')\,\tilde{\Gamma}(k',k-k')\,dk' - 2i\iint dk'\,dq' V(q')\,L_j(k',q,q')[\tilde{\Gamma}(k-q',q') + \tilde{\Gamma}(k,q')]$$
$$- i\iint dk'dq' L_j(k',q,q')\,[V(k'-k+q')\,\tilde{\Gamma}(k-q',q')\,\Gamma(k',k-k'-q') + V(k'-k)\,\tilde{\Gamma}(k,q')\Gamma(k',k-k')].$$

These two sets of coupled equations, one of L_1 and L_2 and the other of L_3, L_4, and L_5 play, respectively, roles in determining the electrical and magnetic properties of the system. Though they appear formidable and do not immediately admit solutions as was the case in Sec. II, all that we require as inputs into the variational expressions are some trial solutions of them; fairly tractable choices of such trial functions can be justified without difficulty within the context of our analysis. A natural starting point would be to take the solutions which follow from the linear approximation as the trial choices. Thus, as a "zeroth order" trial approximation $L_{3t}^{(0)}$, to L_3 as given in Eq. (3.18), we can pick the solution developed in Eq. (2.10):

$$L_{3t}^{(0)}(k,q) = -2iG_t(k+q)\,\Gamma_{zt}(k,q)\,G_t(k). \tag{3.21}$$

That this choice is reasonable is confirmed by recalling that our analysis is in the ladder-bubble scheme so that one can consistently drop all terms that explicitly involve the potential to higher than the first power. The corrections to $L_{3t}^{(0)}$ are precisely of such a form as can be seen by substituting $L_{3t}^{(0)}$ into the right-hand side of Eq. (3.18) to get the next order of approximation, $L_{3t}^{(1)}$ say. The additional terms that appear involve higher powers of the potential and since the trial Lagrange functions are ultimately to be used in the variational expressions where they appear multiplied by terms which are already of $O(V)$ (even with the simplest

possible choices $\Gamma_t = -1$, $\Gamma_{zt} = -1$), such zeroth-order trial approximations are entirely adequate. Exactly similar situations obtain for the other Lagrange functions and, in each case, by inspection of the first terms on the right-hand side of Eqs. (3.16)–(3.20), we can write

$$L_{1t}^{(0)}(k,q,q') = -2iG_t(k+q) \times \Gamma_t(k,q)\, G_t(k)\, \delta(q-q'), \tag{3.22}$$

$$L_{2t}^{(0)}(k,q) = -2i[\tilde{\Gamma}_t(k-q,q) + \tilde{\Gamma}_t(k,q)]\, \Gamma_t(k,q), \tag{3.23}$$

$$L_{4t}^{(0)}(k,q,q') = -iL_{3t}^{(0)}(k,q)\, V(q')\, \tilde{\Gamma}_{zt}(k+q',q), \tag{3.24}$$

$$L_{5t}^{(0)}(k,q) = -2i[\tilde{\Gamma}_{zt}(k-q,q) + \tilde{\Gamma}_{zt}(k,q)]\, \Gamma_{zt}(k,q). \tag{3.25}$$

We note that of the five trial Lagrange functions, one L_{4t}, is of $O(V)$, even in the zeroth-order approximation; hence, it contributes to the variational results only in $O(V^2)$ and can be dropped entirely from our analysis. Physically, what this indicates is that even though magnetic properties of the system depend on the overall density since the Γ_z equation involves Γ, we can proceed to consider the Γ as a given function for this stage of the analysis since variations in Γ (handled by the Lagrange constraint L_4) introduce errors of higher order than are of interest.

IV. VARIATIONAL RESULTS FOR THE DIELECTRIC FUNCTION AND SUSCEPTIBILITY

In Sec. III, we have formally constructed the variational principles for χ and χ_{zz} by setting up the well-defined problem that trial solutions of the original ladder-bubble equations (3.1)–(3.3), and of an adjoint set of equations (3.16)–(3.20), are to be used in evaluating Eqs. (3.14) and (3.15) and we have developed the appropriate trial Lagrange functions in terms of trial estimates of the original Green's and vertex functions. We now proceed to apply these results with simple choices for such estimates as, for instance, the values of these estimates given by standard approximations like the RPA.

Consider first the simple RPA results in Eqs. (3.6)–(3.9). Substituting $\Gamma_t = \Gamma_{\mathrm{RPA}}(q)$ and $G_t = G_0$ into Eq. (3.14) and using Eqs. (3.22) and (3.23) we get

$$\chi_v(q) = 2\Gamma_{\mathrm{RPA}}(q) I(q) - 2\Gamma_{\mathrm{RPA}}^2(q)[J_1(q) + J_2(q)], \tag{4.1}$$

where we have defined

$$J_1(q) \equiv -\int\!\!\int dk\, dk'\, G_0(k+q)\, G_0(k)\, V_s(k'-k) \times G_0(k'+q)\, G_0(k'), \tag{4.2a}$$

$$J_2(q) \equiv -\int\!\!\int dk\, dk'\, G_0^2(k)[G_0(k-q) + G_0(k+q)] \times V_s(k'-k)\, G_0(k'), \tag{4.2b}$$

$$V_s(k'-k) \equiv V(k'-k)/\epsilon_{\mathrm{RPA}}(k'-k). \tag{4.2c}$$

Contrasting Eq. (4.1) with (3.8), we observe the "corrections" in the variational estimate for χ as compared with the RPA value; the corrections are of first order in the screened potential. Correspondingly, the dielectric function is improved from its trial RPA value in Eq. (3.9) to the variational estimate given by Eqs. (3.5) and (4.1):

$$\epsilon_v(q) = [1 + 2V(q)\, I(q)]^2 \{1 + 2V(q)[I(q) - J(q)]\}^{-1}, \tag{4.3}$$

where we have defined

$$J(q) \equiv J_1(q) + J_2(q). \tag{4.4}$$

Likewise, for the magnetic properties, on using $\Gamma_{zt} = \Gamma_{z,\mathrm{RPA}} = -1$, we have

$$[\chi_{zz}(q)]_v = -2[I(q) + J(q)]. \tag{4.5}$$

The above expressions are already interesting because they make contact, in certain interesting limits such as static low momentum transfers ($q_0 = 0$, $\vec{q} \to 0$) with previous results derived by a variational formulation of the HF approximation or by moment-conserving schemes[10] even though we have not as yet used the full power of the variational scheme by having open parameters in terms of which a stationary value is sought. We have merely frozen the trial choice to be the RPA value and then we observe that whereas

$$\lim_{q \to 0} q^2 \epsilon_{\mathrm{RPA}}(q) = 8\pi e^2 I(0), \tag{4.6}$$

we obtain

$$\lim_{q \to 0} q^2 \epsilon_v(q) = 8\pi e^2 I^2(0)[I(0) - J(0)]^{-1}, \tag{4.7}$$

which agrees with results previously derived in more complicated approximations.[3c] The above expressions, which give the compressibility of the system, can be put in a standard form by evaluating the integrals. I and J coincide with functions defined in Ref. 3d, where they have also been evaluated for a certain choice of the screened potential. A slightly simpler version, employing the unscreened potential in J instead of the screened one, has been given in Ref. 3c; the integrals can be cast in the form

$$I(q) = \int \frac{d^3k}{(2\pi)^3} \frac{F_0(\vec{k} + \tfrac{1}{2}\vec{q}) - F_0(\vec{k} - \tfrac{1}{2}\vec{q})}{q_0 - \vec{k}\cdot\vec{q}/m}, \tag{4.8a}$$

$$J_1(q) = \int\!\!\int \frac{d^3k\, d^3k'}{(2\pi)^6} \frac{F_0(\vec{k} + \tfrac{1}{2}\vec{q}) - F_0(\vec{k} - \tfrac{1}{2}\vec{q})}{q_0 - \vec{k}\cdot\vec{q}/m} \times V(\vec{k}' - \vec{k}) \frac{F_0(\vec{k}' + \tfrac{1}{2}\vec{q}) - F_0(\vec{k}' - \tfrac{1}{2}\vec{q})}{q_0 - \vec{k}'\cdot\vec{q}/m}, \tag{4.8b}$$

$$J_2(q) = -\int\!\!\int \frac{d^3k\, d^3k'}{(2\pi)^6} \frac{F_0(\vec{k} + \tfrac{1}{2}\vec{q}) - F_0(\vec{k} - \tfrac{1}{2}\vec{q})}{q_0 - \vec{k}\cdot\vec{q}/m}$$

$$\times V(\vec{k}'-\vec{k})\,\frac{F_0(\vec{k}'+\frac{1}{2}\vec{q})-F_0(\vec{k}'-\frac{1}{2}\vec{q})}{q_0-\vec{k}\cdot\vec{q}/m}\,, \tag{4.8c}$$

where $F_0(\vec{k})$ is the usual Fermi function. These integrals have been evaluated[3c] in the $q\to 0$ limit. In terms of the usual definitions: k_F, the Fermi momentum; n, the electron density,

$$q_{\mathrm{TF}}^2\equiv\frac{6\pi ne^2}{k_F}\,,\quad \alpha^3\equiv\frac{4}{9\pi}\,,\quad \alpha k_F r_s a_0\equiv 1\,, \tag{4.9}$$

they lead to the following familiar values for the compressibility:

$$\lim_{q\to 0} q^2\epsilon_{\mathrm{RPA}}(q)=q_{\mathrm{TF}}^2\,, \tag{4.10}$$

$$\lim_{q\to 0} q^2\epsilon_v(q)=q_{\mathrm{TF}}^2(1-\alpha r_s/\pi)^{-1}. \tag{4.11}$$

The characteristic denominator in Eq. (4.11) is responsible for the familiar mechanical instability that develops in the many electron system in approximations beyond the RPA.

We emphasize the natural occurrence of the combination J_1+J_2 in the variational estimates, a feature of great importance because, as is well known, these integrals are separately divergent and only their sum is finite. This "renormalization" has previously been derived in the HF approximation by cleverly manipulating the energy denominators in G_{HF}.[3d] We note that even with the simplest trial choices of Γ_{RPA} and G_0, the renormalization occurs naturally in the variational formulation through the incorporation of the proper equation for G, Eq. (3.3), as can be verified by tracing J_2 back to Eq. (3.23).

The above results have made contact with previously well-known results derived in an entirely different way. We can immediately proceed further by allowing some flexibility in the choice of the trial functions. The choice we make of taking $\Gamma_t(k,q)$ and $\Gamma_{zt}(k,q)$ to be similar to the RPA values in being functions of q alone but allowing the form of these functions to vary has been used before in the linear approximation.[3] We write

$$\Gamma_t(k,q)=\lambda(q)\Gamma_{\mathrm{RPA}}(q)\,, \tag{4.12a}$$

$$\Gamma_{zt}(k,q)=\mu(q)\Gamma_{z,\mathrm{RPA}}(q)=-\mu(q)\,, \tag{4.12b}$$

where $\lambda(q)$ and $\mu(q)$ are "scaling" factors which will be determined by demanding stationarity of the variational expressions. From Eqs. (3.14), (3.22), and (3.23), we now obtain in place of Eq. (4.1),

$$\chi_v(q)=4\lambda(q)\,\Gamma_{\mathrm{RPA}}(q)\,I(q)+2\lambda^2(q)\Gamma_{\mathrm{RPA}}^2(q)\times\{I(q)[1+2V(q)I(q)]-\mathcal{J}(q)\}\,, \tag{4.13}$$

and from Eqs. (3.15), (3.21), (3.24) and (3.25), we get

$$[\chi_{zz}(q)]_v=-4\mu(q)\,I(q)+2\mu^2(q)[I(q)-\mathcal{J}(q)]\,, \tag{4.14}$$

where

$$\mathcal{J}(q)\equiv\mathcal{J}_1(q)+\mathcal{J}_2(q)\,,$$

and the $\mathcal{J}_i$ are similar to the integrals J_i defined earlier:

$$\mathcal{J}_1(q)\equiv-\iint dk\,dk'\,G_0(k+q)\,G_0(k)\,\lambda(k'-k)\times V_s(k'-k)\,G_0(k'+q)\,G_0(k')\,, \tag{4.15a}$$

$$\mathcal{J}_2(q)\equiv-\iint dk\,dk'\,G_0^2(k)\lambda(k'-k)\,V_s(k'-k)\times[G_0(k-q)+G_0(k+q)]\,G_0(k')\,. \tag{4.15b}$$

We vary Eq. (4.13) with respect to λ to determine the "best" value and this leads to the following integral equation:

$$I(q)+\lambda(q)\Gamma_{\mathrm{RPA}}(q)\{I(q)[1+2V(q)I(q)]-\mathcal{J}(q)\}-\tfrac{1}{2}\lambda^2(q)\Gamma_{\mathrm{RPA}}(q)J(q)=0. \tag{4.16}$$

Solutions of this integral equation [$\mathcal{J}(q)$ involves λ under an integral] are then to be used in Eqs. (4.13) and (4.14). We will not attempt a full solution of this integral equation here but "freezing" the dependence[11] of $\mathcal{J}$ on λ, we solve Eq. (4.16) as a quadratic equation and get

$$\tilde{J}(q)\lambda(q)=1-\tilde{\mathcal{J}}(q)-\{[1-\tilde{\mathcal{J}}(q)]^2-2\tilde{J}(q)\}^{1/2}, \tag{4.17}$$

where we have defined

$$\tilde{J}(q)\equiv J(q)\{I(q)[1+2V(q)I(q)]\}^{-1},\qquad \tilde{\mathcal{J}}(q)\equiv\mathcal{J}(q)\{I(q)[1+2V(q)I(q)]\}^{-1}. \tag{4.18}$$

Similarly, varying Eq. (4.14), we determine $\mu(q)$ to be

$$\mu(q)=I(q)[I(q)-\mathcal{J}(q)]^{-1}. \tag{4.19}$$

Substituting Eq. (4.17) in Eq. (4.13), we obtain

$$J(q)\tilde{J}(q)\chi_v(q)=4I^2(q)\,([1-\tilde{\mathcal{J}}(q)]\{[1-\tilde{\mathcal{J}}(q)]^2-2\tilde{J}(q)\}-\{[1-\tilde{\mathcal{J}}(q)]^2-\tilde{J}(q)\}\times\{[1-\tilde{\mathcal{J}}(q)]^2-2\tilde{J}(q)\}^{1/2})\,. \tag{4.20}$$

Likewise, Eq. (4.19) in Eq. (4.14) gives

$$[\chi_{zz}(q)]_v=-2I^2(q)[I(q)-\mathcal{J}(q)]^{-1}. \tag{4.21}$$

These variational expressions for the density-density correlation function and the spin susceptibility are more accurate than the ones derived earlier. They also contain as a special case results previously derived[3] in the linear HF approximation, which can be recovered by the following replacements that are obvious from inspection; replace $\mathcal{J}$ by J and set J equal to zero in Eqs. (4.17), (4.20), and (4.21). We get as a result

$$\chi_{\mathrm{HF}}(q)=2I^2(q)\{J(q)-I(q)[1+2V(q)I(q)]\}^{-1}, \tag{4.22}$$

$$\chi_{zz,\mathrm{HF}}(q)=-2I^2(q)[I(q)-J(q)]^{-1}\,, \tag{4.23}$$

and, therefore,

$$\epsilon_{HF}(q) = 1 + 2V(q)I^2(q)[I(q) - J(q)]^{-1}. \quad (4.24)$$

These linear results agree precisely with Ref. 3. The difference between the more general results in Eqs. (4.20) and (4.21) and these can be regarded as a contribution from the antiparallel spin correlations which are contained in the former. Note, as expected that the $\epsilon_v(q)$ that follows from Eq. (4.20) in (3.5) differs substantially in its form from $[\chi_{zz}(q)]_v$, whereas the results for $\chi_{zz,HF}(q)$ and $\epsilon_{HF}(q)$ are very similar which is an expression of their neglect of antiparallel spin correlations. The same conclusions follow from examination of the low-momentum limit of these properties of the system. We have, after some algebra, from Eqs. (3.5), (4.17), and (4.20),

$$\lim_{q\to 0} q^2\epsilon_v(q) = \frac{8\pi e^2 I^2(0)}{I(0) - J(0) - \mathcal{J}(0)\{1 - [\mathcal{J}(0)/J(0)]^2\}}, \quad (4.25)$$

whereas

$$\lim_{q\to 0} q^2\epsilon_{HF}(q) = 8\pi e^2 I^2(0)/[I(0) - J(0)]. \quad (4.26)$$

These expressions demonstrate compactly the contribution of the antiparallel spin correlations to the compressibility of the system. Since $\mathcal{J} > J$ as we will shortly argue, we note that the contribution adds a positive term to the characteristic $1 - \alpha r_s/\pi$ denominators given by earlier schemes, that is, the antiparallel correlations seem to lower the compressibility of the system. Also, the compressibility does not become infinite at $r_s = \pi/\alpha \simeq 5.5$ but at a larger value, that is, lower density. The influence of the correlations on the spin susceptibility is, on the other hand, in the opposite direction with the denominator in Eq. (4.21) being smaller than in the corresponding result, Eq. (4.23), of linear approximations. These conclusions are in keeping with the simple physical picture that inclusion of correlations between antiparallel spins will tend to push them apart, thus lowering the Coulomb repulsion and, as a result, the total energy—the system becomes more bound, more stable, that is, less compressible. On the other hand, the paramagnetism is likely to be enhanced when antiparallel spins are kept further apart.

We have tried to express our results so that they appear very similar to the results of well-known linear approximations; this should facilitate quantitative comparisons between them since the integrals have either already been evaluated or are intimately linked to known expressions. We make a few further comments on this matter. The expression for $\lambda(q)$ given in Eq. (4.17) can be simplified on recalling that $J(q)/I(q)$ is known in the $\vec{q}\to 0$ and $\vec{q}\to\infty$ limits (both with $q_0 = 0$). Thus $\tilde{J}(q)$ is seen to vanish as q^2 when $\vec{q}\to 0$ and vanish as $1/q^4$ when $\vec{q}\to\infty$.[3b-3d] It may be expected, therefore, that $\tilde{J}(q)$ is small everywhere and, therefore, $1 - \tilde{\mathcal{J}}(q) \gg \tilde{J}(q)$. This allows us to conclude from Eq. (4.17) that

$$\lambda(q) \simeq [1 - \tilde{\mathcal{J}}(q)]^{-1} \simeq 1 + \tilde{\mathcal{J}}(q) \simeq 1 + \tilde{J}(q). \quad (4.27)$$

Therefore, $\tilde{\mathcal{J}}(q)$ which is, approximately,[11] $\lambda(k_F)\tilde{J}(q)$, is greater than $\tilde{J}(q)$. We further note that since $J(q)/I(q)$ is proportional to $\alpha r_s/\pi$ in both the extreme limits,[3b-3d] $\lambda(k_F)$ has the structure: $1 + c\alpha r_s/\pi$, where c is some positive constant. Thus, Eq. (4.25) becomes

$$\lim_{q\to 0} q^2\epsilon_v(q) = q_{TF}^2[1 - \alpha r_s/\pi + 2c(\alpha r_s/\pi)^2]^{-1}. \quad (4.28)$$

Similarly, from Eq. (4.21), we have

$$[\chi_{zz}(0)]_v = -(mk_F/\pi^2)[1 - \alpha r_s/\pi - c(\alpha r_s/\pi)^2]^{-1}. \quad (4.29)$$

The value of the constant c remains to be determined but we note that it follows from the values of the well-known integrals J and I at k_F. Expressions similar to Eqs. (4.28) and (4.29) have been derived[1] on the basis of the interpolation schemes between high and low densities and it is satisfying that the above analysis of the ladder-bubble scheme leads to formally similar results. Table I summarizes previous results in the literature in terms of our terminology on the structure of the singularities in electrical and magnetic properties. The second entry in the table is the result of the variational solution of the linearized vertex equation with the Thomas-Fermi screened potential, $4\pi e^2/(q^2 + q_{TF}^2)$, in agreement with those quoted in Ref. 1 when the antiparallel spin correlations are completely neglected. Only the third entry (Ref. 1, pp. 307–309) in this table brings out the different effects of antiparallel spin correlations on the compressibility and static spin susceptibility.[12] A comparison of these with Eqs. (4.28) and (4.29) show that our results are at variance with these. In Eqs. (4.28) and (4.29) the value of c will depend on the form of the potential used and its evaluation with screened potentials could be very cumbersome; because of the nature of the integral equation for λ in Eq. (4.16), it could also very well involve terms in $\ln(\alpha r_s/\pi)$. What we have argued is that except for such weak dependences c is essentially a constant, that it is positive, and that the nature of the results in Eqs. (4.28) and (4.29) with contributions of opposite signs to electrical and magnetic properties is physically reasonable. The last entry in the table gives the standard form for the compressibility and spin susceptibility in terms of parameters familiar from the Landau theory of Fermi liquids [Ref. 1, particularly Eqs. (5.27) and (5.28)]. These parameters, F_l^s and F_l^a with $l = 0$ and 1, are related to the symmetric and antisymmetric combinations, respectively, of the strengths, $f_l^{\uparrow\uparrow}$ and $f_l^{\uparrow\downarrow}$, of the interaction between

TABLE I. Singularity structure of the compressibility, $\lim_{q\to 0} q^2\epsilon(q)$, and spin susceptibility, $\chi_{zz}(0)$, in different approximation schemes. α and r_s, which are defined in Eq. (4.9), and F_l are standard quantities from the theory of Fermi liquids.

Approximation	Compressibility	Spin susceptibility
(1) Linearized vertex equation with unscreened Coulomb interaction	$1-\alpha r_s/\pi$	$1-\alpha r_s/\pi$
(2) Linearized vertex with screened Coulomb (Thomas-Fermi screening)	$1-\frac{\alpha r_s}{\pi}\left(1+\frac{\alpha r_s}{\pi}\ln\frac{\alpha r_s/\pi}{1+\alpha r_s/\pi}\right)$	$1-\frac{\alpha r_s}{\pi}\left(1+\frac{\alpha r_s}{\pi}\ln\frac{\alpha r_s/\pi}{1+\alpha r_s/\pi}\right)$
(3) Perturbation-theory–second-order scattering contributions to anti-parallel correlations (Sawada-Brueckner)	$1-\frac{\alpha r_s}{\pi}\left(1+\frac{\alpha r_s}{\pi}(1-\ln 2)\ln r_s\right)$	$1-\frac{\alpha r_s}{\pi}\left(1+\frac{1}{2}\frac{\alpha r_s}{\pi}\ln r_s\right)$
(4) Fermi-liquid theory	$(1+F_0^s)(1+\frac{1}{3}F_1^s)^{-1}$	$(1+F_0^a)(1+\frac{1}{3}F_1^s)^{-1}$

parallel and antiparallel spins (Sec. 1.2 of Ref. 1). The HF and RPA schemes correspond to taking zero for the Fermi liquid parameter for antiparallel spins so that $F_0^s=F_0^a$ and, as a consequence, these schemes give an identical structure for electrical and magnetic properties (as borne out by the first entry in the table). On the other hand, our results take into account the antiparallel spin contributions and thus give different values for F_0^s and F_0^a. In fact, comparing the last row of the table with the denominators in Eqs. (4.21) and (4.25) or, alternatively, Eqs. (4.29) and (4.28), we have

$$(1+F_0^s)(1+\tfrac{1}{3}F_1^s)^{-1}=1-\frac{J(0)}{I(0)}-\frac{\mathcal{J}(0)}{I(0)}\left[1-\left(\frac{\mathcal{J}(0)}{J(0)}\right)^2\right]$$
$$\simeq 1-\frac{\alpha r_s}{\pi}+2c\left(\frac{\alpha r_s}{\pi}\right)^2, \qquad (4.30)$$

$$(1+F_0^a)(1+\tfrac{1}{3}F_1^s)^{-1}=1-\frac{\mathcal{J}(0)}{I(0)}\simeq 1-\frac{\alpha r_s}{\pi}-c\left(\frac{\alpha r_s}{\pi}\right)^2. \qquad (4.31)$$

[As discussed before, replacement of $\mathcal{J}$ by J in these equations leads back to the HF and RPA results. Note that $J(0)/I(0)=\alpha r_s/\pi$.] The above equations make contact between the integrals in this paper and the standard F_l parameters. Numerical evaluation of c can thus be used to obtain the values of F_0^s and F_0^a. We note that our remarks about c being positive are reinforced by these equations because it then follows that $F_0^s>F_0^a$ and this is generally true as illustrated by sample results in Table 1.1 of Ref. 1 (for ^{3}He at 0.28 atm, $F_0^s=10.8$, $F_0^a=-0.67$). We also note that in the theory of Fermi liquids, the F_l parameters are expressed as integrals over functions which obey complicated integral equations similar to the vertex function equations we have considered. Thus, our variational procedure could be applied directly to these equations to obtain variational expressions for F_l. Comparison of such results with the results in this paper would be of interest but we defer this to a later date. The advantage of the vertex function formulation is, of course, that our results are not restricted to the zero-frequency long-wavelength limit (though our discussion in the last few papers has been mainly concerned with this limit simply because of the availability of other results to compare with) but are more generally valid.

We conclude with some remarks about the relevance of these results to the properties of simple metals. The inadequacy of the model of the electron gas with a uniform positive background as a model of metallic behavior has been attributed to shortcomings in its description of both many-body effects and solid-state effects. This paper has addressed itself to the former and has shown that in a consistent many-body theory, the effect of antiparallel spins that is usually neglected by conventional approximations can be incorporated and that it influences the properties of the electron gas in the expected direction. Specific solid-state effects like that of an effective mass for an electron due to its interaction with the lattice and that the positive background is not uniform but localized at lattice sites may also be expected to be important for the description of any real metal; in fact, semiempirical interpolations have been used to argue for corrections to the compressibility and spin susceptibility that are very similar to Eqs. (4.28) and (4.29) though, interestingly, with a negative coefficient in place of the positive c [see Eq. (5.176) and Table 5.2 of Ref. 1]. There has also been a suggestion recently[13] that the lack of translational invariance for any real metal leads to important changes in the properties of the system. Thus, a complete theory of metals involves many complicated contributions, some of which may act in opposite directions. What is hoped is that the approach of this paper, giving a systematic way to handle all the many-body effects, will be a useful guide in unravelling the various complicated contributions into classes of distinct physical origin.

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