

Electron correlations: I. Ground-state results in the high-density regime

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The coupled-cluster or $\exp(S)$ formalism is applied to the problem of correlations in a many-electron system. In this first work in a series of papers we concentrate on exact results and restrict ourselves to various ring approximations applicable essentially to the high-density regime. It is shown that the well-known random-phase approximation (RPA) can be formulated as a nonlinear three-dimensional integral equation for the four-point function S_2 which provides a measure of the two-particle-hole pair component in the true ground-state wave function. Exact analytic solutions are presented for both S_2 and the three-point particle-hole vertex function in the RPA, and their properties are discussed. The Tamm-Dancoff approximation to the ring summation is also formulated, and the analogous exact solutions are presented for the first time. It is demonstrated that both solutions are unique, and a comparison of the two approximations is presented in terms of the correlation energy.

I. INTRODUCTION

As a model of the conduction electrons in a metal, where the periodic potential of the ion lattice is replaced by a uniform positive charge distribution chosen to ensure overall charge neutrality, the electron gas is perhaps the most widely studied of all quantum-mechanical many-body problems. It is well known that many of the most interesting properties of the electron gas basically arise from the long-range nature of the Coulomb interaction between the electrons. The simplicity of the basic Coulomb interaction has also been one of the reasons for studying this system, in the hope that other systems with more complicated long-range components in their interactions will qualitatively share some of its properties.

Owing to the infinite range of the interaction it is clearly of paramount importance for an accurate description of the system to try to include as many as possible of the effects of correlations between the electrons, and it is clear that these will never be negligible, even in the weak-coupling limit. The effective coupling constant r_s is conveniently and conventionally defined to be the ratio of the average interparticle spacing to the only length that can be formed from the parameters of the potential, namely, the Bohr radius. The coupling constant r_s is hence proportional to the parameter e^2 , and is thus essentially the smallness parameter for a perturbation-theoretic treatment. In the high-density limit ($r_s \rightarrow 0$) therefore, the potential represents in some sense a small perturbation, but the strong correlations induced by the potential manifest themselves as a divergence in a naive

application of perturbation theory. It is well known that this divergence is only cured by an infinite partial resummation of the perturbation series. Adherence to the principle of compensation of the most dangerous diagrams then leads to the well-known random-phase approximation (RPA) in which the so-called ring diagrams are summed together.

In the opposite limit of low densities, or the strong-coupling regime, the kinetic energy of the electrons represents a small perturbation on the Coulomb interaction, and as Wigner first pointed out the system then minimizes its energy by the electrons crystallizing on to the sites of a regular (solid) lattice. For some value of the density between these limits there is presumably a transition between the fluid and the solid phases, but it is not known at which critical value of r_s this occurs. Only in the two limiting cases have exact calculations for the correlation energy been performed, resulting, respectively, in a power-series expansion in r_s (interspersed with terms logarithmic in r_s) for high densities, and an expansion in inverse half-integral powers of r_s (plus terms exponentially small in r_s) for low densities. Attempts have been made both to interpolate between these two limits and to extend approximately the exact treatments into the density range of real metals, corresponding to $2 \lesssim r_s \lesssim 6$.

Most attempts to work toward the metallic density regime have started from the high-density side, both since this is the weak-coupling limit, and since it is generally believed that the electrons in real metals lie on the fluid side of the fluid-solid phase transition. One of the earliest of the

modern methods applied to the electron gas was the equations-of-motion approach introduced by Bohm and Pines,¹ where the RPA was first successfully employed in a quantum treatment of the electron gas. This work also led to the introduction of the plasma coordinates (and see Ref. 2). Following this line of approach the techniques of quantum-field theory were soon brought to bear on the electron gas. Thus, Gell-Mann and Brueckner³ were the first to perform the infinite summation of Feynman diagrams necessary to give exactly the first two terms in the high-density expansion of the correlation energy. It was also shown that the approximation of keeping only that infinite class of diagrams considered by Gell-Mann and Brueckner, namely, the so-called ring diagrams, was equivalent to the RPA of Bohm and Pines,¹ and that this was exact in the high-density limit. Equivalent results were obtained by Hubbard⁴ and also by Sawada.⁵ The equivalence of these various calculations, and the role played by the plasmons in each case, was made particularly clear by the work of Sawada *et al.*⁶ A very closely related approach, namely, the dielectric-function formulation, was initiated by Nozières and Pines.⁷ The next term in the high-density expansion was first calculated by DuBois,⁸ and was later recalculated and corrected by Carr and Maradudin.⁹

The earliest attempt at an interpolation formula valid for metallic densities was that of Wigner,¹⁰ who employed his own exact low-density result. More recently, Carr *et al.*^{9,11} have given more exact interpolations based on both the exact low- and high-density results. Most of the methods already described have also been employed to try to extrapolate into the metallic density regime from the high-density side. For example, both Nozières and Pines¹² employing the Bohm-Pines theory of plasma oscillations,¹ and Hubbard⁴ employing a diagrammatic method, have considered incorporating the most important exchange effects arising from fermion statistics, which are missing from the basic RPA treatment. Since these early calculations many other attempts have been made to further improve the results. In particular it became clear that the RPA induces too strong correlations for small interparticle separations. Thus, Singwi *et al.*¹³ invented a method which, by including the correlation effects caused by the two-particle interactions, is thought to provide a good treatment of short-range effects. Within the framework of perturbation theory, similar considerations have led many authors¹⁴⁻¹⁹ to attempt to improve upon the RPA by also including the electron-electron scattering terms (or ladder diagrams) as well as exchange effects. In particular we note that the results of Lowy and Brown¹⁹ agree

very well with those of Singwi *et al.*,¹³ although the methods are quite different.

While these essentially perturbative approaches have the great attraction of enabling one "to keep an eye on the physics" through the use of diagrams, their real drawback is in having at some stage to have to make a guess at "the next most important class of diagrams," or some equivalent procedure, in a physical regime where many of the neglected diagrams may well be equally important. We think it fair to say that there have been few really systematic attempts among the practitioners of the diagram-counting techniques. While the vast majority of the calculations in the literature have been of this broadly perturbation-theoretical kind, there has also been a much smaller number of variational calculations. In this context we mention only the earliest calculations of Edwards²⁰ and Gaskell,²¹ based on a Rayleigh-Schrödinger variational method with a trial wave function of the Jastrow form. Although these variational calculations do not suffer from the same drawbacks already mentioned, they do have the disadvantages that it is difficult both to formulate a theory which is susceptible to systematic improvement and to understand (in terms, say, of the diagrams of perturbation theory) what is the essential physics of a given approximation. Furthermore, the one great advantage of the method, namely the existence of the variational energy bound, is normally lost in practice by the necessity of having to introduce further approximations.

The aim of the present work is to bring a new method to bear on the problem of electron correlations, namely, the $\exp(S)$ method (as it was originally called) or the coupled-cluster formalism (in more modern parlance) of Coester and Kümmel,²²⁻²⁶ to which it has not before been applied, and which we hope to demonstrate retains many of the advantages of the methods outlined above without suffering from the same disadvantages. The coupled-cluster formalism was originally invented to deal with closed-shell atomic nuclei, and calculations by Zabolitzky²⁷ employing the method on such nuclei as ⁴He, ¹⁶O, and ⁴⁰Ca have met with considerable success. A recent review of the formalism with particular emphasis on applications in nuclear physics has been given in Ref. 28. The method has also been essentially reinvented and applied with great success in the realm of quantum chemistry by Čížek and Paldus.²⁹⁻³² It is by now clear that the method provides a powerful tool in the general many-body theory arsenal.

The coupled-cluster formalism re-expresses the general N -body problem in terms of a set of amplitudes $S_n, n = 1, \dots, N$, which provide a measure of the n -particle-hole pair components in the true

ground-state wave function and in terms of which all physical quantities may be expressed, and provides a set of coupled nonlinear equations for these amplitudes. By iterating these equations together it is possible to make contact with the perturbative approaches, and in particular to derive quantities equivalent to those expressible by Goldstone diagrams.³³ It has also been shown³³ that by truncating the equations in a particular manner, one may rederive, for example, the same equations as in the familiar Brueckner-Bethe-Goldstone theory of nuclear matter. Furthermore, one of the present authors has rederived the basic coupled-cluster equations in a manner that especially allows one to intuit the truncations necessary for a particular problem.³⁴

Both from these arguments and from a previous study³⁴ of a simple soluble model which simulates a many-fermion system with long-range forces, it is concluded that the coupled-cluster equations are highly efficient in giving a good description of the true ground state (at least in the weak-coupling regime). The truncation adequate for the case of long-range forces seems to be identical with the "natural" truncation of the coupled-cluster equations, namely to put all amplitudes S_i with $i > n$ equal to zero if we intend to solve the hierarchy of equations up to the n th equation. This truncation from the beginning was the starting point of Čížek²⁹ and was also proposed independently by Coester²⁴ for the case of long-range forces.

The coupled-cluster formalism discussed so far allows one only to calculate the energy of the ground state. It is important for the present applications that further recent developments of the formalism exist which allow one to deal both with excited states and with expectation values of arbitrary operators. For excited states, there now exist two different (but related) formalisms. One is due to Kümmel, Offermann, and Ey³⁵⁻³⁷ who employ a model-space description of the wave functions of the excited states. This method is thought to provide a direct microscopic foundation to the very successful phenomenological shell-model calculations for the excited states of atomic nuclei. An iterative solution of the basic equations of this formalism may be shown to yield the linked valence expansion of Brandow,³⁸ just as the original ground-state equations yield the Goldstone expansion. The other formalism for excited states has been found independently by Emrich,³⁹ who derives a coupled system of eigenvalue equations for the energies and amplitudes of the excitations. It is our subjective feeling that the very elegant formalism of Emrich provides, at least for homogeneous systems, the natural extension of the coupled-cluster formalism to excited states. Finally,

we mention that an evaluation of the density matrix in the coupled-cluster formalism has been given by one of us,⁴⁰ which seems to permit a systematic evaluation of ground-state expectation values of arbitrary operators. This formalism has already been applied^{41,42} to problems in nuclear physics, and a brief outline of the method can be found in Ref. 42.

The above discussion shows that there is a wide scope for application of the coupled-cluster formalism to the problem of electron correlations, and the present work is the first in a series devoted to such applications. The first three papers will be concerned with the electron gas only under the further restrictions that (a) all S_n with $n > 2$ are put equal to zero, which defines our basic so-called SUB2 approximation, and (b) we concern ourselves mainly with the computation of energies. The first two papers are devoted to exact solutions of various further approximations (where we consider only the so-called ring diagrams) which are essentially relevant to the high-density regime. In the present work we treat only the ground state, and in the second paper⁴³ (hereafter referred to as II) we apply the formalism of Emrich to excited states. In a third paper⁴⁴ (hereafter referred to as III) we treat the ground state in both the low-density limit and in the intermediate density regime appropriate to real metals.

In the remainder of this section we give a brief outline of the contents of the present paper. In Sec. II we present a short discussion of the elements of the coupled-cluster ground-state formalism needed for the present work and for future use in III, based mainly on the results and methods of Ref. 34. In Sec. III we formulate within the present formalism the RPA for the two-particle-two-hole amplitude S_2 . We show how this four-point function S_2 can be obtained from a knowledge of the three-point particle-hole vertex function g , which itself is given in the RPA by the solution to a nonlinear integral equation. The correlation energy is obtained by a further integration on g , or equivalently from the two-point proper polarization function, and in so doing we regain the well-known high-density result of Gell-Mann and Brueckner.³ It turns out, as we shall see, that the mathematics needed for the exact solution is very different from and rather more complicated than that needed in the Green's-function formalism, for example, and we present the solution in enough detail to highlight the underlying physics. On the other hand, while we seem to have to work rather hard to obtain results found more easily by alternative techniques, we see that our solution contains more information. Thus we find in the RPA a complete analytic solution for both g and S_2 , and while this

information is not necessary for a calculation of the correlation energy, it should certainly prove useful in other applications, as we shall demonstrate explicitly in II for the particular application to excited states.

Having demonstrated how the formalism may be applied to give known results, we formulate also a further approximation which turns out to be equivalent to the Tamm-Dancoff⁴⁵ approximation (TDA), which is well known in the context of nuclear physics. We show also that the TDA is susceptible to an exact solution for S_2 , and the details of the solution are presented together with the corresponding high-density limit for the correlation energy. Finally, we show that an old approximation for the electron gas due to Macke⁴⁶ completes a natural hierarchy of ring approximations in the coupled-cluster formalism. The various solutions are then compared in more detail in Sec. IV.

II. COUPLED-CLUSTER FORMALISM

We give here a brief review of the coupled-cluster [or exp(S)] formalism so far as it is needed in the present work and for other papers in this series. A full review of the method (but with emphasis on applications in nuclear physics) has appeared recently,²⁸ and some particular considerations concerning long-range forces have been made by one of us elsewhere.³⁴ The following discussion is largely based on the content of Ref. 34.

One of the best ways to understand the physical content of the coupled-cluster formalism, as well as to appreciate both its virtues and limitations, is to start from a formulation in terms of the so-called subsystem amplitudes Ψ_n , $n \leq N$ for a system of N fermions with true ground-state wave function $|\Psi\rangle$. In terms of a model wave function $|\Phi\rangle$, which is the Slater determinant built out of N orthonormalized single-particle states $|\nu_1\rangle, \dots, |\nu_N\rangle$,

$$|\Phi\rangle = a_{\nu_1}^\dagger \cdots a_{\nu_N}^\dagger |0\rangle, \quad (2.1)$$

where $|0\rangle$ is the vacuum state, and $a_{\nu_i}^\dagger$ are a set of fermion creation operators for the states $|\nu_i\rangle$, the subsystem amplitudes are defined as

$$\langle \alpha_1 \cdots \alpha_n | \Psi_n | \nu_1 \cdots \nu_n \rangle_A \\ = \langle \Phi | a_{\nu_1}^\dagger \cdots a_{\nu_n}^\dagger a_{\alpha_n} \cdots a_{\alpha_1} | \Psi \rangle, \quad n \leq N, \quad (2.2)$$

where $|\Psi\rangle$ is considered normalized by $\langle \Phi | \Psi \rangle = 1$. In Eq. (2.2) and henceforth, the labels ν, μ, λ indicate states normally occupied (in $|\Phi\rangle$); the labels σ, ρ, τ indicate states normally unoccupied, and the labels α, β, γ indicate both. Furthermore a subscript A on a ket state, as in Eq. (2.2), indicates an antisymmetrized state

$$|\nu_1 \cdots \nu_n \rangle_A \equiv \sum_P (-1)^P |\nu_1\rangle \cdots |\nu_n\rangle, \quad (2.3)$$

where the index P runs over all permutations and is even or odd according as the permutation of the indices $1, \dots, n$ is even or odd. We note for future use that it is sometimes in practice convenient to consider nonantisymmetrized amplitudes, and hence we consistently use the subscript A wherever necessary. From its definition (2.2), it is clear that the quantity $\langle \alpha_1 \cdots \alpha_n | \Psi_n | \nu_1 \cdots \nu_n \rangle$ represents the amplitude that particles "normally" in states ν_1, \dots, ν_n are in fact in states $\alpha_1, \dots, \alpha_n$, with all other particles in their normally occupied states ν_{n+1}, \dots, ν_N . (It should also be noted that compared to Ref. 34, we have changed the position-vector or \vec{r} space labels $1, \dots, n$ to the present labels $\alpha_1, \dots, \alpha_n$. This clearly changes none of the physical content of the formalism.)

It is now easy to see [and see Eq. (2.8) of Ref. 34] that a knowledge of Ψ_1 and Ψ_2 is sufficient to calculate the exact ground-state energy E ($\equiv \langle \Phi | H | \Psi \rangle$), where $H \equiv T + V$ is the Hamiltonian, and we have used the condition $\langle \Phi | \Psi \rangle = 1$,

$$E = \sum_\nu \langle \nu | T \Psi_1 | \nu \rangle + \frac{1}{2} \sum_{\nu\nu'} \langle \nu\nu' | V \Psi_2 | \nu\nu' \rangle_A, \quad (2.4)$$

assuming the particles interact only via a two-body potential V . The notation employed in Eq. (2.4) and hereafter implies that complete sets of states may be freely inserted as necessary, e.g.,

$$\langle \nu\nu' | V \Psi_2 | \nu\nu' \rangle = \sum_{\alpha\alpha'} \langle \nu\nu' | V | \alpha\alpha' \rangle \langle \alpha\alpha' | \Psi_2 | \nu\nu' \rangle. \quad (2.5)$$

In order to derive the formal coupled-cluster equations, one may now proceed as in Ref. 34 by writing down as a first step, the Schrödinger equations for the amplitudes Ψ_n ,

$$\langle \Phi | a_{\nu_1}^\dagger \cdots a_{\nu_n}^\dagger a_{\alpha_n} \cdots a_{\alpha_1} H | \Psi \rangle \\ = E \langle \alpha_1 \cdots \alpha_n | \Psi_n | \nu_1 \cdots \nu_n \rangle_A. \quad (2.6)$$

What is then needed is a decomposition of the amplitudes Ψ_n which allows one to eliminate all macroscopic terms (i.e., those terms which are proportional to N) in the essentially microscopic equations. This is formally achieved by introducing the so-called correlation amplitudes S_n (for $n \geq 2$), as is considered in Sec. II B of Ref. 34. Alternatively, one may simply write

$$|\Psi\rangle = e^S |\Phi\rangle, \quad (2.7a)$$

where

$$S = \sum_{n=1}^N S_n, \quad (2.7b)$$

$$S_n = (n!)^{-2} \sum_{\substack{\rho_1 \cdots \rho_n \\ \nu_1 \cdots \nu_n}} \langle \rho_1 \cdots \rho_n | S_n | \nu_1 \cdots \nu_n \rangle_A \\ \times a_{\rho_1}^\dagger \cdots a_{\rho_n}^\dagger a_{\nu_n} \cdots a_{\nu_1}, \quad (2.7c)$$

in analogy to perturbation theory, where Eqs. (2.7) merely express the linked-cluster theorem for the wave function. Insertion of Eqs. (2.7) into Eq. (2.2) immediately yields the following decompositions:

$$\langle \alpha | \Psi_1 | \nu \rangle = \langle \alpha | \nu \rangle + \langle \alpha | S_1 | \nu \rangle, \quad (2.8a)$$

$$\langle \alpha_1 \alpha_2 | \Psi_2 | \nu_1 \nu_2 \rangle_A = (\langle \alpha_1 | \Psi_1 | \nu_1 \rangle \langle \alpha_2 | \Psi_1 | \nu_2 \rangle)_A \\ + \langle \alpha_1 \alpha_2 | S_2 | \nu_1 \nu_2 \rangle_A, \quad (2.8b)$$

$$\langle \alpha_1 \alpha_2 \alpha_3 | \Psi_3 | \nu_1 \nu_2 \nu_3 \rangle_A \\ = (\langle \alpha_1 | \Psi_1 | \nu_1 \rangle \langle \alpha_2 | \Psi_1 | \nu_2 \rangle \langle \alpha_3 | \Psi_1 | \nu_3 \rangle)_A \\ + S_{123} (\langle \alpha_1 \alpha_2 | S_2 | \nu_1 \nu_2 \rangle \langle \alpha_3 | \Psi_1 | \nu_3 \rangle)_A \\ + \langle \alpha_1 \alpha_2 \alpha_3 | S_3 | \nu_1 \nu_2 \nu_3 \rangle_A, \quad (2.8c)$$

where the symbol S_{123} generates the sum of all cyclic permutations of the labels $\alpha_1, \alpha_2, \alpha_3$, and the antisymmetrization indicated by the subscript A is performed on the ket states. A general decomposition of the Ψ_n in terms of the S_m ($m \leq n$) is given in Eq. (2.16) of Ref. 34. It is worthwhile to consider the above decompositions in some detail. Equation (2.8a) shows that $\langle \alpha | S_1 | \nu \rangle$ is that part of the amplitude $\langle \alpha | \Psi_1 | \nu \rangle$ which is *not* given by the single-particle amplitude $\langle \alpha | \nu \rangle \equiv \delta_{\alpha\nu}$. As in this situation all *other* normally occupied states are in fact occupied, the Pauli principle enforces that the label α in the amplitude $\langle \alpha | S_1 | \nu \rangle$ must equal some

normally unoccupied label. Similar considerations apply to *all* correlation amplitudes S_n , which is reflected in the ansatz (2.7) where only normally unoccupied state labels occur in the bra labels of the functions $\langle |S_n| \rangle$. From Eq. (2.8b) it is seen that $\langle |S_2| \rangle$ is that part of the two-body subsystem amplitude $\langle | \Psi_2 | \rangle$ which cannot be described by one-body subsystem amplitudes $\langle | \Psi_1 | \rangle$, and it is this observation that provides the basis for calling $\langle |S_2| \rangle$ the two-body correlation amplitude. Similarly, Eq. (2.8c) shows that $\langle |S_3| \rangle$ is that part of the amplitude $\langle | \Psi_3 | \rangle$ which cannot be described in terms of one- and two-body amplitudes $\langle | \Psi_1 | \rangle$ and $\langle |S_2| \rangle$. These considerations can clearly be extended to the relationship between arbitrary $\langle | \Psi_n | \rangle$ and $\langle |S_n| \rangle$.

What is clear from the above discussion is that the amplitudes $\langle |S_n| \rangle$ describe correlations only to the extent that these occur within an n -body subsystem. As in such an n -body subsystem all of the remaining $(N-n)$ particles are in their normally occupied single-particle states, this means that to be of use the physical system under consideration must in some sense have the feature of being close to such an idealization. The precise manner in which this has to be so is hard to specify, but we will take up this point again after having written down the dynamical equations which connect the defined amplitudes. These equations now follow from Eq. (2.6) and the decompositions indicated in Eqs. (2.8). The reader interested in the technical details of the derivations may consult Ref. 34.

Using Eqs. (2.28b)–(2.30) of Ref. 34, the *exact* one- and two-body equations may be written

$$\langle \alpha_1 | T \Psi_1 | \nu_1 \rangle + \sum_{\nu'} \langle \alpha_1 \nu | V \Psi_2 | \nu_1 \nu' \rangle_A + \sum_{\nu} \langle \alpha_1 \nu | T(2) S_2 | \nu_1 \nu \rangle_A \\ + \frac{1}{2} \sum_{\nu\nu'} \langle \alpha_1 \nu \nu' | V(23) [S_2(13) \Psi_1(2) + S_2(12) \Psi_1(3) + S_3(123)] | \nu_1 \nu \nu' \rangle_A = \sum_{\nu} h_{\nu\nu_1} \langle \alpha_1 | \Psi_1 | \nu \rangle \quad (2.9)$$

and

$$\langle \rho_1 \rho_2 | [T(1) + T(2)] S_2 | \nu_1 \nu_2 \rangle_A - \sum_{\nu} (h_{\nu\nu_1} \langle \rho_1 \rho_2 | S_2 | \nu \nu_2 \rangle_A + h_{\nu\nu_2} \langle \rho_1 \rho_2 | S_2 | \nu_1 \nu \rangle_A) \\ = - \left(\langle \rho_1 \rho_2 | V \Psi_2 | \nu_1 \nu_2 \rangle_A + \frac{1}{2} \sum_{\nu\nu'} \langle \rho_1 \rho_2 | S_2 | \nu \nu' \rangle_A \langle \nu \nu' | V \Psi_2 | \nu_1 \nu_2 \rangle_A + \sum_{\nu} \langle \rho_1 \rho_2 \nu | T(3) S_3 | \nu_1 \nu_2 \nu \rangle_A \right. \\ + \sum_{\nu} \langle \rho_1 \rho_2 \nu | V(13) [S_2(23) \Psi_1(1) + S_2(12) \Psi_1(3) + S_3(123)] | \nu_1 \nu_2 \nu \rangle_A \\ + \sum_{\nu} \langle \rho_1 \rho_2 \nu | V(23) [S_2(13) \Psi_1(2) + S_2(12) \Psi_1(3) + S_3(123)] | \nu_1 \nu_2 \nu \rangle_A \\ + \frac{1}{2} \sum_{\nu\nu'} \langle \rho_1 \rho_2 \nu \nu' | V(34) [S_2(13) S_2(24) + S_2(23) S_2(14) \\ \left. + S_3(123) \Psi_1(4) + S_3(124) \Psi_1(3) + S_4(1234)] | \nu_1 \nu_2 \nu \nu' \rangle_A \right). \quad (2.10)$$

In Eqs. (2.9) and (2.10) we have used the convention that the integers in parentheses after a particular operator refer that operator to those quantum labels in the associated bra or ket in the corresponding numerical positions (counting from the left), e.g., $\langle \rho_1 \rho_2 | T(1) = \langle \rho_1 | T \otimes \langle \rho_2 |$, $\langle \rho_1 \rho_2 | T(2) = \langle \rho_1 | \otimes \langle \rho_2 | T$; but $\langle \rho_2 \rho_1 | T(1) = \langle \rho_2 | T \otimes \langle \rho_1 |$, and $\langle \rho_2 \rho_3 \rho_4 | V(13) = \langle \rho_2 \rho_4 | V \otimes \langle \rho_3 |$. This rule has to be used in connection with the insertion of unit operators as in Eq. (2.5) in order to derive explicit expressions. The quantity $h_{\nu_1 \nu_2}$ appearing in Eqs. (2.9) and (2.10) is denoted as the hole energy, and is defined by

$$h_{\nu_1 \nu_2} = \langle \nu_1 | T \Psi_1 | \nu_2 \rangle + \sum_{\nu'} \langle \nu_1 \nu' | V \Psi_2 | \nu_2 \nu' \rangle_A. \quad (2.11)$$

We shall not need the equations for S_n for $n > 2$, but we note that the general structure is that the equation for S_n involves both S_{n+1} and S_{n+2} . In order to use the equations in practice the hierarchy must somehow be truncated. The truncation alluded to in Sec. I of setting all S_i equal to zero for $i > n$ we shall henceforth call the SUB n approximation. It is clear that the SUB1 approximation [i.e., Eq. (2.6) with $S_2 = S_3 = 0$] is just the familiar Hartree-Fock approximation, by the following argument. The SUB1 approximation is equivalent to solving the Schrödinger equation with the ansatz $|\Psi\rangle = e^{S_1} |\Phi\rangle$, and a familiar theorem of Thouless⁴⁷ ensures that any determinantal state $|\Phi'\rangle$ can be expressed in terms of an arbitrary determinant $|\Phi\rangle$ (not orthogonal to $|\Phi'\rangle$) by means of the transformation $|\Phi'\rangle = e^{S_1} |\Phi\rangle$. It is seen that the hole energy in this case is just the Hartree-Fock energy. From this one may also suspect that the hole energy will play a special role in the two-body equation, as will prove to be the case in III.

As indicated in Sec. I, we aim to treat the electron gas in the SUB2 approximation, namely, the system of equations (2.9) and (2.10) with the approximation $S_n = 0$, $n \geq 3$, which thus comprise a closed and soluble set of equations for the amplitudes $\langle |S_1| \rangle$ and $\langle |S_2| \rangle$. It is again clear that the solution so obtained is equivalent to solving the Schrödinger equation with the ansatz $|\Psi\rangle = e^{(S_1 + S_2)} |\Phi\rangle$, and from this point of view the approximation is the natural generalization of the Hartree-Fock approach [although by computing the energy from Eq. (2.4) one loses the upper-bound property].

In our discussion subsequent to Eqs. (2.8) we indicated that in order for the SUB2 approximation to be valid it would seem that the physical system under consideration must have something in common with a state where all but two particles are in normally occupied single-particle states. We now see, however, that this is not such a severe limitation as might originally have been supposed.

Thus, the subsystem amplitude

$$\langle \alpha_1 \alpha_2 | \Psi_2 | \nu_1 \nu_2 \rangle_A = \langle \Phi | a_{\nu_1}^\dagger a_{\nu_2}^\dagger a_{\alpha_2} a_{\alpha_1} | \Psi \rangle$$

is computed by using the very complex total wave function $|\Psi\rangle$. What makes the formalism useful (from this point of view) is that the subsystems are allowed fully to interact among themselves through a dynamics determined by the resulting SUB2 equations.

We now restrict ourselves for further discussion to an infinite homogeneous system of spin- $\frac{1}{2}$ particles of mass m interacting through a (pairwise) spin-independent local potential, which we write in momentum space as

$$\begin{aligned} \langle \vec{k}_1 s_1, \vec{k}_2 s_2 | V | \vec{k}_3 s_3, \vec{k}_4 s_4 \rangle \\ = V(\vec{k}_1 - \vec{k}_3) \delta_{\vec{k}_1 + \vec{k}_2, \vec{k}_3 + \vec{k}_4} \delta_{s_1 s_3} \delta_{s_2 s_4}. \end{aligned} \quad (2.12)$$

For such a system we choose our single-particle basis to consist of plane-wave states with quantum labels specified as

$$\begin{aligned} \nu \equiv (\vec{k}, s), \quad |\vec{k}| < k_F, \\ \rho \equiv (\vec{k}, s), \quad |\vec{k}| > k_F, \end{aligned} \quad (2.13)$$

where, as in Eq. (2.12), s is a spin label with the possible values \uparrow or \downarrow , \vec{k} is the wave number of the plane-wave state, and $\hbar k_F$ is the Fermi momentum. It is clear that the one-body equation (2.9) now becomes trivial, since both the states $|\Phi\rangle$ and $|\Psi\rangle$ are assumed to be eigenstates of the total momentum operator \vec{P} with $\langle \vec{P} \rangle = 0$, and hence $S_1 = 0$ from Eqs. (2.7) and (2.13). We further introduce the convenient notation

$$S_{2; \vec{k}_1 \vec{k}_2}^{s_1 s_2}(\vec{q}) \equiv \langle \vec{k}_1 + \vec{q}, s_1; \vec{k}_2 - \vec{q}, s_2 | S_2 | \vec{k}_1 s_1; \vec{k}_2 s_2 \rangle_A, \quad (2.14)$$

where we have implicitly used conservation of both total momentum and third component of spin. From general grounds it is clear that so far as the spin indices are concerned, in the absence of any external applied "magnetic" fields (as assumed here), there are only two independent functions for given \vec{k}_1 , \vec{k}_2 , and \vec{q} , namely, the parallel case $S_2^{\uparrow\uparrow} \equiv S_2^{\downarrow\downarrow}$, and the antiparallel case $S_2^{\uparrow\downarrow} \equiv S_2^{\downarrow\uparrow}$, which are however themselves generally unequal.

It is now not difficult to evaluate explicitly the basic SUB2 approximation equation for S_2 , namely, Eq. (2.10) with $S_3 = S_4 = 0$. We find, after a considerable amount of regrouping of the terms, the reasons for which will become clearer presently, that our basic SUB2 equation for S_2 may be written

$$\begin{aligned} (\hbar^2/2m)(|\vec{k}_1 + \vec{q}|^2 + |\vec{k}_2 - \vec{q}|^2 - \vec{k}_1^2 - \vec{k}_2^2) S_{2; \vec{k}_1 \vec{k}_2}^{s_1 s_2}(\vec{q}) \\ + T_{\text{RPA}} + T_{\text{RPAEX}} + T_{\text{CHP}} + T_{\text{CPP}} + T_{\text{CLAD}} \\ + T_{\text{PHA}} + T_{\text{PHB}} + T_{\text{EE1}} + T_{\text{EE2}} = 0, \end{aligned} \quad (2.15)$$

where

$$T_{\text{RPA}} = V(q) \left(1 + \sum_{\vec{k}\sigma} S_{2;\vec{k}_1\vec{k}}^{s_1\sigma}(\vec{q}) n(k) \bar{n}(\vec{k} - \vec{q}) \right) \times \left(1 + \sum_{\vec{k}'\sigma'} S_{2;\vec{k}'\vec{k}_2}^{\sigma's_2}(\vec{q}) n(k') \bar{n}(\vec{k}' + \vec{q}) \right), \quad (2.16)$$

and where the functions $n(k)$ and $\bar{n}(k)$ are defined in terms of the usual unit-step function $\Theta(x)$,

$$\Theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x < 0, \end{cases} \quad (2.17)$$

by

$$n(k) \equiv \Theta(k_F - k), \quad \bar{n}(k) \equiv \Theta(k - k_F) \quad (2.18)$$

$$T_{\text{RPAEX}} = -\delta_{s_1 s_2} V(q_{\text{ex}}) \times \left(1 + \sum_{\vec{k}\sigma} S_{2;\vec{k}_1\vec{k}}^{s_1\sigma}(\vec{q}_{\text{ex}}) n(k) \bar{n}(\vec{k} - \vec{q}_{\text{ex}}) \right) \times \left(1 + \sum_{\vec{k}'\sigma'} S_{2;\vec{k}'\vec{k}_2}^{\sigma's_2}(\vec{q}_{\text{ex}}) n(k') \bar{n}(\vec{k}' + \vec{q}_{\text{ex}}) \right), \quad (2.19)$$

where the exchange momentum transfer \vec{q}_{ex} is defined by

$$\vec{q}_{\text{ex}} \equiv \vec{k}_2 - \vec{k}_1 - \vec{q}, \quad (2.20)$$

$$T_{\text{CHP}} = - \left(NV(0) - \sum_{\vec{k}} V(\vec{k}_1 - \vec{k}) n(k) + \sum_{\vec{k}\sigma} V(q') S_{2;\vec{k}_1\vec{k}}^{s_1\sigma}(\vec{q}') n(k) \bar{n}(\vec{k} - \vec{q}') \bar{n}(\vec{k}_1 + \vec{q}') \right) S_{2;\vec{k}_1\vec{k}_2}^{s_1 s_2}(\vec{q}) - \left(NV(0) - \sum_{\vec{k}} V(\vec{k}_2 - \vec{k}) n(k) + \sum_{\vec{k}\sigma} V(q') S_{2;\vec{k}_1\vec{k}_2}^{\sigma s_2}(\vec{q}') n(k) \bar{n}(\vec{k} + \vec{q}') \bar{n}(\vec{k}_2 - \vec{q}') \right) S_{2;\vec{k}_1\vec{k}_2}^{s_1 s_2}(\vec{q}), \quad (2.21)$$

$$T_{\text{CPF}} = + \left(NV(0) - \sum_{\vec{k}} V(\vec{k}_1 + \vec{q} - \vec{k}) n(k) - \sum_{\vec{k}\sigma} V(\vec{k}_1 + \vec{q} - \vec{k}) S_{2;\vec{k}_1\vec{k}}^{s_1\sigma}(\vec{q}) (\vec{k}_1 + \vec{q} - \vec{k}) n(k) n(k') \bar{n}(\vec{k} + \vec{k}' - \vec{k}_1 - \vec{q}) \right) S_{2;\vec{k}_1\vec{k}_2}^{s_1 s_2}(\vec{q}) + \left(NV(0) - \sum_{\vec{k}} V(\vec{k} - \vec{k}_2 + \vec{q}) n(k) - \sum_{\vec{k}\sigma} V(\vec{k} - \vec{k}_2 + \vec{q}) S_{2;\vec{k}_1\vec{k}}^{\sigma s_2}(\vec{q}) (\vec{k} - \vec{k}_2 + \vec{q}) n(k) n(k') \bar{n}(\vec{k} + \vec{k}' - \vec{k}_2 + \vec{q}) \right) S_{2;\vec{k}_1\vec{k}_2}^{s_1 s_2}(\vec{q}), \quad (2.22)$$

$$T_{\text{CLAD}} = \sum_{\vec{q}'} V(\vec{q} - \vec{q}') S_{2;\vec{k}_1\vec{k}_2}^{s_1 s_2}(\vec{q}') \bar{n}(\vec{k}_1 + \vec{q}') \bar{n}(\vec{k}_2 - \vec{q}') + \sum_{\vec{k}} V(k) S_{2;\vec{k}_1+\vec{k},\vec{k}_2-\vec{k}}^{s_1 s_2}(\vec{q} - \vec{k}) n(\vec{k}_1 + \vec{k}) n(\vec{k}_2 - \vec{k}) + (1 - \frac{1}{2} \delta_{s_1 s_2}) \sum_{\vec{k}\sigma} V(\vec{k} - \vec{q}') S_{2;\vec{k}_1+\vec{k},\vec{k}_2-\vec{k}}^{s_1 s_2}(\vec{q} - \vec{k}) S_{2;\vec{k}_1\vec{k}_2}^{s_1 s_2}(\vec{q}) n(\vec{k}_1 + \vec{k}) n(\vec{k}_2 - \vec{k}) \bar{n}(\vec{k}_1 + \vec{q}') \bar{n}(\vec{k}_2 - \vec{q}'), \quad (2.23)$$

$$T_{\text{PHA}} = - \sum_{\vec{k}} V(\vec{k}_2 - \vec{k}) S_{2;\vec{k}_1\vec{k}}^{s_1 s_2}(\vec{q}) n(k) \bar{n}(\vec{k} - \vec{q}) - \sum_{\vec{k}} V(\vec{k}_1 - \vec{k}) S_{2;\vec{k}_1\vec{k}_2}^{s_1 s_2}(\vec{q}) n(k) \bar{n}(\vec{k} + \vec{q}), \quad (2.24)$$

$$T_{\text{PHB}} = - \sum_{\vec{k}} V(\vec{k}_2 - \vec{k}) S_{2;\vec{k}_1\vec{k}}^{s_1 s_2}(\vec{q}) (\vec{k} + \vec{q} - \vec{k}_2) n(k) \bar{n}(\vec{k}_1 + \vec{q} - \vec{k}_2 + \vec{k}) - \sum_{\vec{k}} V(\vec{k}_1 - \vec{k}) S_{2;\vec{k}_1\vec{k}_2}^{s_1 s_2}(\vec{q}) (\vec{k}_1 + \vec{q} - \vec{k}) n(k) \bar{n}(\vec{k}_2 - \vec{q} - \vec{k}_1 + \vec{k}), \quad (2.25)$$

$$T_{\text{EE1}} = - \sum_{\vec{k}\sigma} V(\vec{k}' - \vec{k} + \vec{q}) S_{2;\vec{k}_1\vec{k}}^{s_1\sigma}(\vec{q}) S_{2;\vec{k}'\vec{k}_2}^{\sigma s_2}(\vec{q}) n(k) n(k') \bar{n}(\vec{k} - \vec{q}) \bar{n}(\vec{k}' + \vec{q}), \quad (2.26)$$

and finally,

$$T_{\text{EE2}} = + \sum_{\vec{k}\vec{k}'} V(\vec{k}' - \vec{k} + \vec{q}_{\text{ex}}) \left(\delta_{s_1 s_2} \sum_{\sigma} S_{2;\vec{k}_1\vec{k}}^{s_1\sigma}(\vec{q}_{\text{ex}}) S_{2;\vec{k}'\vec{k}_2}^{\sigma s_2}(\vec{q}_{\text{ex}}) + \delta_{s_1, -s_2} S_{2;\vec{k}_1\vec{k}}^{s_1 s_2}(\vec{k} + \vec{q} - \vec{k}_2) S_{2;\vec{k}'\vec{k}_2}^{s_1 s_2}(\vec{k}_1 + \vec{q} - \vec{k}') \right) n(k) n(k') \bar{n}(\vec{k} - \vec{q}_{\text{ex}}) \bar{n}(\vec{k}' + \vec{q}_{\text{ex}}). \quad (2.27)$$

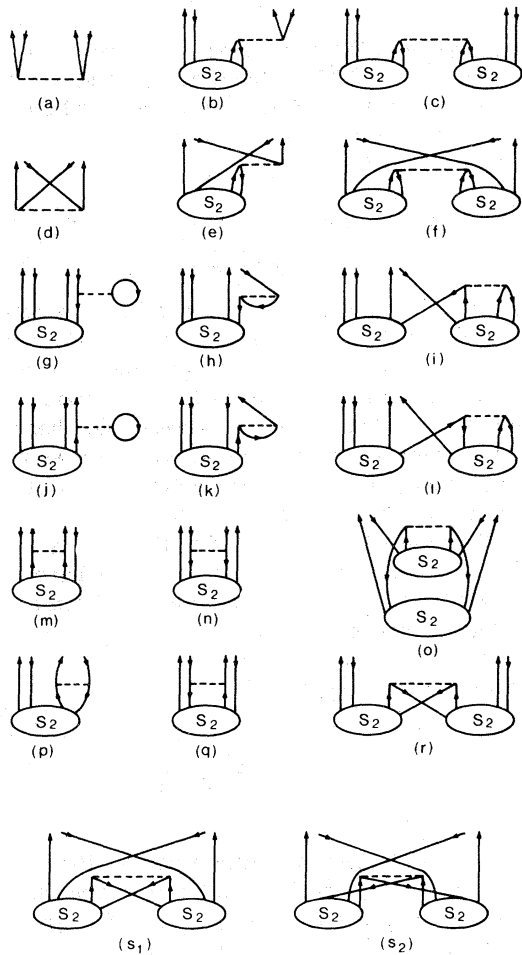


FIG. 1. Diagrammatic representation of the various terms in the SUB2 equation (2.15) for S_2 . Note that the asymmetric diagrams (b), (e), (g)–(l), (p), and (q) each represent two separate terms; one as shown and another obtained by mirror reflection. The terms (s_1) and (s_2) apply only to the parallel and antiparallel spin cases, respectively.

We now wish to stress that although the basic SUB2 equation (2.15) for S_2 appears to be highly complicated analytically, its underlying structure is remarkably simple. We therefore examine each of the terms in more detail, and in so doing explain the reasoning behind their nomenclature. Apart from the first kinetic energy (KE) term, each of the remaining terms is also illustrated diagrammatically in Fig. 1. Apart from the sign of the terms (rules for which we do not give), a suitable labeling of the diagrams (using conservation of momentum and of third component of spin at each vertex) will readily demonstrate to the reader the obvious rules for their construction and their equivalence to the various analytic forms

given above. We note only that lines with arrows pointing upwards (downwards) are to be strictly associated with "particle states" ("hole states"), i.e., with normally unoccupied (occupied) states with momenta outside (inside) the Fermi sphere. The diagrams are thus "time-ordered" in the sense of Goldstone perturbation theory, about which we shall have more to say later.

The terms labeled RPA are represented pictorially by the diagrams (a)–(c) of Fig. 1, and it is clear that they are responsible for generating the so-called ring (or bubble) diagrams. It is well known that summing only the ring diagrams is equivalent to the RPA, whence the choice of name. In the remainder of the present work we shall explicitly demonstrate that the further (drastic) approximation to Eq. (2.15) of keeping only the KE and RPA terms, setting the remainder to zero, leads to an equation which is exactly soluble, and which reproduces all of the known RPA results. Similarly, the RPAEX terms which contribute only in the parallel-spin case, are shown in diagrams (d)–(f) of Fig. 1, and these clearly generate the exchange corrections to the RPA caused by the fermion statistics. We note that diagrams (a) and (d), which represent, respectively, the direct and exchange bare potential, are the sole driving terms in Eq. (2.15). The terms labeled CHP, shown in diagrams (g)–(i) of Fig. 1 are all of the form of an insertion into one of the two hole lines of the amplitude S_2 . They thus generate (in this approximation) the complete-hole-potential (CHP) corrections to the unperturbed or bare KE of the hole states. The diagrams (g), (h), and (i) are referred to individually as the Hartree-hole-potential (HHP), the Fock-hole-potential (FHP), and simply the hole-potential (HP) terms, respectively. The CPP terms (j)–(l) analogously generate the complete-particle-potential (CPP) insertions, and are again respectively distinguished as the Hartree-particle potential (HPP), the Fock-particle potential (FPP), and simply the particle potential (PP). The three terms labeled CLAD are shown in diagrams (m)–(o) of Fig. 1. It is clear that they are responsible for generating the complete sum of ladder diagrams for two-particle and two-hole scattering in the many-body medium, and hence again the choice of name. Diagrams (m) and (n) taken individually, generate the particle-particle ladder sum and hole-hole ladder sum, respectively, while diagram (o) generates the mixed particle-particle and hole-hole ladder terms. Again to distinguish them, we refer to diagram (m) as the PPLAD term (or in view of its usual importance in comparison to the other two as simply the LAD term), to diagram (n) as the HHLAD term, and to diagram (o) as the MLAD

term. Similarly, the terms labeled PHA and PHB which are represented pictorially by Figs. 1(p) and 1(q), respectively, generate the two sorts of particle-hole ladder diagrams which we distinguish by the labels *A* and *B*. Finally the two terms EE1 and EE2 are extra exchange (EE) terms required by Fermi statistics. The term EE1 is shown in diagram (r) of Fig. 1; while the term EE2 in the case of parallel spins is shown in diagram (s_1) and in the case of antiparallel spins in diagram (s_2).

We stress again that the basic SUB2 approximation expressed by Eq. (2.15) is exact apart from neglecting the interactions with higher-order subsystems. Otherwise, *all* two-body effects are included, and it is now clear why the equation at first sight looks so complex. In perturbation-theoretical terms we are effectively summing an enormous class of diagrams in the SUB2 approximation. As stated in Sec. I, it has formally been shown elsewhere³³ how to obtain quantities equivalent to those expressible by the time-ordered Goldstone diagrams of time-independent perturbation theory. From our previous discussion this equivalence should now be intuitively obvious when we realize that a Goldstone diagram for the wave function, for example, is always referred to the state $|\Phi\rangle$, and it is always implied that all of the nonparticipating particles (i.e., the "missing" lines in the diagram) are in their normally occupied single-particle states. The analogy with our amplitudes $\langle|\Psi_n\rangle|$ is then almost trivial. In the same vein we also note that the equivalence of the present coupled-cluster approach with the Green's-function approach based on the Feynman-Dyson time-dependent perturbation theory is considerably more complicated. This Green's function formalism can also be expressed diagrammatically in terms of non-time-ordered or Feynman diagrams which have no direct counterpart in our approach. We note for example that the three CLAD terms of diagrams (m)–(o) of Fig. 1 could be represented by a single non-time-ordered diagram in the Green's-function approach. Similar "simplifications" occur elsewhere in the Green's-function approach, but as pointed out by one of the present authors⁴⁸ in a different context such advantages are always offset by accompanying disadvantages. In this context we finally remark that the structure of the basic SUB2 equation (2.15) for S_2 is that of a "quadratic" integral equation. It is seen that in order to generate the terms involving "backward propagation" in time it is necessary for the formalism to involve terms at least bilinear in S_2 , and hence in this sense the formalism achieves this minimally.

The purpose of the remainder of this work is now to apply Eq. (2.15) to the electron gas, and in particular to study the RPA and some allied approximations. A fuller study of the equation is then deferred to III.

III. APPLICATION TO THE ELECTRON GAS

A. General comments

We now wish to use the general formalism outlined in Sec. II in the case of the uniform electron gas. As usual we consider a large number N of electrons enclosed in a volume Ω with a rigid uniformly distributed positive background chosen to ensure overall charge neutrality. Since we are interested only in the bulk properties, the system is studied in the thermodynamic limit where both N and Ω become infinite such that the density $\rho = N/\Omega$ remains constant. The electrons have mass m and charge e , and the total Hamiltonian may thus be written

$$H \equiv H_0 + V = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i < j} \sum_{\vec{k} \neq 0} \frac{4\pi e^2}{\Omega k^2} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)}, \quad (3.1)$$

where in the Coulomb potential term V , the Fourier component $\vec{k} = 0$ is excluded on account of the neutralizing positive background. The ground-state eigenfunction Φ of the kinetic energy operator H_0 is just the usual Slater determinant built from doubly occupying the $\frac{1}{2}N$ plane-wave states with momenta $k < k_F$, where the Fermi momentum k_F is given by

$$k_F = (3\pi^2 \rho)^{1/3}. \quad (3.2)$$

As usual we also define an average interparticle spacing r_0 by

$$\rho = \left(\frac{4}{3}\pi r_0^3\right)^{-1}, \quad (3.3)$$

and the dimensionless parameter r_s by

$$r_s = r_0/a_0, \quad (3.4)$$

in terms of the Bohr radius $a_0 = \hbar^2/me^2$. Defining E_0 to be the expectation value of the full Hamiltonian (3.1) in the noninteracting ground state Φ , and ϵ_0 to be the corresponding energy per electron expressed in Rydbergs,

$$E_0 = \langle\Phi|H|\Phi\rangle = \epsilon_0 N e^2 / 2a_0, \quad (3.5)$$

it is trivial to show that ϵ_0 may be evaluated as,

$$\epsilon_0 = 2.21/r_s^2 - 0.916/r_s,$$

where the two terms correspond, respectively, to the kinetic energy of the unperturbed filled Fermi

sea, and the second term is the Fock exchange energy [the usual direct Hartree term being zero in this case because $V(\vec{k}=0)=0$]. The difference between the exact ground-state energy ϵ (expressed again in Rydbergs per electron) and ϵ_0 is known as the correlation energy

$$\epsilon_c = \epsilon - \epsilon_0, \quad (3.6)$$

and its calculation is one of the main subjects of the remainder of this work.

From Eqs. (2.4) and (2.8) and using $S_1=0$, it is clear that the correlation energy E_c may be expressed in terms of S_2 by

$$E_c = \frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2}^{k_F} \sum_{\sigma_1, \sigma_2} \langle \vec{k}_1 \sigma_1, \vec{k}_2 \sigma_2 | V S_2 | \vec{k}_1 \sigma_1, \vec{k}_2 \sigma_2 \rangle_A, \quad (3.7)$$

or, in an approximation where S_2 is spin-independent, by

$$E_c = \frac{8\pi e^2}{\Omega k_F^2} \sum_{\vec{k}_1 \in \Gamma} \sum_{-\vec{k}_2 \in \Gamma} \sum_{q \neq 0} \frac{1}{q^2} S_{2; \vec{k}_1 \vec{k}_2}(\vec{q}), \quad (3.8)$$

where in Eq. (3.8) and henceforth all momenta are considered to be dimensionless variables, having been scaled by k_F , and where the restrictions on the \vec{k}_1 and \vec{k}_2 sums are defined by

$$\vec{k} \in \Gamma \Rightarrow \begin{cases} |\vec{k}| < 1, \\ |\vec{k} + \vec{q}| > 1. \end{cases} \quad (3.9)$$

It is thus clear that any approximation for S_2 generates a corresponding approximation for the correlation energy. What we wish to do in the remainder of this section is to consider various approximations to S_2 from our basic equations (2.15)–(2.27).

It is well known that summation of the so-called ring diagrams is vital to remove the divergence in the order-by-order perturbation expansions that arises from the long-range nature of the Coulomb potential, and which immediately arises in second-order perturbation theory. In Sec. IIIB we use our formalism to include all of the ring diagrams, a result which we shall show is fully equivalent to the RPA. In Sec. IIIC we solve a simplified (linearized) set of ring equations which is equivalent to summing only the forward-going in time (in the Goldstone time-ordered sense) ring diagrams, and which is identical in this case to the Tamm-Dancoff⁴⁵ approximation. So far as we are aware, we obtain exact results in this case for the first time. Finally, in Sec. IIIC we consider a further approximation which completes a natural hierarchy of ring equations, and which we show is equivalent to an approximation due originally to Macke⁴⁶ (MA).

B. RPA ring equations

From our basic SUB2 approximation equation (2.15) we now select only those terms which lead to the most general ring diagrams. By reference to Fig. 1 it is clear that these are the terms corresponding to diagrams (a)–(c) of the figure for both S_2^{++} and S_2^{+-} . Thus, from our basic SUB2 equation (2.15) and from Eqs. (3.1)–(3.4), and defining $S_2^{++} = S_2^{+-} = S_2$ in this approximation, we find that (what we now denote as) the RPA equation for S_2 is

$$S_{2; \vec{k}_1 \vec{k}_2}^R(\vec{q}) = -\alpha \gamma_s \frac{4}{3\pi N} \frac{1}{\vec{q} \cdot (\vec{k}_1 - \vec{k}_2 + \vec{q})} \times \frac{1}{q^2} [1 + 2f_{\vec{k}_1}^R(\vec{q})][1 + 2f_{-\vec{k}_2}^R(\vec{q})], \quad (3.10)$$

where

$$\alpha \equiv (4/9\pi)^{1/3}, \quad (3.11)$$

and the function $f_{\vec{k}_1}^R(\vec{q})$ is defined by

$$f_{\vec{k}_1}^R(\vec{q}) \equiv \sum_{-\vec{k}_2 \in \Gamma} S_{2; \vec{k}_1 \vec{k}_2}(\vec{q}). \quad (3.12)$$

The superscript (or subscript, as convenient) R used in Eq. (3.10) will henceforth be used consistently to indicate that the quantity under discussion is evaluated in the RPA. The RPA equation (3.10) is illustrated diagrammatically in Fig. 2. In writing Eq. (3.10) we have used the equality

$$S_{2; \vec{k}_1 \vec{k}_2}(\vec{q}) = S_{2; -\vec{k}_2, -\vec{k}_1}(\vec{q}), \quad (3.13)$$

which follows from the definition of Eq. (2.14) and Galilean invariance, to write

$$\sum_{\vec{k}_1 \in \Gamma} S_{2; \vec{k}_1 \vec{k}_2}(\vec{q}) = f_{-\vec{k}_2}(\vec{q}). \quad (3.14)$$

Using Eqs. (3.10) and (3.12) together yields the equation for $f_{\vec{k}_1}^R(\vec{q})$,

$$f_{\vec{k}_1}^R(\vec{q}) = -\frac{4\alpha \gamma_s}{3\pi N q^2} \sum_{-\vec{k}_2 \in \Gamma} \frac{1}{\vec{q} \cdot (\vec{k}_1 - \vec{k}_2 + \vec{q})} \times [1 + 2f_{\vec{k}_1}^R(\vec{q})][1 + 2f_{-\vec{k}_2}^R(\vec{q})]. \quad (3.15)$$

Defining the general particle-hole vertex function $g(\vec{k})$ as

$$g_{\vec{k}}^{\pm}(\vec{k}) \equiv g(\vec{k}) \equiv 1 + 2f_{\vec{k}}^{\pm}(\vec{q}), \quad (3.16)$$

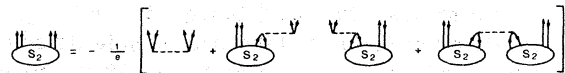


FIG. 2. Diagrammatic representation of the RPA equation for S_2 .

and changing the sum to an integral as usual by

$$\sum_{\vec{k}} \rightarrow \Omega k_F^3 (2\pi)^{-3} \int d\vec{k}, \quad (3.17)$$

we find that Eq. (3.15) may be rewritten

$$g_R(\vec{k}_1) = 1 - \frac{1}{2\pi\beta} g_R(\vec{k}_1) \times \int_{\Gamma} d\vec{k}_2 \frac{g_R(\vec{k}_2)}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2 + \vec{q})}, \quad (3.18)$$

where

$$\beta(q) \equiv \beta = \frac{2\pi^2 \hbar^2}{m\Omega k_F} \frac{1}{V(q k_F)} = \frac{\pi q^2}{2\alpha r_s}. \quad (3.19)$$

For many purposes it is more convenient to define new (dimensionless) and more symmetric momentum variables \vec{k}_1 and \vec{k}_2 by

$$\vec{k}_1 = \vec{k}_1 - \frac{1}{2} \vec{q}, \quad \vec{k}_2 = -\vec{k}_2 + \frac{1}{2} \vec{q}. \quad (3.20)$$

We denote quantities defined in terms of these new variables by a tilde, thus

$$g(\vec{k}_1) = g(\vec{k}_1 - \frac{1}{2} \vec{q}) \equiv \tilde{g}(\vec{k}_1), \\ S_{2; \vec{k}_1 \vec{k}_2}(\vec{q}) = S_{2; \vec{k}_1 - (1/2)\vec{q}, -\vec{k}_2 + (1/2)\vec{q}}(\vec{q}) \\ \equiv \tilde{S}_{2; \vec{k}_1 \vec{k}_2}(\vec{q}), \quad (3.21)$$

and in terms of which Eq. (3.18) may be written

$$\tilde{g}_R(\vec{k}_1) = 1 - \frac{1}{2\pi\beta} \tilde{g}_R(\vec{k}_1) \\ \times \int_{\Gamma} d\vec{k}_2 \frac{\tilde{g}_R(\vec{k}_2)}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)}, \quad \vec{k}_1 \in \tilde{\Gamma}, \quad (3.22)$$

where

$$\{\vec{k} \in \tilde{\Gamma}(\vec{k}) \equiv \tilde{\Gamma}\} \Rightarrow \begin{cases} |\vec{k} - \frac{1}{2} \vec{q}| < 1, \\ |\vec{k} + \frac{1}{2} \vec{q}| > 1. \end{cases} \quad (3.23)$$

We shall regard Eq. (3.22), which is a nonlinear integral equation for the RPA particle-hole vertex function $\tilde{g}_R(\vec{k})$, as the basic RPA equation in the coupled-cluster formalism, since all other quantities of interest may be obtained from it. Thus, using Eqs. (3.10), (3.16), and (3.21), we have that \tilde{S}_2^R can be expressed as

$$\tilde{S}_{2; \vec{k}_1 \vec{k}_2}^R(\vec{q}) = -\frac{2}{3\beta N} \frac{1}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)} \tilde{g}_R(\vec{k}_1) \tilde{g}_R(\vec{k}_2), \quad (3.24)$$

in the physical regime $\vec{k}_1 \in \tilde{\Gamma}$ and $\vec{k}_2 \in \tilde{\Gamma}$. The purpose of the remainder of this subsection is thus to obtain the *exact* solution to Eq. (3.22) and to discuss its general properties.

As it stands, Eq. (3.22) is a quadratic integral equation for $\tilde{g}_R(\vec{k})$, and the first step in its solution is to bring it into linear form. This can be achieved as follows. The equation is first multiplied throughout by the factor $[\vec{q} \cdot (\vec{k}_1 + \vec{k})]^{-1}$, and

then integrated on the variable $\vec{k}_1 \in \tilde{\Gamma}$. After some trivial algebra, this gives

$$\int_{\tilde{\Gamma}} \frac{d\vec{k}_1}{\vec{q} \cdot (\vec{k}_1 + \vec{k})} = \int_{\tilde{\Gamma}} \frac{d\vec{k}_1 \tilde{g}_R(\vec{k}_1)}{\vec{q} \cdot (\vec{k}_1 + \vec{k})} \\ + \frac{1}{2\pi\beta} \int_{\tilde{\Gamma}} \frac{d\vec{k}_1 \tilde{g}_R(\vec{k}_1)}{\vec{q} \cdot (\vec{k}_1 + \vec{k})} \int_{\tilde{\Gamma}} \frac{d\vec{k}_2 \tilde{g}_R(\vec{k}_2)}{\vec{q} \cdot (\vec{k}_2 - \vec{k})} \\ - \frac{1}{2\pi\beta} \int_{\tilde{\Gamma}} \frac{d\vec{k}_2 \tilde{g}_R(\vec{k}_2)}{\vec{q} \cdot (\vec{k}_2 - \vec{k})} \int_{\tilde{\Gamma}} \frac{d\vec{k}_1 \tilde{g}_R(\vec{k}_1)}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)}. \quad (3.25)$$

In the second and third terms on the right-hand side of Eq. (3.25) we now repeatedly substitute from Eq. (3.22) written as

$$\int_{\tilde{\Gamma}} \frac{d\vec{k}_2 \tilde{g}_R(\vec{k}_2)}{\vec{q} \cdot (\vec{k}_2 - \vec{k})} = 2\pi\beta \left(\frac{1}{\tilde{g}_R(\vec{k})} - 1 \right), \quad (3.26)$$

which leads straightforwardly to the functional relation

$$[\tilde{g}_R(\vec{k}) \tilde{g}_R(-\vec{k})]^{-1} = \tilde{K}_R(\vec{k}), \quad (3.27)$$

where the known function $\tilde{K}_R(\vec{k})$ is defined by the relation

$$\tilde{K}_R(\vec{k}) \equiv 1 + \frac{1}{2\pi\beta} \int_{\tilde{\Gamma}} d\vec{k}_1 \left(\frac{1}{\vec{q} \cdot (\vec{k}_1 + \vec{k})} + \frac{1}{\vec{q} \cdot (\vec{k}_1 - \vec{k})} \right). \quad (3.28)$$

Substitution of Eq. (3.27) into our original equation (3.22) leads immediately to the *linear* integral equation for $\tilde{g}_R(\vec{k})$,

$$\tilde{K}_R(\vec{k}) \tilde{g}_R(\vec{k}) = 1 + \frac{1}{2\pi\beta} \int_{\tilde{\Gamma}} \frac{d\vec{k}' \tilde{g}_R(\vec{k}')}{\vec{q} \cdot (\vec{k}' - \vec{k})}. \quad (3.29)$$

We note that although we have achieved our goal of linearizing the original integral equation for $\tilde{g}_R(\vec{k})$, the equation is now a *singular* integral equation in the physical regime $\vec{k} \in \tilde{\Gamma}(\vec{k})$ since the kernel becomes infinite at all values $\vec{k}' = \vec{k}$. Thus, the kernel of the equation is not square integrable and the usual Fredholm theory of linear integral equations cannot be applied.

Happily, however, Eq. (3.29) is still susceptible to an exact solution, but in order to proceed further it is important to choose the correct coordinate system. The function $\tilde{g}_R(\vec{k})$ is in reality a function of both the vector \vec{k} , and the vector \vec{q} which we have suppressed for ease of notation. By Galilean invariance the only independent scalars are thus κ^2 , q^2 , and $\vec{k} \cdot \vec{q}$, and continuing to suppress the implicit dependence on q , we write $\tilde{g}_R(\vec{k}) \equiv \tilde{g}_R(\vec{k} \cdot \vec{q}, \kappa^2)$. We note, however, from the defining equation (3.28) that $\tilde{K}_R(\vec{k})$ is independent of the scalar κ^2 , and hence it is clear by inspection that Eq. (3.29) has a solution $\tilde{g}_R(\vec{k}) \equiv \tilde{g}_R(\vec{k} \cdot \vec{q})$, independent of κ^2 . It is therefore clear that the natural coordinate system in which to solve Eq.

(3.29) is a cylindrical polar system with axis along the direction \hat{q} , and for obvious reasons of symmetry with origin at the midpoint of the axis joining the centers of the two unit Fermi spheres implied by the integration regime $\tilde{\Gamma}$. In these cylindrical polar coordinates (x, ρ, Θ) , where x

$\equiv \vec{k} \cdot \hat{q}$, the integrations expressed in Eqs. (3.28)–(3.29) may be written

$$\int_{\tilde{\Gamma}} d\vec{k} f(x) = 2\pi q \int_{\tilde{L}} dx \tilde{N}(x) f(x), \quad (3.30)$$

for an arbitrary function $f(x)$, where

$$\tilde{N}(x > 0) = \begin{cases} x, & 0 \leq x \leq 1 - \frac{1}{2}q, \quad q < 2, \\ [1 - (\frac{1}{2}q - x)^2]/2q, & 1 - \frac{1}{2}q \leq x \leq 1 + \frac{1}{2}q, \quad q < 2, \\ [1 - (\frac{1}{2}q - x)^2]/2q, & \frac{1}{2}q - 1 \leq x \leq \frac{1}{2}q + 1, \quad q \geq 2, \\ 0, & \text{otherwise,} \end{cases} \quad (3.31a)$$

and for future use we define

$$\tilde{N}(-x) = -\tilde{N}(x), \quad (3.31b)$$

and where

$$x \in \tilde{L} \Rightarrow \begin{cases} 0 \leq x \leq \frac{1}{2}q + 1, & q < 2; \\ \frac{1}{2}q - 1 \leq x \leq \frac{1}{2}q + 1, & q \geq 2. \end{cases} \quad (3.32)$$

Using Eqs. (3.30)–(3.31) with Eq. (3.28) leads to the explicit expression for $\tilde{K}_R(\vec{k})$,

$$\tilde{K}_R(\vec{k}) \equiv \tilde{K}_R(x) = 1 + \frac{1}{2\beta q} \left(2q + [1 - (\frac{1}{2}q + x)^2] \ln \left| \frac{\frac{1}{2}q + 1 + x}{\frac{1}{2}q - 1 + x} \right| + [1 - (\frac{1}{2}q - x)^2] \ln \left| \frac{\frac{1}{2}q + 1 - x}{\frac{1}{2}q - 1 - x} \right| \right), \quad (3.33)$$

$$\vec{k} \cdot \hat{q} = x,$$

which is valid for *all* values of q .

Similarly, Eq. (3.29) may be written in these coordinates for $\tilde{g}_R(\vec{k} \cdot \hat{q}) \equiv \tilde{g}_R(x)$ as

$$\tilde{K}_R(x) \tilde{g}_R(x) = 1 + \frac{1}{\beta} \int_{\tilde{L}} dx' \frac{\tilde{N}(x') \tilde{g}_R(x')}{x' - x}, \quad x \in \tilde{L}. \quad (3.34)$$

We note that at this point the RPA problem has been reduced to finding the solution of the one-dimensional singular integral equation (3.34). This equation is almost of the standard Muskhelishvili–Omnès-type,⁴⁹ and we shall only sketch such further steps in its solution as are necessary to illuminate the physics of the approximation.

In order to solve Eq. (3.34), it appears to be necessary to make an appeal to analytic continuation at some stage and having realized this it is easiest to do so immediately. Defining a function $\tilde{K}_R(z)$ of the complex variable z , by

$$\begin{aligned} \tilde{K}_R(z) &\equiv 1 + \frac{1}{\beta} \int_{\tilde{L}} dx' \tilde{N}(x') \left(\frac{1}{x' + z} + \frac{1}{x' - z} \right) \\ &= 1 + \frac{1}{\beta} \left[1 + \frac{1}{2q} [1 - (\frac{1}{2}q + z)^2] \ln \left(\frac{\frac{1}{2}q + z + 1}{\frac{1}{2}q + z - 1} \right) \right. \\ &\quad \left. + \frac{1}{2q} [1 - (\frac{1}{2}q - z)^2] \ln \left(\frac{\frac{1}{2}q - z + 1}{\frac{1}{2}q - z - 1} \right) \right], \end{aligned} \quad (3.35)$$

it is straightforward to show that

$$\tilde{K}_{R\pm}(x) \equiv \tilde{K}_R(x \pm i\eta) = \tilde{K}_R(x) \pm i\pi\beta^{-1} \tilde{N}(x), \quad (3.36)$$

where η is a positive infinitesimal, and $\tilde{K}_R(x)$ and $\tilde{N}(x)$ are as defined in Eqs. (3.33) and (3.31), respectively. We can thus define a function $\tilde{g}_R(z)$ for arbitrary z in the complex plane by

$$\tilde{K}_R(z) \tilde{g}_R(z) = 1 + \frac{1}{\beta} \int_{\tilde{L}} dx' \frac{\tilde{N}(x') \tilde{g}_R(x')}{x' - z}, \quad (3.37)$$

and by comparison of Eqs. (3.34) and (3.37), and making use of Eq. (3.36), it is clear that in the physical regime $x \in \tilde{L}$,

$$\tilde{g}_R(x) = \lim_{y \rightarrow 0} \tilde{g}_R(x \pm iy), \quad x \in \tilde{L}. \quad (3.38)$$

Finally, defining a new function $\phi(z)$ by

$$\phi(z) \equiv \tilde{g}_R(z) \tilde{K}_R(z), \quad (3.39)$$

and writing

$$h_R(x) \equiv (i\pi/\beta) \tilde{N}(x) / \tilde{K}_{R+}(x), \quad (3.40)$$

we may rewrite Eq. (3.37) as

$$\phi_+(x) = 1 + \frac{1}{i\pi} \int_{\tilde{L}} dx' \frac{h_R(x') \phi_+(x')}{x' - x - i\eta}, \quad x \in \tilde{L}. \quad (3.41)$$

In this form, Eq. (3.41) may now be solved by standard methods⁴⁹ to give the general solution

$$\phi(z) = 1 - \frac{e^{u^R(z)}}{2\pi i} \int_{\tilde{L}} dx' \frac{e^{-u_+^R(x')} - e^{-u_-^R(x')}}{x' - z} + \tilde{P}(z)e^{u^R(z)}, \quad (3.42)$$

where

$$u^R(z) \equiv \frac{1}{2\pi i} \int_{\tilde{L}} dx' \frac{\text{Ln}[1/G_R(x')]}{x' - z}, \quad (3.43)$$

$$G_R(x) \equiv 1 - 2h_R(x), \quad (3.44)$$

and where the symbol Ln indicates any value of the multivalued logarithmic function which is continuous on \tilde{L} . It should be noted that the general solution of Eq. (3.42) is not unique since it contains the function $\tilde{P}(z)$, which is defined to be any function analytic in the entire complex plane with the possible exceptions of singularities at either or both of the end points of the integration interval \tilde{L} . Also it is clear that in order not to run into trouble with possible branch points of the Ln function in Eq. (3.43) we must further require that $G_R(z) \neq 0$ for $z \in \tilde{L}$, which is readily verified in our particular case. Thus, using Eqs. (3.40) and (3.44), we have

$$1/G_R(x) \equiv e^{2i\delta_R(x)} = \tilde{K}_{R+}(x)/\tilde{K}_{R-}(x), \quad (3.45)$$

where $\delta_R(x)$ is real, and is given by

$$\tilde{K}_{R\pm}(x) = |\tilde{K}_{R\pm}(x)| e^{\pm i\delta_R(x)}, \quad (3.46)$$

or equivalently,

$$\begin{aligned} \delta_R(x) &= -\delta_R(-x) = \text{Tan}^{-1} \left(\frac{\text{Im}\tilde{K}_{R+}(x)}{\text{Re}\tilde{K}_{R+}(x)} \right) \\ &= \text{Tan}^{-1} \left(\frac{\pi\tilde{N}(x)}{\beta\tilde{K}_R(x)} \right), \end{aligned} \quad (3.47)$$

and where to be consistent with the use of the Ln function in Eq. (3.43), the Tan^{-1} function in Eq. (3.47) indicates any value of the multivalued inverse tangent function which is continuous on \tilde{L} .

The integral term in Eq. (3.42) may readily be simplified by considering the contour integral of the function $e^{-u(z')}/(z' - z)$ with respect to the variable z' around the contour comprising the circle at infinity indented at the real axis to exclude the cut \tilde{L} . Comparison of the direct evaluation with the result obtained using Cauchy's theorem and the defining equation (3.43) leads trivially to the result

$$\tilde{g}_R(z) = [e^{u^R(z)}/\tilde{K}_R(z)][1 + \tilde{P}(z)]. \quad (3.48)$$

There remains for us therefore only to try to eliminate the unknown function $\tilde{P}(z)$. It should be realized however that we have no *a priori* knowledge of whether our original equation (3.22) indeed has a unique solution, although this will turn out to be the case. What is certainly true however

is that the derived equation (3.29) does not have a unique solution. The only method now open to us to attempt to eliminate the unknown function $\tilde{P}(z)$ is to ensure that the solution (3.48) does indeed satisfy the original equation (3.22). Somewhat more directly we may also require that the solution (3.48) satisfies the functional relation (3.27), or better, its generalization

$$\tilde{g}_R(z)\tilde{g}_R(-z) = 1/\tilde{K}_R(z), \quad (3.49)$$

which is proved analogously.

Before proceeding with this derivation, however, it is necessary to inquire into the analytic structure of the function $\text{Ln}\tilde{K}_R(z)$, which is intimately connected with the function $u(z)$ from Eqs. (3.43) and (3.45). It is clear from Eq. (3.35) that $\tilde{K}_R(z)$ is analytic in the entire complex z plane except for cuts along $z \in (\tilde{L} + \tilde{L}')$, where \tilde{L}' is the reflection of the segment \tilde{L} about the y axis (i.e., $x \in \tilde{L}' \Leftrightarrow -x \in \tilde{L}$). Clearly, the only additional singularities in the function $\text{Ln}\tilde{K}_R(z)$ will be logarithmic branch-points at any possible zeros of the function $\tilde{K}_R(z)$. It is trivial to show that the only possible zeros of $\tilde{K}_R(z)$ occur on the real axis outside the cuts \tilde{L} and \tilde{L}' . From Eq. (3.33) we see that the only possible zeros of $\tilde{K}_R(z)$ are at $z = \pm x_0^R$, where $x_0^R = x_0^R(q) > \max(\tilde{L}) = \frac{1}{2}q + 1$ is the positive root (if any) of the equation

$$\begin{aligned} -1 &= \frac{\alpha\gamma_s}{\pi q^3} \left[2q + [1 - (x_0^R + \frac{1}{2}q)^2] \ln \left(\frac{x_0^R + \frac{1}{2}q + 1}{x_0^R + \frac{1}{2}q - 1} \right) \right. \\ &\quad \left. + [1 - (x_0^R - \frac{1}{2}q)^2] \ln \left(\frac{x_0^R - \frac{1}{2}q - 1}{x_0^R - \frac{1}{2}q + 1} \right) \right], \\ &\quad x_0^R > \frac{1}{2}q + 1. \end{aligned} \quad (3.50)$$

It is also not difficult to show that Eq. (3.50) has either one or no solution, according as $q \leq q_{\max}^R$ or $q > q_{\max}^R$, respectively, where q_{\max}^R is given by

$$x_0(q_{\max}^R) = \frac{1}{2}q_{\max}^R + 1, \quad (3.51)$$

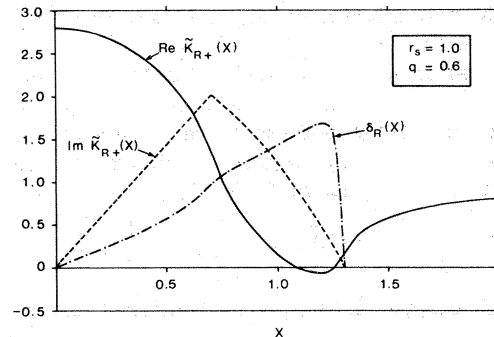


FIG. 3. Real and imaginary parts of the function $\tilde{K}_{R+}(x)$ and the phase angle $\delta_R(x)$ for $r_s = 1$ and momentum transfer $q = 0.6 > q_{\max}^R = 0.560$.

or, using Eq. (3.45),

$$(q_{\max}^R)^2 = \frac{\alpha r_s}{\pi} \left[(2 + q_{\max}^R) \ln \left(1 + \frac{2}{q_{\max}^R} \right) - 2 \right], \quad (3.52)$$

which is readily shown to have a unique solution for any value of r_s . The structure of the real and imaginary parts of $\tilde{K}_{R+}(x)$ is shown in Figs. 3 and 4, together with the phase angle $\delta_R(x)$ of Eq. (3.47) for the two cases $q > q_{\max}^R$ and $q < q_{\max}^R$. To be specific we have chosen the value $r_s = 1$ for which Eq. (3.52) has the solution $q_{\max}^R = 0.560$, and again to be specific we have chosen values of $q < 2$, although nothing of significance changes for $q > 2$. It should also be noted that we have now restricted our-

selves to work on the branch of the Tan^{-1} function in Eq. (3.47), where $\delta_R(z) \rightarrow 0$ when $z \rightarrow \infty$, and this branch will always be implied henceforth. The important thing to note about the function $\delta_R(x)$ is the differing behavior for $q > q_{\max}^R$ or $q < q_{\max}^R$. In the former case $0 < \delta_R(x) < \pi$, and $\delta_R(x) = 0$ for $x \geq \frac{1}{2}q + 1$, whereas in the latter case $\delta_R(x) = \pi$ for $\frac{1}{2}q + 1 \leq x < x_0^R$, and this behavior is intimately connected with the respective absence or presence of the zero at $x = x_0^R$ in the function $\tilde{K}_R(x)$. These points are further illustrated in Fig. 5, again for $r_s = 1$.

Returning now to our general solution $\tilde{g}_R(z)$ it is straightforward to show from Eqs. (3.43), (3.45), and (3.48) that

$$\tilde{g}_R(z) \tilde{g}_R(-z) = \frac{[1 + \tilde{P}(z)][1 + \tilde{P}(-z)]}{\tilde{K}_R^2(z)} \exp \left(\frac{1}{2\pi i} \int_{\tilde{L} + \tilde{L}'} dx' \frac{\text{Ln} \tilde{K}_{R+}(x') - \text{Ln} \tilde{K}_{R-}(x')}{x' - z} \right). \quad (3.53)$$

The integral in Eq. (3.53) can now be simplified by considering the obvious contour integral taken around a contour comprising the whole circle at infinity, indented only to exclude the entire real axis. Using the results above on the analytic structure of the function $\text{Ln} \tilde{K}_R(z)$ together with Cauchy's theorem, it is found by comparison with Eq. (3.49) that

$$1 = [1 + \tilde{P}(z)][1 + \tilde{P}(-z)] \begin{cases} 1, & q \geq q_{\max}^R; \\ \frac{(1 + \frac{1}{2}q - z)(1 + \frac{1}{2}q + z)}{(x_0^R - z)(x_0^R + z)}, & q < q_{\max}^R. \end{cases} \quad (3.54)$$

Remembering that the function $\tilde{P}(z)$ must be every-

where analytic except for possible singularities at the end points of \tilde{L} [viz., $\max(0, \frac{1}{2}q - 1)$ and $(\frac{1}{2}q + 1)$], Eq. (3.54) immediately yields

$$1 + \tilde{P}(z) = \begin{cases} 1, & q \geq q_{\max}^R, \\ (x_0^R - z)/(1 + \frac{1}{2}q - z), & q < q_{\max}^R, \end{cases} \quad (3.55)$$

where the negative solution has been discounted by reference to Eq. (3.37) in the limit $z \rightarrow \infty$. Comparison with Eq. (3.48) then yields the unique solution

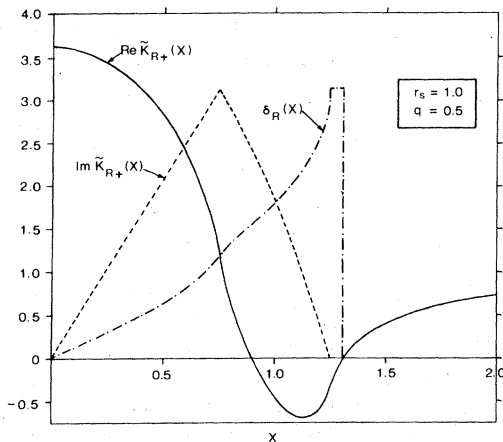


FIG. 4. Same as Fig. 3, but at a momentum transfer $q = 0.5 < q_{\max}^R = 0.560$.

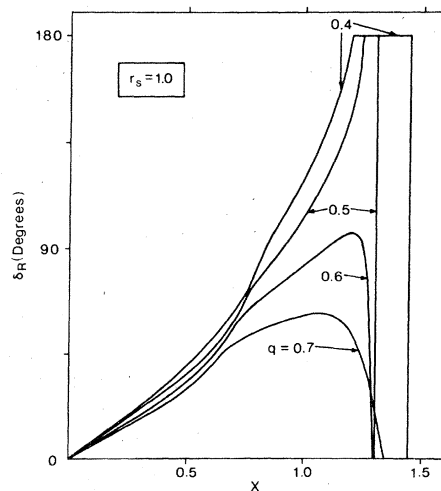


FIG. 5. Phase angle $\delta_R(x)$ at $r_s = 1$, for various values of the momentum transfer q .

$$\bar{g}_R(z) = \frac{1}{\bar{K}_R(z)} \exp\left(\frac{1}{\pi} \int_{\bar{L}} dx' \frac{\delta_R(x')}{x' - z}\right) \times \begin{cases} 1, & q \geq q_{\max}^R, \\ \frac{x_0^R - z}{1 + \frac{1}{2}q - z}, & q < q_{\max}^R, \end{cases} \quad (3.56a)$$

which by reference to Fig. 5 and the discussion of it can be rewritten in the equivalent form

$$\bar{g}_R(z) = \frac{1}{\bar{K}_R(z)} \exp\left(\frac{1}{\pi} \int_0^\infty dx' \frac{\delta_R(x')}{x' - z}\right), \quad (3.56b)$$

which is valid for *all* values of q , and where the effective upper limit on the integral is $\max(q/2 + 1, x_0^R)$. Two further equivalent expressions which can be constructed from Eqs. (3.56a) and (3.56b) by using the functional relation (3.49) are

$$\bar{g}_R(z) = \exp\left(-\frac{1}{\pi} \int_{\bar{L}} dx' \frac{\delta_R(x')}{x' + z}\right) \times \begin{cases} 1, & q \geq q_{\max}^R; \\ \frac{z + \frac{1}{2}q + 1}{z + x_0^R}, & q < q_{\max}^R; \end{cases} \quad (3.56c)$$

$$\bar{E}_R(y) \equiv \bar{K}_R(iy)$$

$$= 1 + \frac{1}{\beta} \left\{ 1 + \frac{1}{2q} (1 - \frac{1}{4}q^2 + y^2) \ln \left(\frac{(\frac{1}{2}q + 1)^2 + y^2}{(\frac{1}{2}q - 1)^2 + y^2} \right) + y \left[\tan^{-1} \left(\frac{\frac{1}{2}q - 1}{y} \right) - \tan^{-1} \left(\frac{\frac{1}{2}q + 1}{y} \right) \right] \right\}, \quad (3.57)$$

and where in Eq. (3.57) the symbol \tan^{-1} now indicates the principal value of the inverse tangent function, defined to lie in the interval $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$. This last form for $\bar{g}_R(x)$ is particularly suited to numerical computation since it contains a non-singular integrand, does not depend on the parameter $x_0^R(q)$, and is independent of whether $q \geq 2$. We also add that values in the physical regime $z \in \bar{L}$ are readily obtained by making use of Eq. (3.38).

Having obtained the general unique solution to the RPA ring equations in our formalism, we now wish for future use to discuss some of its properties. We start by considering the analytic structure of $\bar{g}_R(z)$, which is most readily investigated by considering Eq. (3.56c). Thus, $\bar{g}_R(z)$ is seen to be a function analytic in the entire complex z plane cut along \bar{L}' with the exception (for $q < q_{\max}$ only) of a simple pole at $z = -x_0^R$. In particular, $\bar{g}_R(z)$ is analytic over the physical regime \bar{L} and does not have a pole at $z = +x_0^R$.

It is readily verified that $\bar{g}_R(x)$ is a monotonically increasing function of x for $x > 0$, with a value at

and

$$\bar{g}_R(z) = \exp\left(-\frac{1}{\pi} \int_0^\infty dx' \frac{\delta_R(x')}{x' + z}\right), \quad (3.56d)$$

and where in each of Eqs. (3.56a)–(3.56d), $\delta_R(x)$ as given by Eq. (3.47) is continuous for $\min(\bar{L}) \leq x \leq \max(\frac{1}{2}q + 1, x_0^R)$, with values between 0 and π , and zero elsewhere on the positive real axis, as illustrated in Fig. 5. Strictly speaking we should still verify that the solution expressed by any of the above equivalent forms actually satisfies our original nonlinear integral equation. Suffice it to say that this may fairly readily be performed.

For many purposes, one final form for $\bar{g}_R(z)$ is useful, which is readily obtained by performing an obvious contour rotation

$$\bar{g}_R(z) = \exp\left(-\frac{z}{2\pi} \int_{-\infty}^\infty dy \frac{\ln \bar{E}_R(y)}{y^2 + z^2}\right) \times \begin{cases} 1, & \text{Re } z > 0, \\ 1/\bar{K}_R(z), & \text{Re } z < 0, \end{cases} \quad (3.56e)$$

where, from Eq. (3.35),

the origin given by

$$\bar{g}_R(0) = \left[1 + \frac{1}{\beta} \left(1 + \frac{1}{q} (1 - \frac{1}{4}q^2) \ln \left| \frac{q+2}{q-2} \right| \right) \right]^{-1/2}, \quad (3.58)$$

and which approaches unity as x approaches infinity. Its limiting behavior for small x is determined by the following expressions:

$$\bar{g}_R(x) \xrightarrow{x \rightarrow 0^+} \begin{cases} \bar{g}_R(0) [1 - \beta^{-1} \bar{g}_R^2(0) x \ln x + O(x)], & q < 2; \\ \bar{g}_R(0) [1 + O(x)], & q > 2. \end{cases} \quad (3.59)$$

The limiting behavior for large values of the momentum transfer q is also of interest, and it is important to realize that we shall actually be less interested in this limit when x remains constant but rather as $x/q \rightarrow \frac{1}{2}$, since we are basically interested in the physical regime specified by Eq. (3.23). It is easy to verify that the general limit is given by

$$\tilde{g}_R(x) \xrightarrow[q \rightarrow \infty]{x/q \rightarrow c} 1 - \frac{8\alpha r_s}{3\pi(1+2c)} q^{-4} + O(q^{-6}) \quad (3.60)$$

for arbitrary value of the constant c .

Using Eqs. (3.8), (3.12), (3.16), (3.17), and (3.21), it is readily shown that the correlation energy expressed as an energy per particle in units of rydbergs in the RPA is given by

$$\epsilon_c^{\text{RPA}} = \frac{3}{8\pi^3\alpha r_s} \int \frac{d\vec{q}}{q^2} \int_{\bar{\Gamma}} d\vec{k} [\tilde{g}_R(\vec{k}) - 1]. \quad (3.61)$$

The integrations in Eq. (3.61) can presumably now be performed by inserting any of the exact relations (3.56a)–(3.56e). It is, however, much simpler

to use Eq. (3.29) to derive the relation

$$\int_{\bar{\Gamma}} d\vec{k}' \tilde{g}_R(\vec{k}') = \lim_{z \rightarrow \infty} \{2\pi\beta qz [1 - \tilde{K}_R(z) \tilde{g}_R(z)]\}. \quad (3.62)$$

Use of Eqs. (3.61)–(3.62), together with the trivial relation

$$\begin{aligned} \int_{\bar{\Gamma}} d\vec{k} &= 2\beta q \int_{\bar{L}} dx \operatorname{Im} \tilde{K}_{R+}(x) \\ &= 2\beta q \int_0^\infty dy [\tilde{E}_R(y) - 1] \end{aligned} \quad (3.63)$$

and the various exact results of Eqs. (3.56) leads to the various forms for the RPA correlation energy

$$\epsilon_c^{\text{RPA}} = \left(\frac{3}{2\pi}\right) \left(\frac{1}{\alpha r_s}\right)^2 \int_0^\infty q^3 dq \int_0^\infty dx \left[\operatorname{Tan}^{-1} \left(\frac{\operatorname{Im} \tilde{K}_{R+}(x)}{\operatorname{Re} \tilde{K}_{R+}(x)} \right) - \operatorname{Im} \tilde{K}_{R+}(x) \right] \quad (3.64a)$$

$$= \left(\frac{3}{2\pi}\right) \left(\frac{1}{\alpha r_s}\right)^2 \int_0^\infty q^3 dq \left\{ \int_{\bar{L}} dx \left[\operatorname{Tan}^{-1} \left(\frac{\operatorname{Im} \tilde{K}_{R+}(x)}{\operatorname{Re} \tilde{K}_{R+}(x)} \right) - \operatorname{Im} \tilde{K}_{R+}(x) \right] + \pi \left[x_0^R - \left(\frac{1}{2}q + 1\right) \right] \Theta(q_{\max}^R - q) \right\} \quad (3.64b)$$

$$= \left(\frac{3}{2\pi}\right) \left(\frac{1}{\alpha r_s}\right)^2 \int_0^\infty q^3 dq \int_0^\infty dy [\ln \tilde{E}_R(y) - \tilde{E}_R(y) + 1], \quad (3.64c)$$

where $\Theta(x)$ is the usual unit-step function, defined to be one (zero) if x is greater (less) than zero. The last of the above forms is precisely the well-known expression for the RPA correlation energy as first derived by Gell-Mann and Brueckner,³ and the other forms have also been shown to be equivalent by Hubbard⁴ and Sawada *et al.*⁵

While (3.64c) is most convenient for the numerical evaluation of the RPA correlation energy (since it is independent of x_0^R), we can usefully consider Eq. (3.64b) further to enquire into the physical role of the constant $x_0^R = x_0^R(q)$. We may rewrite the two terms in Eq. (3.64b) as

$$\epsilon_c^{\text{RPA}} = \epsilon_{c;\text{cont}}^{\text{RPA}} + \epsilon_{c;\text{pl}}^{\text{RPA}}, \quad (3.65)$$

where the first term corresponds to the contribution from the x integration over the regime \bar{L} , and the second term arises from the term involving x_0^R . It is clear in this form that the term $\epsilon_{c;\text{cont}}^{\text{RPA}}$ arises from the physical regime \bar{L} , corresponding to the particle-hole continuum for which $|\tilde{k} + \frac{1}{2}\tilde{q}| > 1$ and $|\tilde{k} - \frac{1}{2}\tilde{q}| < 1$. The second-term $\epsilon_{c;\text{pl}}^{\text{RPA}}$ clearly then arises from an unphysical (for bare particle-hole pairs) region in momentum space. From Eq. (3.64b) it is easy to rewrite this latter contribution (to the total energy) as

$$E_{c;\text{pl}}^{\text{RPA}} = \frac{1}{2} \sum_{\vec{q}}^{q_{\max}} \left(\hbar \omega_{\text{pl}}(q) - \frac{\hbar^2}{2m} [(q + k_F)^2 - k_F^2] \right), \quad (3.66)$$

$$\hbar \omega_{\text{pl}}(q) \equiv (\hbar^2 k_F / m) q x_0^R(q),$$

where q has temporarily been restored to a variable with proper dimensions. In this form it is clearly seen that this piece of the correlation energy is just that arising from the plasma oscillations or *plasmons* with frequency $\omega_{\text{pl}}(q)$ and is given as the difference between the zero-point energy of this oscillation and the value this energy approaches as the coupling is turned off ($e^2 \rightarrow 0$ or equivalently $r_s \rightarrow 0$). This latter limit is simply from Eqs. (3.50) and (3.66):

$$\lim_{r_s \rightarrow 0} \hbar \omega_{\text{pl}}(q) = (\hbar^2 / 2m) [(q + k_F)^2 - k_F^2] \quad (3.67)$$

as required, which is just the upper limit of the particle-hole pair excitation continuum for a given q . We thus see from Eq. (3.66) that $x_0^R = x_0^R(q)$ essentially measures the plasmon dispersion curve. This result is perhaps not unexpected if we refer back to the analytic structure of the three-point or particle-hole vertex function $\tilde{g}_R(z)$, which analytic behavior is also reflected in

the four-point two-particle-two-hole function \tilde{S}_2^R from Eq. (3.24). Thus we recall that $\tilde{g}_R(z)$ has the cut \tilde{L}' and the (possible) pole at $z = -x_0^R$. By analogy with ordinary two-body potential scattering we would expect that the cut is a reflection of the particle-hole scattering continuum and the pole corresponds to a bound state, and this interpretation is now seen to be correct, except that we realize the bound state is not a two-body bound state but a true (many particle-hole) collective excitation of the many-body system. The analogy with potential theory can in fact usefully be extended. For example, the behavior of the "phase-shift" angle $\delta_R(x)$ shown in Fig. 5 with respect to whether the system sustains a plasmon or not for a particular momentum q , bears obvious analogy to Levinson's theorem⁵⁰ for two-body potential scattering. It is not difficult to formulate exactly the quasi-Levinson theorem for this many-body situation, although we shall not attempt to do so here.

It is perhaps also worth pointing out that the function $\tilde{K}_R(z)$ which plays such an important role in our solution is no more than the dielectric function well known from the Green's-function techniques (and see, e.g., Ref. 51). In the Green's-function analysis of time-dependent perturbation theory one can define a proper polarization insertion $\Pi^*(\tilde{q}, \omega)$ which renormalizes the bare static potential $V(\tilde{q})$ into a generally nonstatic (or equivalently energy-dependent) effective potential $\mathcal{V}(\tilde{q}, \omega)$ by

$$\mathcal{V}(\tilde{q}, \omega) = \frac{V(\tilde{q})}{1 - V(\tilde{q})\Pi^*(\tilde{q}, \omega)} \equiv \frac{V(\tilde{q})}{\epsilon(\tilde{q}, \omega)}, \quad (3.68)$$

where $\epsilon(\tilde{q}, \omega)$ is the dielectric response function. In the Green's-function theory it is shown that replacing Π^* by its lowest order approximation generates the RPA, and it is readily seen [cf. our Eq. (3.35) and Eqs. (12.36) and (12.45) of Ref. 51] that

$$\tilde{K}_R(z) \equiv \epsilon_{\text{RPA}}(\tilde{q}, qz). \quad (3.69)$$

In order to compare our results with the later TDA results we also consider taking the high-density ($r_s \rightarrow 0$) limit of Eq. (3.64c). The calculation is straightforward and is identical to that given by Gell-Mann and Brueckner,³ and we quote only the well-known result

$$\epsilon_c^{\text{RPA}} \xrightarrow{r_s \rightarrow 0} A \ln r_s + B_R + O(r_s \ln r_s), \quad (3.70a)$$

$$A = (2/\pi^2)(1 - \ln 2) \approx 0.0622,$$

$$B_R = (2/\pi^2)(1 - \ln 2)[\ln(4\alpha/\pi) + \langle \ln R \rangle_{\text{av}} - \frac{1}{2}] + \delta,$$

where

$$\langle \ln R \rangle_{\text{av}} \equiv \int_{-\infty}^{\infty} dy R^2 \ln R / \int_{-\infty}^{\infty} dy R^2 \approx -0.551,$$

$$R \equiv R(y) \equiv \frac{1}{2} \lim_{a \rightarrow 0} \{\beta [\tilde{E}_R(y) - 1]\} \\ = 1 - y \tan^{-1}(1/y), \quad (3.70b)$$

and δ is the finite piece of the (logarithmically divergent) second-order direct contribution $\epsilon_a^{(2)}$ after the logarithmic divergence has been properly removed

$$\delta \equiv \epsilon_a^{(2)} - \left(-\frac{12}{\pi^3} \int_0^{\infty} dy \int_0^1 \frac{dq}{q} R^2 \right) \\ = \lim_{\epsilon \rightarrow 0} \left(-\frac{4}{\pi^2} (1 - \ln 2) \ln \epsilon - \frac{3}{8\pi^5} \right. \\ \left. \times \int_{\epsilon}^{\infty} \frac{d\tilde{q}}{q^4} \int_{\tilde{\Gamma}} d\tilde{k}_1 \int_{\tilde{\Gamma}} d\tilde{k}_2 \frac{1}{\tilde{q} \cdot (\tilde{k}_1 + \tilde{k}_2)} \right) \\ \approx -0.0508. \quad (3.70c)$$

Putting these results together leads to the asymptotic expression

$$\epsilon_c^{\text{RPA}} \xrightarrow{r_s \rightarrow 0} 0.0622 \ln r_s - 0.142 + O(r_s \ln r_s). \quad (3.71)$$

Finally, it is well known³ that to get the first two terms in the above asymptotic expression exactly, one need only add to the RPA result the second-order exchange contribution $\epsilon_2^{(b)}$ evaluated exactly by Onsager⁵² as

$$\epsilon_2^{(b)} = \frac{1}{3} \ln 2 - (3/2\pi^2)\zeta(3) \approx 0.0484. \quad (3.72)$$

One thus obtains the exact result

$$\epsilon_c \xrightarrow{r_s \rightarrow 0} 0.0622 \ln r_s - 0.094 + O(r_s \ln r_s). \quad (3.73)$$

It is not difficult to show that in this high-density limit the plasmons contribute only to the constant term in Eq. (3.73), and by explicit evaluation⁶ we find

$$\epsilon_{c; \text{pl}}^{\text{RPA}} \xrightarrow{r_s \rightarrow 0} \frac{3}{2\pi^2} \int_1^{\infty} dx_0^R f^2(x_0^R), \\ f(x) \equiv x \ln[(x+1)/(x-1)] - 2, \quad (3.74)$$

which integral can be evaluated analytically⁵² to give

$$\epsilon_{c; \text{pl}}^{\text{RPA}} \xrightarrow{r_s \rightarrow 0} \frac{1}{3} - 2/\pi^2 \approx 0.1307. \quad (3.75)$$

C. TDA ring equations

In Sec. IIIB we have explicitly solved the S_2 equations in the RPA. It is clear from iteration of Eq. (3.10), or its pictorial representation in Fig. 2, that the RPA sums all the most general ring diagrams and that the general intermediate state in the RPA consists of an arbitrary (even) number of particle-hole pairs. An equivalent way of describing the RPA is thus to say that the intermediate states considered are restricted to those obtained by creating or destroying (bare) particle-hole pairs from the noninteracting ground state, and in this form the RPA is also well known in the context of nuclear spectroscopy. Here one is interested, for example, in the calculation of collective excitations in closed-shell nuclei, where the ground state is supposed to be, to a good zeroth approximation, the closed-shell Hartree-Fock state; i.e., a Slater determinant built from the self-consistent Hartree-Fock single-particle (or shell-model) basis. One then arrives at the RPA by, for example, linearizing the equations of motion by keeping only those matrix elements which connect an excited state to the ground state by creating or destroying particle-hole pairs in the ground state. A further approximation is also well known in this context, which makes the further restriction that one considers only those states reached by creating particle-hole pairs from the ground state, i.e., the further approximation is made that the ground state has no particle-hole pair components. For historical reasons this has become known in the literature as the Tamm-Dancoff⁴⁵ approximation. These authors were in fact concerned with a field-theoretic treatment of a system of mesons and nucleons, which they solved within such a truncated basis as described above, and the general approach has been employed both previously and since by many other authors.

Within the present context the TDA is now easy to formulate. Thus we consider the subset of ring diagrams, wherein every intermediate state consists of just two particle-hole pairs. Equivalently, within the language of Goldstone perturbation theory, the TDA consists of taking only those ring diagrams propagating forwards in time from the time the first two particle-hole pairs were created, whereas the RPA enlarges the class to the rings propagating either forwards or backwards in time. From Fig. 2 it is now clear that the only term in the RPA which is responsible for backward propagation is the last term quadratic in \tilde{S}_2 , and omission of this term leads to the TDA.

At this point it is worth pointing out that one knows many examples in many-body theory where

an approximation is worsened rather than improved by the addition of extra diagrams, particularly at intermediate values of the effective coupling constant, and thus it is not *a priori* obvious whether the TDA is a worse approximation than the RPA for nonvanishing values of r_s . Furthermore the TDA has to our knowledge never before been applied to the electron gas. Finally, since the TDA turns out also to be susceptible to an exact solution in this case, and since exact results in many-body theory are rare, and can often be used as a yardstick against which to measure more elaborate methods, we consider it worthwhile to consider further.

Just as above we used the index R to indicate quantities evaluated in the RPA, we now use the index T (subscript or superscript) for the corresponding quantities in the TDA. From the above discussion, it is clear that the basic TDA ring equation is the "linearized" version of Eq. (3.15),

$$\tilde{f}_{\vec{k}_1}^T(\vec{q}) = -\frac{1}{4\pi\beta} \int_{\vec{r}} d\vec{k}_2 \frac{1}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)} \times [1 + 2\tilde{f}_{\vec{k}_1}^T(\vec{q}) + 2\tilde{f}_{\vec{k}_2}^T(\vec{q})], \quad (3.76)$$

or in terms of the TDA particle-hole vertex function \tilde{g}_T , defined by Eq. (3.16),

$$\tilde{g}_T(\vec{k}_1) = 1 - \frac{1}{2\pi\beta} \int_{\vec{r}} d\vec{k}_2 \frac{1}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)} \times [\tilde{g}_T(\vec{k}_1) + \tilde{g}_T(\vec{k}_2) - 1]. \quad (3.77)$$

Defining the functions $\tilde{K}_T(\vec{k})$ and $\tilde{Z}(\vec{k})$ by

$$\tilde{K}_T(\vec{k}) \equiv 1 + \tilde{Z}(\vec{k}) \equiv 1 + \frac{1}{2\pi\beta} \int_{\vec{r}} \frac{d\vec{k}'}{\vec{q} \cdot (\vec{k}' + \vec{k})}, \quad (3.78)$$

the basic TDA equation (3.77) can be recast in the form

$$\tilde{K}_T(\vec{k}_1)\tilde{g}_T(\vec{k}_1) = \tilde{K}_T(\vec{k}_1) - \frac{1}{2\pi\beta} \int_{\vec{r}} d\vec{k}_2 \frac{\tilde{g}_T(\vec{k}_2)}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)} \quad (3.79)$$

in terms of the solution to which the TDA approximant for \tilde{S}_2 may be written

$$\tilde{S}_{2; \vec{k}_1 \vec{k}_2}^T(\vec{q}) = -(2/3\beta N) [1/\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)] \times [\tilde{g}_T(\vec{k}_1) + \tilde{g}_T(\vec{k}_2) - 1]. \quad (3.80)$$

By exactly the same reasoning as in the RPA case, we again come to the conclusion that $\tilde{g}_T(\vec{k})$ is a function only of the scalar variables q^2 and $\vec{k} \cdot \vec{q}$, and is independent of κ^2 . Continuing to suppress the dependence on q , we write $\tilde{g}_T(\vec{k}) \equiv \tilde{g}_T(\vec{k} \cdot \vec{q})$

henceforward. By choosing the same cylindrical polar coordinate system as in the RPA case, Eq. (3.80) may be reduced to a one-dimensional integral equation for $\tilde{g}_T(x \equiv \tilde{k} \cdot \hat{q})$,

$$\tilde{K}_T(z) \tilde{g}_T(z) = \tilde{K}_T(z) - \frac{1}{\beta} \int_{\tilde{L}} dx' \tilde{N}(x') \frac{\tilde{g}_T(x')}{x' + z}, \quad (3.81)$$

with

$$\tilde{K}_T(z) \equiv 1 + \tilde{Z}(z) \equiv 1 + \frac{1}{\beta} \int_{\tilde{L}} dx' \frac{\tilde{N}(x')}{x' + z}, \quad (3.82)$$

where we have again analytically continued our equation into the complex z plane, and where the function $\tilde{N}(x)$ and the symbol \tilde{L} have the same meaning as in Eqs. (3.31)–(3.32). Equation (3.81) is now a nonsingular linear integral equation in the physical regime $z = x \in \tilde{L}$, but as in the RPA case it is convenient to turn it into a singular equation in order to solve it analytically, and we do this as before by deriving a relation between $\tilde{g}_T(z)$ and $\tilde{g}_T(-z)$. Starting with Eq. (3.81), and performing an essentially similar analysis as in the RPA case, it is fairly straightforward to show that $\tilde{g}_T(z)$ satisfies the functional relation

$$\tilde{g}_T(z) + \tilde{g}_T(-z) = 1 + 1/\tilde{K}_T(z) \tilde{L}_T(z), \quad (3.83)$$

where

$$\tilde{L}_T(z) \equiv \tilde{K}_T(-z), \quad (3.84)$$

which is just the TDA analog of the RPA result (3.49). This result can now be used to rewrite Eq. (3.81) in the form

$$\tilde{L}_T(z) \tilde{g}_T(z) = \frac{1}{\tilde{K}_T(z)} + \frac{1}{\beta} \int_{\tilde{L}} dx' \tilde{N}(x') \frac{\tilde{g}_T(x')}{x' - z}, \quad (3.85)$$

which is the TDA analog of the RPA equation (3.37). It is again clear that in the physical regime $x \in \tilde{L}$,

$$\tilde{g}_T(x) = \lim_{y \rightarrow 0} \tilde{g}_T(x \pm iy), \quad x \in \tilde{L}. \quad (3.86)$$

Equation (3.85) is again of the standard Muskhelishvili–Omnès type, and the well-known theory of this class of singular equations (and see Ref. 49) leads to the general solution

$$\begin{aligned} \tilde{L}_T(z) \tilde{g}_T(z) = & \frac{1}{\tilde{K}_T(z)} - \frac{\Pi(z) e^{u^T(z)}}{2\pi i} \\ & \times \int_{\tilde{L}} dx' \frac{e^{-u^T_+(x')} - e^{-u^T_-(x')}}{\Pi(x') \tilde{K}_T(x') (x' - z)} \\ & + p(z) \Pi(z) e^{u^T(z)}, \end{aligned} \quad (3.87)$$

where $u^T(z)$ is defined analogously to $u^R(z)$ in Eq. (3.43), with

$$G_T(x) = \tilde{L}_T_-(x) / \tilde{L}_T_+(x) \equiv e^{-2i\delta_T(x)}, \quad x \in \tilde{L} \quad (3.88)$$

and

$$\Pi(z) = (z - a)^{-n_1} (z - b)^{-n_2}, \quad (3.89)$$

where a and b are, respectively, the lower and upper end points of the regime \tilde{L} , and the integers n_1 and n_2 are defined by

$$n_1 = -\pi^{-1} \delta_T(a), \quad n_2 = \pi^{-1} \delta_T(b). \quad (3.90)$$

We again note that solution (3.87) is not unique since it contains the function $p(z)$, which is an arbitrary polynomial.

Again, in order to simplify the result (3.87) by performing the obvious contour integral, it is necessary to consider the analytic structure of the function $\text{Ln} \tilde{L}_T(z)$. From either the defining relations (3.82) and (3.84), or from the explicit result

$$\tilde{L}_T(z) = \begin{cases} 1 + \frac{1}{2\beta q} \left[[1 - (z - \frac{1}{2}q)^2] \ln \left(\frac{z - 1 - \frac{1}{2}q}{z - 1 + \frac{1}{2}q} \right) + 2qz \ln \left(\frac{z - 1 + \frac{1}{2}q}{z} \right) - q(z - 1) \right], & q < 2, \\ 1 + \frac{1}{2\beta q} \left[[1 - (z - \frac{1}{2}q)^2] \ln \left(\frac{z - \frac{1}{2}q - 1}{z - \frac{1}{2}q + 1} \right) - 2(z - \frac{1}{2}q) \right], & q \geq 2, \end{cases} \quad (3.91)$$

it is not difficult to show that the function $\text{Ln} \tilde{L}_T(z)$ has the following properties: (i) it contains the branch cut \tilde{L} of $\tilde{L}_T(z)$, and (ii) the (possible) extra branch point at $z = +x_0^T$, due to the (possible) zero in $\tilde{L}_T(z)$, $\tilde{L}_T(x_0^T) = 0$, where $x_0^T = x_0^T(q) > \frac{1}{2}q + 1$. This zero exists only for $q \leq q_{\text{max}}^T$, where q_{max}^T is given by

$$x_0^T(q_{\text{max}}^T) = \frac{1}{2} q_{\text{max}}^T + 1, \quad (3.92)$$

(iii) otherwise $\text{Ln} \tilde{L}_T(z)$ is analytic in the cut plane, and (iv) $\tilde{L}_T(z) \rightarrow 1$ when $z \rightarrow \infty$. Using this information it is readily shown that $u^T(z)$ may be evaluated explicitly as

$$e^{u^T(z)} = \tilde{L}_T(z) \times \begin{cases} 1, & q > q_{\text{max}}^T, \\ (\frac{1}{2}q + 1 - z)/(x_0^T - z), & q \leq q_{\text{max}}^T, \end{cases} \quad (3.93)$$

and working on the same branch of the Ln function as in the RPA case, the integers n_1 and n_2 in Eq. (3.90) may be specified as

$$n_1 = 0, \quad n_2 = \Theta(q_{\max}^T - q). \quad (3.94)$$

Equations (3.93) and (3.94) may now be used to simplify the result given in Eq. (3.87). By considering the contour integral of the obvious integrand around a contour comprising the imaginary axis and the infinite semicircle in the right half-plane, indented at the real axis to exclude the cut \bar{L} , one finally arrives at the solution

$$\tilde{g}_T(z) = 1 + \left(\frac{1}{\bar{K}_T(z)\bar{L}_T(z)} - 1 \right) \Theta(-\text{Re}z) + \frac{z}{2\pi} \int_{-\infty}^{\infty} \frac{dy}{y^2 + z^2} \left(\frac{1}{\bar{K}_T(iy)\bar{L}_T(iy)} - 1 \right), \quad (3.95)$$

where the arbitrary polynomial $p(z)$ in Eq. (3.87) has again been evaluated by insisting that the solutions both satisfy the functional relation (3.83) and approach unity as z tends to infinity, as is readily observed from our original Eq. (3.81). Equation (3.95) again specifies completely the unique TDA solution, and should be compared with its RPA counterpart (3.56e). Both for completeness and for future use, we also give the TDA counterparts of the RPA results expressed in Eqs. (3.56a)–(3.56d). These relations, fully equivalent to Eq. (3.95) are derived from this result by performing various contour distortions, and using the functional relation (3.83):

$$\begin{aligned} \tilde{g}_T(z) &= \frac{1}{\bar{K}_T(z)\bar{L}_T(z)} + \frac{\Theta(q_{\max}^T - q)}{(x_0^T - z)} \frac{1}{\bar{K}_T(x_0^T)\bar{L}'_T(x_0^T)} - \frac{1}{2\pi i} \int_{\bar{L}} \frac{dx'}{x' - z} \frac{1}{\bar{K}_T(x')} \left(\frac{1}{\bar{L}_{T+}(x')} - \frac{1}{\bar{L}_{T-}(x')} \right) \\ &= \frac{1}{\bar{K}_T(z)\bar{L}_T(z)} - \frac{1}{2\pi i} \int_0^{\infty} \frac{dx'}{x' - z} \frac{1}{\bar{K}_T(x')} \left(\frac{1}{\bar{L}_{T+}(x')} - \frac{1}{\bar{L}_{T-}(x')} \right) \\ &= 1 - \frac{\Theta(q_{\max}^T - q)}{(x_0^T + z)} \frac{1}{\bar{K}_T(x_0^T)\bar{L}'_T(x_0^T)} + \frac{1}{2\pi i} \int_{\bar{L}} \frac{dx'}{x' + z} \frac{1}{\bar{K}_T(x')} \left(\frac{1}{\bar{L}_{T+}(x')} - \frac{1}{\bar{L}_{T-}(x')} \right) \\ &= 1 + \frac{1}{2\pi i} \int_0^{\infty} \frac{dx'}{x' + z} \frac{1}{\bar{K}_T(x')} \left(\frac{1}{\bar{L}_{T+}(x')} - \frac{1}{\bar{L}_{T-}(x')} \right), \end{aligned} \quad (3.96)$$

where

$$\tilde{L}'_T(x_0^T) = \left. \frac{d\bar{L}_T(x)}{dx} \right|_{x=x_0^T} \quad (3.97)$$

By analogy with Eq. (3.61) we can now evaluate the correlation energy in the TDA as

$$\epsilon_c^{\text{TDA}} = \frac{3}{\pi} \left(\frac{1}{\alpha r_s} \right) \int_0^{\infty} q dq \int_{\bar{L}} dx \bar{N}(x) [\tilde{g}_T(x) - 1], \quad (3.98)$$

which is readily evaluated in the two equivalent forms, by direct substitution of the exact solution from either Eq. (3.95) or the third of Eqs. (3.96),

$$\begin{aligned} \epsilon_c^{\text{TDA}} &= \left(\frac{3}{2\pi} \right) \left(\frac{1}{\alpha r_s} \right)^2 \int_0^{\infty} q^3 dq \left[\frac{1}{2i} \int_{\bar{L}} dx' \left(\frac{\bar{K}_T(x') - 1}{\bar{K}_T(x')} \right) \left(\frac{1}{\bar{L}_{T+}(x')} - \frac{1}{\bar{L}_{T-}(x')} \right) \right. \\ &\quad \left. - \pi \frac{\bar{K}_T(x_0^T) - 1}{\bar{K}_T(x_0^T)\bar{L}'_T(x_0^T)} \Theta(q_{\max}^T - q) \right] \end{aligned} \quad (3.99a)$$

$$= \left(\frac{3}{4\pi} \right) \left(\frac{1}{\alpha r_s} \right)^2 \int_0^{\infty} q^3 dq \int_0^{\infty} dy \left(\frac{1}{\bar{K}_T(iy)\bar{L}_T(iy)} - 1 \right) [\bar{K}_T(iy) + \bar{L}_T(iy) - 2]. \quad (3.99b)$$

The two terms in Eq. (3.99a) again correspond respectively to the contributions from the particle-hole continuum and the plasmons, whereas Eq. (3.99b) is more convenient for numerical integration. The evaluation of ϵ_c^{TDA} in the high-density limit may be derived from Eq. (3.99b) in a straightforward fashion. The result after a certain

amount of tedious algebra is

$$\epsilon_c^{\text{TDA}} \xrightarrow{r_s \rightarrow 0} A \ln r_s + B_T + O(r_s \ln r_s), \quad (3.100a)$$

where A is identical to the RPA value in Eq. (3.70a), and

$$B_T = (2/\pi^2) (1 - \ln 2) [\ln(2\alpha/\pi) + \kappa] + \delta, \quad (3.100b)$$

where δ is as given in Eq. (3.70c), and

$$\kappa = \left\{ \int_0^\infty dy R^2 \left[\frac{1}{2} \ln(R^2 + I^2) + \left(\frac{R^2 - I^2}{2IR} \right) \tan^{-1} \left(\frac{I}{R} \right) \right] \right\} / \int_0^\infty dy R^2$$

$$R \equiv R(y) = 1 - y \tan^{-1}(1/y), \quad (3.100c)$$

$$I \equiv I(y) = \frac{1}{2} y \ln(1 + 1/y^2).$$

Numerical integration yields a value $\kappa = -0.1670$, which gives the final expression

$$\epsilon_c^{\text{TDA}} \xrightarrow{r_s \rightarrow 0} 0.0622 \ln r_s - 0.1298 + O(r_s \ln r_s). \quad (3.101)$$

D. MA ring equations

As we have already seen the RPA can be represented as summing the most general ring diagrams in their entirety, while the TDA sums only that subset in which the rings propagate only forward in time from the instant the first two particle-hole pairs are created. There is one further approximation which has been used in the context of the electron gas many years ago by Macke,⁴⁶ and which was motivated by earlier work of Wigner.¹⁰ Here one also considers the rings to propagate only forward in time, but further restricts the class of diagrams to those in which a given pair of the original two particle-hole pairs created remains for all subsequent times in its original state, i.e., suffers no subsequent scattering. Within the context of the present formalism this Macke approximation (MA) is readily seen to correspond diagrammatically not only to omitting the term quadratic in S_2 in Fig. 2 as in the TDA, but also either one of the terms linear in S_2 on the right-hand side of Fig. 2.

Using the index (subscript or superscript) M now to indicate quantities evaluated in this MA, it is clear from the above discussion that the basic MA ring equation, by analogy to Eqs. (3.15) and (3.76), is

$$\tilde{f}_{\vec{k}_1}^M(\vec{q}) = -\frac{1}{4\pi\beta} \int_{\vec{r}} d\vec{k}_2 \frac{1}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)} [1 + 2\tilde{f}_{\vec{k}_1}^M(\vec{q})] \quad (3.102)$$

or, in terms of the MA particle-hole vertex function \tilde{g}_M defined as in Eq. (3.16),

$$\tilde{g}_M(\vec{k}_1) = 1 - \frac{1}{2\pi\beta} \int_{\vec{r}} d\vec{k}_2 \frac{1}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)} \tilde{g}_M(\vec{k}_1), \quad (3.103)$$

in terms of the solution to which the MA approximant for S_2 is

$$\tilde{S}_{2;\vec{k}_1\vec{k}_2}^M(\vec{q}) = -\frac{2}{3\beta N} \frac{\tilde{g}_M(\vec{k}_1)}{\vec{q} \cdot (\vec{k}_1 + \vec{k}_2)}. \quad (3.104)$$

It is clear both from the discussion above and the explicit expression of Eq. (3.104) that the MA destroys the symmetry of $\tilde{S}_{2;\vec{k}_1\vec{k}_2}(\vec{q})$ under the interchange $\vec{k}_1 \leftrightarrow \vec{k}_2$, although this symmetry can be restored if necessary by symmetrizing Eq. (3.104).

The solution of Eq. (3.103) is now trivial, and gives in our, by now familiar, variables

$$\tilde{g}_M(z) = 1/\tilde{K}_T(z), \quad (3.105)$$

where $\tilde{K}_T(z)$ is the TDA dielectric function defined in Eq. (3.78). We note that $\tilde{g}_M(z)$ has identical analytic structure to $\tilde{g}_T(z)$, namely, the same plasmon pole at $z = -x_0^T$, and the particle-hole continuum cut corresponding to $z \in \tilde{L}'$.

The correlation energy in the MA is immediately given by comparison with Eq. (3.98) as

$$\epsilon_c^{\text{MA}} = \frac{3}{\pi} \left(\frac{1}{\alpha r_s} \right) \int_0^\infty q dq \int_{\tilde{L}} dx \tilde{N}(x) \left(\frac{1}{\tilde{K}_T(x)} - 1 \right). \quad (3.106)$$

It is straightforward to derive the high-density limit of this expression, viz.,

$$\epsilon_c^{\text{MA}} \xrightarrow{r_s \rightarrow 0} \delta + \frac{3}{\pi^2} \int_0^1 x dx J \ln \left(\frac{2\alpha r_s}{\pi} J \right), \quad (3.107)$$

$$J \equiv J(x) = \int_0^1 \frac{y dy}{y+x} = 1 - x \ln \left(1 + \frac{1}{x} \right),$$

where again δ is given by Eq. (3.70c). This expression is identical to that given by Gell-Mann and Brueckner³ for the MA, whose by numerical integration quote the final result

$$\epsilon_c^{\text{MA}} \xrightarrow{r_s \rightarrow 0} 0.0622 \ln r_s - 0.174 + O(r_s \ln r_s). \quad (3.108)$$

We note that the result (3.107), without the second-order correction term δ , is also just that given by Lührmann.³⁴

IV. COMPARISONS AND CONCLUSIONS

For a comparison of the RPA and TDA results it is most convenient to consider the contributions to the correlation energy ϵ_c arising from the different values of the momentum transfer q . Thus, we define a function $\epsilon(q)$, such that

$$\epsilon_c = \int_0^\infty dq \epsilon(q), \quad (4.1)$$

and the RPA and TDA values of this function are correspondingly given by Eqs. (3.64) and (3.99). It is easy to show that the large- q (or short-range) limits of this quantity are identical in both approximations and are given by

$$\lim_{q \rightarrow \infty} \epsilon_{\text{RPA}}(q) = \lim_{q \rightarrow \infty} \epsilon_{\text{TDA}}(q) = -(8/3\pi^2)(1/q^4), \quad (4.2)$$

whereas the small- q (or long-range) limits are given by

$$\begin{aligned} \epsilon_{\text{RPA}}(q) &\xrightarrow{q \rightarrow 0} -(3/2\pi)q/\alpha r_s, \\ \epsilon_{\text{TDA}}(q) &\xrightarrow{q \rightarrow 0} -(3/4\pi)q/\alpha r_s. \end{aligned} \quad (4.3)$$

The common short-range limit is hardly surprising since to this leading order only the common second-order ring diagram contributes. What is more interesting is how rapidly in fact this limit is approached, as is illustrated in Fig. 6. It is seen that for both RPA and TDA at both $r_s=1$ and $r_s=6$, the $\epsilon(q)$ curves have already healed to their asymptotic limits within a few percent at $q=2$. What is more, the RPA and TDA values heal together even more rapidly than this, even for $r_s=6$. For small values of r_s this is to be expected, since it is clear from our previous discussion that in perturbation-theoretical terms the RPA and TDA differ only in fourth- and higher-order terms, but it is quite surprising at values of r_s as high as 6. It is clear both from our high-density limits expressed in Eqs. (3.71) and (3.101), and from Fig. 6, that the overall effect of the ring terms containing backward-going propagation, is attractive. Actual values of the correlation energy in both approximations are shown in Table I for various values of r_s . It is clear that while the ring terms containing backward propagation are not negligible, they contribute only (8–12)% of the total ring contribution to the correlation energy over the range in r_s from 1 to 6.

While the RPA taken together with the second-order exchange term gives exactly the first two terms in the high-density expansion for the correlation energy, we certainly do not expect it to

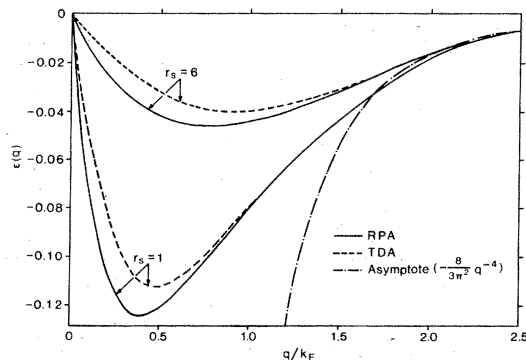


FIG. 6. Function $\epsilon(q)$ in the RPA and TDA at the values $r_s=1$ and $r_s=6$. The common short-range asymptote of Eq. (4.2) is also shown.

TABLE I. Correlation energy ϵ_c of the electron gas in the RPA and TDA.

r_s	ϵ_c^{RPA}	ϵ_c^{TDA}
1	-0.1576	-0.1464
2	-0.1236	-0.1129
3	-0.1055	-0.0952
4	-0.0936	-0.0836
5	-0.0849	-0.0753
6	-0.0782	-0.0689

be a good approximation in the intermediate regime. Thus, quite apart from ignoring the simple effects of exchange [Fig. 1(d)] we have ignored even in the SUB2 approximation (i) all of the combined particle-particle and hole-hole ladder terms [generated by diagrams (m)–(o) of Fig. 1], some at least of which are important for short-range effects; (ii) the generalized self-energy correction terms [generated by diagrams (g)–(l) of Fig. 1]; (iii) a class of ring-exchange diagrams [generated by diagrams (d)–(f) of Fig. 1]; and (iv) a class of additional exchange terms [generated by the remaining diagrams of Fig. 1] which includes the particle-hole ladder terms (p) and (q). It will remain the task for future papers in this series (particularly III) systematically to examine the effects caused by these various terms.

After the present work was completed, we learned of a recent paper of Freeman⁵³ in which essentially the same coupled-cluster formalism as used here is applied to the electron gas in the ring approximations. Freeman considered both the RPA and what he calls a linearized RPA (equivalent to our TDA), but he was unable to obtain exact solutions in either case. His numerical results however are in perfect agreement with ours. Freeman also considers the incorporation of exchange effects arising from the ring diagrams, but he treats only the incomplete case where in terms of diagrams for the ground-state energy only the latest (in time) potential line is exchanged, with all other interactions retaining their accompanying "direct" rings. We have checked that our exact RPA and TDA solutions also agree with his numerical results for this simple treatment of exchange. We do not present results for this case however since we believe that meaningful results on the effects of exchange on the RPA, for example, can only be given by considering them in their entirety, i.e., by including the entire set of RPA exchange diagrams generated by incorporating Figs. 1(d), 1(e), and 1(f), which we consider separately in III.

It is also interesting to note that in the absence of an exact solution to his RPA equation [equivalent

to our Eq. (3.10)], Freeman⁵³ is led to assert that nonlinear equations of the RPA type will have multiple solutions, and in particular he claims that the numerical solution he obtains by numerical iteration is not unique. In view of our having shown that the RPA solution is unique, it is clear that this assertion is simply not true in this case. It is also true that both the full SUB2 approximation for S_2 and many other approximations to it involve nonlinear equations, and Freeman further suggests that all such equations will have multiple solutions, and that "the other solutions may provide useful approximations for some of the excited states of the system." For several reasons we remain sceptical of this suggestion. While we cannot prove in general that the full SUB2 equation for S_2 , or any particular approximation to it, does have a unique solution, our experience suggests that either such equations will have unique solutions that describe the unique (approximation to the) ground state as in the RPA discussed here, or if a nonuniqueness does occur, that physical considerations will usually dictate that only one of the mathematical solutions is physically tenable and that the remainder must normally be discarded. With regard to the latter possibility we argue on the following grounds. In the first place we know already of at least two cases where nonunique solutions do occur. One of these is the analogous RPA considered here but for a system of bosons. In this case (and see III), the equation for S_2 is a simple algebraic quadratic equation. Only one of the two roots passes over to the pertur-

bative solution, and the other nonperturbative solution must certainly be discarded since it is unbounded. Another case is the soluble fermion model discussed by one of the present authors.³⁴ Here again it is shown that for an N -particle problem, a complete SUB n description leads to multiple solutions, and furthermore that the non-ground-state solutions only give even an approximate description of the excited states if $n \approx N$. In summary, what seems clear to us is that any possible multiple solutions of a SUB n approximation with $n \ll N$ are extremely unlikely to provide a good description of collective excitations, although it must remain an open question as to whether some of the extra solutions might provide a good description of m -body excitations with $m \leq n$. In any case we feel that it is more sensible to study excited states with a formalism which is particularly designed to do so, rather than with the coupled-cluster approach described here. Thus in II we study the excited states of the electron gas employing such an approach, and which uses our analytic RPA solution for S_2 obtained here as input.

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