Higher Random-Phase Approximations in the Many-Body Problem

H. SUHL AND N. R. WERTHAMER*

Bell Telephone Laboratories, Murray Hill, New Jersey, and Department of Physics,
University of California, Berkeley, California

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The usual random-phase approximation combined with an equations-of-motion technique for the many-electron problem is extended, yielding many of the known results of series summation methods in a straightforward manner. The method should apply to other types of many-body problems as well.

INTRODUCTION

IN recent years the approach to the ground-state problem of the free electron gas known as the "random-phase approximation"[1] (hereafter called RPA) has been vindicated by rigorous partial summation of perturbation series.[2-7] It was shown, particularly in reference 3, that at high electron densities the dominant term in the correlation energy may be derived either by formal summation of the most divergent integrals in the expansion in powers of the interaction parameter, or else by a consistent application of the RPA.

However, the summation methods have also answered questions that are out of reach of the ordinary RPA. Two cases in point are the damping of plasma oscillations,[8] and the Du Bois result for the ground-state energy of a free electron gas.[8] Similarly, the result of Gell-Mann[9] for the specific heat of an electron gas is inaccessible from the RPA, which would predict only the Hartree-Fock single-particle exchange correction with its logarithmic singularity near the Fermi surface,

and hence zero specific heat.[10] This paper demonstrates that at least some of these defects of the RPA can be remedied by extending it just one step.[11] Specifically, we demonstrate that the extension reproduces the result of Du Bois[8] for the ground state energy, and the result of Gell-Mann[9] for the specific heat of a degenerate electron gas.

Our procedure is based on the well-known fact that if O is an operator such that its commutator with the Hamiltonian H satisfies

$$[H,O]=\omega O, \tag{1}$$

then $O\psi_G$ is an excited eigenstate of the system, with excitation energy ω above the energy of the true ground-state ψ_G. This is seen by operating on ψ_G with both sides of Eq. (1). As an example, one may consider the motion of a hole in an existing electron cloud. In that case, ω (or rather its derivative), as the momentum of the added electron approaches the Fermi momentum, is the quantity needed in a calculation of the specific heat. It then seems natural to try for O the operator C_λ which destroys an electron with momentum λ.[12] One then finds

* National Science Foundation Predoctoral Fellow.
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[8] D. F. Du Bois, Ann. Phys. **7**, 174 (1959); **8**, 24 (1959).
[9] M. Gell-Mann, Phys. Rev. **106**, 369 (1957).

[10] The ordinary RPA, when used to decompose the electron motions into collective modes and screened single-particle motions, will of course lead to an at least qualitatively correct modification of the Hartree-Fock energy; the point here is that the RPA applied directly to the motion of an excess electron (or hole) does not.

[11] H. Suhl, Bull. Am. Phys. Soc. **5**, 279 (1960).

[12] Actually the spin index, σ, can be considered as incorporated into the momentum subscript provided we alter the definition (11) of the potential to read

$$v(\mathbf{pqrs}) \equiv \tfrac{1}{2}[v(\mathbf{p-r})\delta_{\sigma_p,\,\sigma_r} - v(\mathbf{p-s})\delta_{\sigma_p,\,\sigma_s}]\delta_{\mathbf{p+q,r+s}}.$$

that the commutator with the kinetic energy part of H is consistent with Eq. (1), while the commutator with the potential energy is not. We have

$$H = \sum_k \varepsilon_k C_k^* C_k$$
$$- \frac{2\pi e^2}{\Omega} \sum_{k,k',p\neq 0} \frac{1}{p^2} C_{k+p}^* C_{k'-p}^* C_k C_{k'} \equiv K + V, \quad (2)$$

and

$$[H,C_\lambda] = -\varepsilon_\lambda C_\lambda + \frac{4\pi e^2}{\Omega} \sum_{k,p\neq 0} \frac{1}{p^2} C_{k+p}^* C_{\lambda+p} C_k. \quad (3)$$

In fact, only in trivial cases is there an exact relation like (1). The ordinary RPA now proceeds by retaining, of the offending triple terms, only those which may be "linearized," i.e., those in which the momentum subscript of one of the two C's coincides with that of the single C^*. The resultant combination is replaced by its expectation value in the ground state. Equation (1) then takes the form

$$\omega = -\varepsilon_\lambda + \frac{4\pi e^2}{\Omega} \sum_{p\neq 0} n_{\lambda+p}/p^2 \equiv -\varepsilon_\lambda'. \quad (4)$$

The expectation value $n_{\lambda+p}$ in the true ground state is not known. Therefore, it is usual to make the further approximation that the n's may be replaced by their values appropriate to the ground state of the non-interacting gas, that is by unity below, and zero above, the Fermi surface. The excitation energy then becomes equal to the ordinary Hartree-Fock separation energy. A familiar difficulty now results: The sum has a derivative with logarithmic singularity when $\lambda = k_F$, the Fermi momentum, leading to a zero in the density of states and therefore zero specific heat. The reason is of course that the Coulomb interaction should be shielded so as to yield a finite limit as $p \to 0$. The work of Gell-Mann based on a summation of selected terms in a perturbation series, effectively produced a shielding.

On the other hand, we may also remove the difficulty by retaining in the commutator (3) not only the usual RPA terms, but also all the residual terms of the form

$$C_{k+p}^* C_{\lambda+p} C_k, \quad k \neq \lambda, \quad (5)$$

as well as the fluctuations,

$$\delta n_{\lambda+p} C_\lambda \equiv (n_{\lambda+p} - C_{\lambda+p}^* C_{\lambda+p}) C_\lambda, \quad (6)$$

about the RPA terms normally retained. Next we form the commutators of these quantities with H and demand that they be, respectively, equal to $\omega C_{k+p}^* C_{\lambda+p} C_k$ and $\omega \delta n_{\lambda+p} C_\lambda$, for reasons to be explained presently. Consider first the commutator

$$[H, C_{k+p}^* C_{\lambda+p} C_k].$$

The kinetic energy portion of this commutator is again simply proportional to $C_{k+p}^* C_{\lambda+p} C_k$. But the commutator with the potential energy leads to a superposition of terms of the form $C^* C^* C C C$. At this point we make

what may be termed the "second random-phase approximation" in the following way. Of the quintuple terms $C^* C^* C C C$ we retain only two restricted classes:

I. Terms in which the momentum subscript of *one* of the C^*'s coincides with that of one of the C's, replacing this $C^* C$ combination by its expectation value n in the true ground state.

II. Terms in which the total momentum (i.e., the sum of the subscripts) of two C^*'s equals the sum of the subscripts of two C's. Any such $C^* C^* C C$ combination will in general have a nonvanishing expectation value m in the true ground state, since it carries zero net momentum.

Procedure I leaves us with triple terms times average occupation numbers, which product may be regarded as the "reaction" of the medium. Procedure II leaves us with a single C (and because of momentum conservation it must be C_λ), multiplied by an m number; this we regard as a "driving" term. All quintuple terms that do not conform with I or II are discarded.

Disregarding the fluctuation terms (6) for the moment, we see that the equations

$$[H, C_\lambda] = \omega C_\lambda,$$
$$[H, C_{k+p}^* C_{\lambda+p} C_k] = \omega C_{k+p}^* C_{\lambda+p} C_k, \quad (7)$$

form a closed system, quintuple terms having been discarded. We may solve the second of Eqs. (7) for the triples in terms of the "driving" term C_λ, and substitute the solution in the first of Eqs. (7). We thereby obtain a new quasi-energy ε_λ' (or in the general case of a bounded system, a quasi-Hamiltonian). The new ε_λ' turns out to incorporate the correct shielding and yields a density of states in agreement with the series result of Gell-Mann.

The fluctuation terms turn out to have no effect on the shielding problem. Should they be needed in more general cases, they can be included by supplementing Eqs. (7) with

$$[H, \delta n_{\lambda+p} C_\lambda] = \omega \delta n_{\lambda+p} C_\lambda, \quad (7')$$

and manipulating the commutator according to rules I and II. Then Eqs. (7) and (7') allow triple and fluctuation terms to be eliminated in favor of the single hole, again yielding a quasi-energy or Hamiltonian.

Two different types of m values may be distinguished under rule II: one in which the subscript of each of the two C^*'s is exactly matched by the subscript of one of the two C's, and another (more numerous) type in which the restriction is merely to net momentum zero. The former class is simply the product of two n numbers (corrected for fluctuation), and m's of this type will always be finite even in the limit of vanishing interaction. The latter type differs from zero only in the presence of the interaction. It will be shown that the series results for the specific heat and the Du Bois result for the ground state energy follow only if such averages are neglected. For the superconducting case, on the

other hand, the inclusion of such averages is of the essence (see Conclusions), since some of them have the form $\langle C_k{}^*C_{-k}{}^*C_{k'}C_{-k'}\rangle$.

One may ask what meaning is to be attached to solving for an operator C^*CC in terms of the operator C. This procedure is purely formal; what is really meant is that the Eqs. (7) and (7') are to be diagonalized by forming appropriate linear superpositions of C, C^*CC, and δnC. The coefficients in the superposition turn out to satisfy exactly the same Eqs. (7), (7'), but with the matrix of the whole set replaced by the transposed matrix. Our procedure thus amounts to "dressing" the state $C\psi_G$ with triples, etc.; in this sense it is a version of the Tamm-Dancoff method, but a Tamm-Dancoff method that considers excitations above the true ground state, not the Fermi state. Beginning with the Fermi state, in fact, gives results that in the first few orders do *not* agree with the series results.

A remark about self-consistency is in order here: We have spoken of averages $\langle C^*C\rangle$ in the ground state as though these were known. In actual fact, we take them to be occupation numbers appropriate to the non-interacting gas, wherever we expect the result for physical reasons to be insensitive to deviations from these numbers. But there exists the possibility of doing better, at least in principle. We note that $\langle C^*C\rangle$ is the overlap integral of $C\psi_G$ with itself. Now $C\psi_G$ is not an eigenstate of the system, but it may be expanded in terms of the eigenstates $(C+\sum C^*CC)\psi_G$ of set (7) [supplemented by (7') if necessary]. Then $\langle C^*C\rangle$ is just the sum of the squares of the expansion coefficients. These, however, are themselves nontrivial functions of $\langle C^*C\rangle$ and so a set of self-consistent, nonlinear equations for these averages is obtained. Similar remarks apply to averages such as $\langle C^*C^*CC\rangle$ which are overlap integrals of $CC\psi_G$. These are expansible in terms of eigenfunctions made up of two holes, two holes with an electron-hole pair, etc. No attempt at solving such self-consistent equations is actually made in this paper.

SPECIFIC HEAT OF THE ELECTRON GAS

As the simplest specific example of the method outlined in the previous section, we may calculate the single-particle excitation energies of a degenerate Coulomb gas. This spectrum finds application in computing the specific heat of the gas, which is inversely proportional to the derivative of the separation energy, or single-particle energy at the Fermi surface. We show that our method reproduces the well-known results of Gell-Mann.[9] We also investigate in detail the fluctuations of number operators from their expectation values, and justify for large systems the contraction of these operators described above.

It proves convenient at this point to alter the notation slightly. We write the Hamiltonian for this problem

$$H=\sum_k \varepsilon_k C(\mathbf{k};\mathbf{k})$$
$$-\tfrac{1}{2}\sum_{k_1k_2k_3k_4} v(\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4)C(\mathbf{k}_1\mathbf{k}_2;\mathbf{k}_3\mathbf{k}_4). \quad (8)$$

We further adopt the notations

$$C(\mathbf{pq}\cdots;\mathbf{rs}\cdots)\equiv C_p{}^*C_q{}^*\cdots C_rC_s\cdots; \quad (9)$$

$$\varepsilon(\mathbf{pq}\cdots;\mathbf{rs}\cdots)\equiv \varepsilon_p+\varepsilon_q+\cdots-\varepsilon_r-\varepsilon_s-\cdots, \quad (10)$$

where ε_p is the kinetic energy $p^2/2m$;

$$v(\mathbf{pqrs})\equiv\tfrac{1}{2}[v(\mathbf{p}-\mathbf{r})-v(\mathbf{p}-\mathbf{s})]\delta_{p+q,r+s}, \quad (11)$$

where $v(\mathbf{p})$ is the Fourier transform of the two-body potential, which for the Coulomb interaction with neutralizing positive background is given by

$$v(\mathbf{p})=4\pi e^2\hbar^2/\Omega p^2 \quad \text{if} \quad \mathbf{p}\neq 0$$
$$=0 \quad\quad\quad \text{if} \quad \mathbf{p}=0. \quad (12)$$

The volume of the system is denoted by Ω. Spin indices have been ignored for notational simplicity.[12]

We choose to consider the effect of an added hole, of momentum λ. The equation of motion (1) for this hole in our new notation becomes

$$\omega C_\lambda=[H,C_\lambda]=-\varepsilon_\lambda C_\lambda+\sum_{\lambda_1\lambda_2\lambda_3} v(\lambda\lambda_1\lambda_2\lambda_3)C(\lambda_1;\lambda_2\lambda_3)$$

$$=-[\varepsilon_\lambda-\sum_k n_k v(\mathbf{k}-\lambda)]C_\lambda$$

$$+\sum_{\lambda_1\lambda_2\lambda_3}{}' v(\lambda_1-\lambda_3)C(\lambda_1;\lambda_2\lambda_3)$$

$$-\sum_k v(\mathbf{k}-\lambda)[n_k-C(\mathbf{k};\mathbf{k})]C_\lambda, \quad (13)$$

where the prime on the summation means $\lambda_1\neq\lambda_2\neq\lambda_3$.

The approach to this equation of the usual RPA, and its attendant difficulties, were discussed in the previous section. To extend the RPA we write equations of motion for the remaining terms in Eq. (13). We first do this for the last term, which involves the fluctuations of $C(\mathbf{k};\mathbf{k})$ about its mean value. The equation of motion reads

$$\omega[n_k-C(\mathbf{k};\mathbf{k})]C_\lambda=[H,(n_k-C(\mathbf{k};\mathbf{k}))C_\lambda]$$

$$=[n_k-C(\mathbf{k};\mathbf{k})][-\varepsilon_\lambda C_\lambda+\sum_{\lambda_1\lambda_2\lambda_3} v(\lambda\lambda_1\lambda_2\lambda_3)C(\lambda_1;\lambda_2\lambda_3)]$$

$$-[\sum_{k_1k_2k_3k_4} v(\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4)(\delta_{k,k_1}-\delta_{k,k_3})C(\mathbf{k}_1\mathbf{k}_2;\mathbf{k}_3\mathbf{k}_4)]C_\lambda. \quad (14)$$

Since we expect the fluctuation to be small, we need only calculate it approximately; making contractions on the

right-hand side of Eq. (14) is thus assumed valid. We further discard all remaining terms involving the product of five creation and destruction operators as being of higher order. The resulting equation becomes

$$[\varepsilon_\lambda+\omega][n_{\bf k}-C({\bf k};{\bf k})]C_\lambda \cong -(1-n_{\bf k}-n_\lambda)\sum_{\lambda_2\lambda_3} v(\lambda{\bf k}\lambda_2\lambda_3)C({\bf k};\lambda_2\lambda_3)$$

$$+2(n_{\bf k}-n_\lambda)\sum_{\lambda_1\lambda_3} v(\lambda\lambda_1{\bf k}\lambda_3)C(\lambda_1;{\bf k}\lambda_3)+n_{\bf k}(2n_{\bf k}-1)v({\bf k}-\lambda)C_\lambda. \quad (15)$$

Substituting the resulting expression for the fluctuation into Eq. (13), we find

$$\omega C_\lambda = -\left\{\varepsilon_\lambda-\sum_{\bf k} n_{\bf k}v({\bf k}-\lambda)\left[1-\frac{v({\bf k}-\lambda)(2n_{\bf k}-1)}{\varepsilon_\lambda+\omega}\right]\right\}C_\lambda$$

$$+\sum_{\lambda_1\lambda_2\lambda_3} v(\lambda_1-\lambda_3)\left[1-\frac{2(n_{\bf k}-n_\lambda)v(\lambda\lambda_1{\bf k}\lambda_3)+(1-n_{\bf k}-n_\lambda)v(\lambda-\lambda_1)}{\varepsilon_\lambda+\omega}\right]C(\lambda_1;\lambda_2\lambda_3). \quad (16)$$

But since in a cube of side $\Omega^{\frac{1}{3}}$, we have $p\gtrsim\hbar\Omega^{-\frac{1}{3}}$, and since

$$\varepsilon_\lambda+\omega\cong\sum_{\bf k} n_{\bf k}v({\bf k}-\lambda)\sim e^2k_F/\hbar,$$

therefore   (17)

$$v({\bf p})/(\varepsilon_\lambda+\omega)\lesssim\Omega^{-\frac{1}{3}}\hbar/k_F\sim N^{-\frac{1}{3}}.$$

Thus for a large number of electrons, N, in the system, the fluctuation terms are negligible. From now on, therefore, we will feel justified in making contractions whenever possible.

Turning now to the remaining term in Eq. (13), we write an equation of motion for a particle-plus-pair excitation. Evaluating the commutator, making all possible contractions, and discarding uncontractable products of five creation and destruction operators, we find

$$\omega C(\lambda_1;\lambda_2\lambda_3)=[H,C(\lambda_1;\lambda_2\lambda_3)]\cong\{\varepsilon(\lambda_1;\lambda_2\lambda_3)-\sum_{\bf k} n_{\bf k}[v({\bf k}-\lambda_1)-v({\bf k}-\lambda_2)-v({\bf k}-\lambda_3)]-(1-n_{\lambda_2}-n_{\lambda_3})v(\lambda_2-\lambda_3)\}$$

$$\times C(\lambda_1;\lambda_2\lambda_3)-\sum_{{\bf k}_3{\bf k}_4}' v(\lambda_2\lambda_3{\bf k}_3{\bf k}_4)(1-n_{\lambda_2}-n_{\lambda_3})C(\lambda_1;{\bf k}_3{\bf k}_4)-2\sum_{{\bf k}_2{\bf k}_4}' [v(\lambda_2{\bf k}_2\lambda_1{\bf k}_4)(n_{\lambda_1}-n_{\lambda_2})$$

$$\times C({\bf k}_2;{\bf k}_4\lambda_3)-v(\lambda_3{\bf k}_2\lambda_1{\bf k}_4)(n_{\lambda_1}-n_{\lambda_3})C({\bf k}_2;{\bf k}_4\lambda_2)]$$

$$-2v(\lambda_1\lambda\lambda_2\lambda_3)[n_{\lambda_1}(1-n_{\lambda_2}-n_{\lambda_3})+n_{\lambda_2}n_{\lambda_3}]C_\lambda. \quad (18)$$

This integral equation for a triple may be substantially simplified by noting that it occurs in Eq. (13) multiplied by a Coulomb potential factor. Since that factor is singular for $\lambda_1=\lambda_3$, to a good approximation we need only substitute an expression for the triple valid in this region. Thus, retaining in its kernel only terms singular as $\lambda_1-\lambda_3\to 0$, our equation for a triple now reads

$$[\varepsilon(\lambda_1;\lambda_2\lambda_3)-\omega]C(\lambda_1;\lambda_2\lambda_3)$$

$$\cong\sum_{{\bf k}_2{\bf k}_4} v(\lambda_1-\lambda_3)(n_{\lambda_1}-n_{\lambda_3})C({\bf k}_2;\lambda_2{\bf k}_4)$$

$$+v(\lambda_1-\lambda_3)[n_{\lambda_2}(n_{\lambda_1}-n_{\lambda_3})-n_{\lambda_1}(1-n_{\lambda_3})]C_\lambda. \quad (19)$$

An additional, somewhat *ad hoc*, justification for the approximations leading to Eq. (19) comes from noting that the Hartree-Fock separation energy has an infinite derivative because of the singularity of the Coulomb potential in the exchange term; if the potential were shielded, the specific heat would be finite. In obtaining the approximate Eq. (19), we have in fact discarded only terms which do not contribute to shielding the exchange self-energy. If we further restrict ourselves just to calculating this shielding, so as to obtain consistently the lowest order nonzero specific heat, then we must also discard the terms in Eq. (19) of the form $n(1-n)$. These latter terms, furthermore, lead in Eq. (13) to one higher power of the coupling parameter e^2 than the others. Although the potential factor in them is not shielded in this order, it is anticipated that retaining quintuple terms in Eq. (18), at least to lowest approximation, supplies the desired shielding.

In this event, Eq. (19) can be solved algebraically:

$$\sum_{\lambda_1\lambda_3} C(\lambda_1;\lambda_2\lambda_3)$$

$$=n_{\lambda_2}v(\lambda-\lambda_2)\chi(\lambda_2,\lambda)/[1-v(\lambda-\lambda_2)\chi(\lambda_2,\lambda)], \quad (20)$$

where

$$\chi(\lambda_2,\lambda)\equiv\sum_{\lambda_1\lambda_3} (n_{\lambda_1}-n_{\lambda_3})/[\varepsilon(\lambda_1;\lambda_2\lambda_3)-\omega], \quad (21)$$

the summation being restricted by the condition $\lambda + \lambda_1 = \lambda_2 + \lambda_3$.

Substituting this result into Eq. (13), we find

$$\omega C_\lambda = -\{\varepsilon_\lambda - \sum_k n_k v(\mathbf{k} - \lambda)/$$
$$[1 - v(\mathbf{k} - \lambda)\chi(\mathbf{k},\lambda)]\}C_\lambda. \quad (22)$$

Thus the exchange self-energy is indeed shielded, χ being nonzero for $\mathbf{k} = \lambda$.

In order to match explicitly this expression for ω with that of Gell-Mann's paper,[9] we must retain in a consistent manner only the same low orders in the coupling as is done there. This involves the approximate replacements:

(a) $\chi(\mathbf{k},\lambda) \rightarrow \chi(\lambda,\lambda)$, (shielding term replaced by its value for vanishing momentum transfer).

(b) $\omega \rightarrow -\varepsilon_\lambda$ in the denominator of χ.

(c) $n \rightarrow$ its value in the unperturbed Fermi state.

When these are carried out, Eq. (22) corresponds precisely to the result of Gell-Mann.

THE GROUND STATE VS FERMI STATE

Point (c) requires very careful consideration. An exact evaluation of χ would require a knowledge of the expectation values n_k in the *true* ground state. Replacing them by values appropriate to the Fermi state assumes that χ is not a very sensitive functional of the actual distribution for n's. At this point we stress the profound difference between our present result and what would have been obtained had we based the excitations on the Fermi state (instead of the true ground state), simply diagonalizing the Hamiltonian within the manifold formed by $C\psi_F$ and all states $C^*CC\psi_F$. In that case, the formula for χ would have read

$$- \sum_{\lambda_1 > k_F; \lambda_3 < k_F} [\varepsilon(\lambda_1; \lambda_2\lambda_3) - \omega]^{-1}, \quad (23)$$

only "half" the present result.

This point becomes particularly striking in the case of an attractive potential. The equations of motion for "Cooper pairs" $C_k^* C_{-k}^*$, when operating on the true ground state, lead (in the ordinary RPA) to a characteristic equation for a collective root ω. The characteristic equation depends on the distribution of n's; if

these are taken to have Fermi values, the possible roots ω are $\pm i\eta$, where η is real. This indicates that the Fermi state is unstable against addition of two particles. On the other hand, diagonalizing the Hamiltonian within the manifold of all states $C_k^* C_{-k}^* \psi_F$ leads to bound eigenstates of the kind discovered by Cooper.[13]

GROUND-STATE ENERGY OF THE ELECTRON GAS

A further example of the application of the extended RPA to the electron gas problem is the computation of the ground-state energy. It is well known[14] that this quantity may be obtained from the spectrum of single-particle excitations by a suitable integration with respect to density, but for our purposes it is more instructive to investigate ground-state properties by the equally well-known[15] method of calculating the dielectric constant, in which the ground-state energy, for example, is related to the response of the system to a given imposed change in density. Both approaches are especially suited to, and in fact necessitated by, the equations of motion technique we are using, which can only yield the spectrum of excited states above the correct, but not directly calculable, ground state.

Specifically, we apply by external means a density wave $a(\lambda) \exp[i\hbar^{-1}(\lambda \cdot \mathbf{r} - \omega t)] + \text{cc}$ of wave number λ and frequency ω. The interaction of this density wave with the gas leads to an additional term in the Hamiltonian

$$v(\lambda) A \sum_k C(\mathbf{k} - \lambda; \mathbf{k}) + \text{cc}, \quad (24)$$

where

$$A \equiv a(\lambda) e^{-i\omega t/\hbar}. \quad (25)$$

A dielectric constant $\epsilon(\lambda,\omega)$ is defined by Nozières and Pines[15] as the ratio of the perturbation to the total density response with wave number λ, and we shall adhere to this definition:

$$\epsilon(\lambda,\omega) \equiv A / [A + \sum_{\lambda'} C(\lambda' + \lambda; \lambda')]. \quad (26)$$

The difference in ground-state energies of interacting and noninteracting systems is then shown[15] to depend on the analytic properties of the dielectric constant through the equation:

$$\Delta E = -\lim_{\eta \to 0} \int_0^{e^2} \frac{de'^2}{e'^2} \sum_\lambda \frac{1}{2\pi} \int_0^\infty d\omega \, \text{Im} \frac{1}{\epsilon(\lambda, \omega + i\eta)} - \frac{1}{2}N \sum_\lambda v(\lambda). \quad (27)$$

Thus the ground-state energy is obtainable once we have an expression for a density element $C(\lambda' + \lambda; \lambda')$; but this we calculate approximately using the equation of motion method along with contractions, as outlined in the

[13] L. N. Cooper, Phys. Rev. **104**, 1189 (1956).
[14] J. J. Quinn and R. A. Ferrell, Phys. Rev. **112**, 812 (1958).
[15] P. Nozières and D. Pines, Nuovo cimento **9**, 470 (1958).

Introduction. Making use of the general formula of the Appendix,

$$\omega C(\lambda'+\lambda;\lambda') = [H, C(\lambda'+\lambda, \lambda')] = \{\varepsilon(\lambda'+\lambda;\lambda') + \sum_k n_k[v(k-\lambda')-v(k-\lambda-\lambda')]\}$$

$$\times C(\lambda'+\lambda;\lambda') - \sum_k [v(\lambda)-v(k-\lambda')](n_{\lambda'+\lambda}-n_{\lambda'})C(k+\lambda;k) - v(\lambda)(n_{\lambda'+\lambda}-n_{\lambda'})A$$

$$+\sum_k v(k-\lambda') \sum_{k'k''} [C(\lambda'+\lambda, k'; kk'')-C(k+\lambda, k''; \lambda'k')]. \quad (28)$$

After some algebraic manipulations, we find for the quantity of interest in Eq. (26):

$$\sum_{\lambda'} C(\lambda'+\lambda;\lambda') = \frac{1}{1-v(\lambda)\chi(\lambda)}\left\{v(\lambda)\chi(\lambda)A + \sum_{\lambda_1\lambda_3} v(\lambda_1-\lambda_3)\left[\frac{1}{\varepsilon(\lambda_1+\lambda;\lambda_1)-\omega}-\frac{1}{\varepsilon(\lambda_3+\lambda;\lambda_3)-\omega}\right]\right.$$

$$\left.\times[(n_{\lambda_3+\lambda}-n_{\lambda_3})C(\lambda_1+\lambda;\lambda_1)-\sum_{\lambda_2\lambda_4} C(\lambda_1+\lambda, \lambda_2; \lambda_3\lambda_4)]\right\}, \quad (29)$$

where we define

$$\chi(\lambda)\equiv\sum_{\lambda'}(n_{\lambda'+\lambda}-n_{\lambda'})/[\varepsilon(\lambda'+\lambda;\lambda')-\omega]. \quad (30)$$

If the last term in (29) were absent, this would represent a linear inhomogeneous integral equation for $C(\lambda'+\lambda;\lambda')$; an approximate solution has been shown[7,15] to reproduce the results of Gell-Mann and Brueckner,[2] and Sawada and Brout,[3-5] for the ground-state energy. By taking terms of the form $C(\lambda_1+\lambda, \lambda_2; \lambda_3\lambda_4)$ into account, however, we obtain the higher-order corrections computed by Du Bois.[8]

A consistent treatment of the last term is again to write an equation of motion for it. However, since it is of higher order, we may treat its motion approximately; because of the singular nature of the Coulomb potential at vanishing momentum transfer, the term only contributes strongly for $\lambda_1-\lambda_3=\lambda_4-\lambda_2\cong 0$. Hence in the equation of motion, we need only retain terms prominent in this region. A further approximation is to discard terms which couple the quadruple to itself, instead of to pairs; they lead merely to additional shielding, unnecessary in the order to which Du Bois has worked. We then find, again referring to the Appendix,

$$\omega C(\lambda_1\lambda_2; \lambda_3\lambda_4) = [H, C(\lambda_1\lambda_2; \lambda_3\lambda_4)]\cong\varepsilon(\lambda_1\lambda_2; \lambda_3\lambda_4)C(\lambda_1\lambda_2; \lambda_3\lambda_4) - v(\lambda_2-\lambda_4)\{[n_{\lambda_4}(1-n_{\lambda_1}-n_{\lambda_2})+n_{\lambda_1}n_{\lambda_2}]$$

$$\times C(\lambda_1+\lambda_2-\lambda_4; \lambda_3) - [n_{\lambda_2}(1-n_{\lambda_3}-n_{\lambda_4})+n_{\lambda_3}n_{\lambda_4}]C(\lambda_1; \lambda_3+\lambda_4-\lambda_2)\}, \quad (31)$$

so that

$$\sum_{\lambda_2\lambda_4} C(\lambda_1+\lambda, \lambda_2; \lambda_3\lambda_4) = \sum_{\lambda_2\lambda_4} \frac{v(\lambda_2-\lambda_4)}{\varepsilon(\lambda_1+\lambda, \lambda_2; \lambda_3\lambda_4)-\omega}\{[n_{\lambda_1+\lambda}(n_{\lambda_2}-n_{\lambda_4})+n_{\lambda_4}(1-n_{\lambda_2})]$$

$$\times C(\lambda_3+\lambda; \lambda_3) + [n_{\lambda_3}(n_{\lambda_2}-n_{\lambda_4})-n_{\lambda_2}(1-n_{\lambda_4})]C(\lambda_1+\lambda; \lambda_1)\}. \quad (32)$$

The summation is restricted by the condition $\lambda_1+\lambda_2=\lambda_3+\lambda_4$.

Inserting this result into Eq. (29), we reobtain an integral equation for the density response. However, pair correlations which shield the potential at small distances have already been included, so that it is legitimate to provide an iterative solution. Substituting on the right-hand side

$$C(\lambda'+\lambda;\lambda')\cong\frac{v(\lambda)}{1-v(\lambda)\chi(\lambda)}\frac{n_{\lambda'+\lambda}-n_{\lambda'}}{\varepsilon(\lambda'+\lambda;\lambda')-\omega}\cdot A, \quad (33)$$

we have

$$\sum_{\lambda'} C(\lambda'+\lambda;\lambda')/A\cong\frac{v(\lambda)}{1-v(\lambda)\chi(\lambda)}\left\{\chi(\lambda)+\frac{\chi^{(1)}(\lambda)}{1-v(\lambda)\chi(\lambda)}+\chi^{(2)}(\lambda)\right\}, \quad (34)$$

where

$$\chi^{(1)}(\lambda)\equiv\frac{1}{2}\sum_{\lambda_1\lambda_3} v(\lambda_1-\lambda_3)\left[\frac{1}{\varepsilon(\lambda_1+\lambda;\lambda_1)-\omega}-\frac{1}{\varepsilon(\lambda_3+\lambda;\lambda_3)-\omega}\right]^2(n_{\lambda_1+\lambda}-n_{\lambda_1})(n_{\lambda_3+\lambda}-n_{\lambda_3}), \quad (35)$$

and

$$\chi^{(2)}(\lambda)\equiv\sum_{\lambda_1\lambda_2\lambda_3\lambda_4} v(\lambda_1-\lambda_3)v(\lambda_2-\lambda_4)\left[\frac{1}{\varepsilon(\lambda_1+\lambda;\lambda_1)-\omega}-\frac{1}{\varepsilon(\lambda_3+\lambda;\lambda_3)-\omega}\right]\frac{n_{\lambda_3+\lambda}-n_{\lambda_3}}{\varepsilon(\lambda_3+\lambda;\lambda_3)-\omega}$$

$$\times\left[\frac{n_{\lambda_1+\lambda}(n_{\lambda_2}-n_{\lambda_4})+n_{\lambda_4}(1-n_{\lambda_2})}{\varepsilon(\lambda_1+\lambda, \lambda_2; \lambda_3\lambda_4)-\omega}+\frac{n_{\lambda_1}(n_{\lambda_2}-n_{\lambda_4})+n_{\lambda_4}(1-n_{\lambda_2})}{\varepsilon(\lambda_3+\lambda, \lambda_4; \lambda_1\lambda_2)-\omega}\right]\delta_{\lambda_1+\lambda_2, \lambda_3+\lambda_4}. \quad (36)$$

Equation (34) now matches Du Bois' Eq. (C2)[8] if we make the identifications

$$\chi \leftrightarrow -Q_0, \quad \chi^{(1)} \leftrightarrow -Q^{(1)}, \quad \chi^{(2)} \leftrightarrow -Q^{(2)}. \quad (37)$$

The first two of these correspondences may be verified in detail from Du Bois' Eqs. (1.39) and (A4), provided our occupation numbers n are given their values in the Fermi state. However, Du Bois does not give an explicit expression for $Q^{(2)}$. As Du Bois points out, *for purposes of calculating the ground-state energy in this approximation*, the effect of $Q^{(2)}$ (being additive) may be calculated by the usual third-order perturbation theory.

Note added in proof. At the suggestion of Dr. DuBois, we re-examined $\chi^{(2)}$, and found that we had omitted one contribution to it. This additional contribution is

$$\sum_{\lambda'} \frac{n_{\lambda'+\lambda} - n_{\lambda'}}{\varepsilon(\lambda'+\lambda; \lambda') - \omega}$$

$$\times \left\{ \sum_k v(k-\lambda') \left[\frac{n_{k+\lambda} - n_k}{\varepsilon(\lambda'+\lambda; \lambda') - \omega} - \frac{n_{k+\lambda} - n_k}{\varepsilon(k+\lambda; k) - \omega} \right] \right\}^2$$

and arises from the need for iterating the term $C(\lambda_1+\lambda; \lambda_1)$ in Eq. (29) to one order higher than that implied by Eq. (33).

Also we wish to point out a self-consistent set of misprints in Appendix C of reference 8. The development following Eq. (C2) reads correctly provided the second and third terms within the square brackets of this equation are interchanged.

CONCLUSIONS

It must be emphasized that in spite of its apparent success in reproducing results previously obtained by perturbation theory, the present procedure is subject to the same criticisms as similar "truncation" methods that have been suggested in the past: The "expansion parameter" is not given. It is not clear what criterion should be used in the decision to terminate the chain of equations at a particular stage. Thus the stage to which the process was carried in this paper was the lowest which contained the results of perturbation theory, but it also contained a good deal more. The extra information was not needed in the expansion in the first few powers of the interaction parameter, and at this point it is not clear in what critical direction the extra information improves the result. However, further experimentation with the method may throw light on these more fundamental aspects.

The case of superconductivity may prove particularly interesting. Following the Bardeen-Cooper-Schrieffer[16] theory of superconductivity, one will here retain averages, not only of C_k*C_k, but also of $C_k*C_{-k}*$ and $C_{-k}C_k$. The ordinary RPA amended in this way has already been studied by Anderson.[17] For the added particle

problem it yields two coupled equations for $C_\lambda*$ and $C_{-\lambda}$, with excitation energy equal to the familiar square root expression. Retention of the terms neglected in RPA leads to coupled equations linking $C_\lambda*$ and $C_{-\lambda}$ with terms of the forms $C*CC$, $C*C*C$, $C*C*C*$, and CCC. Eliminating the latter four terms in favor of the former two should improve the excitation spectrum. We may conjecture what this process means physically by again considering the normal case. There the $C*CC$ terms were driven by C_λ, and in solving for $C*CC$, the sums were replaced by integrals. Then, as a first approximation, the energy was replaced by the uncorrected energy ε_λ in the solution. The replacement of summation by integration picks out the collective response of the medium to C_λ (it is easily seen that in the approximation of section two, the corresponding natural frequency is the plasma frequency plus a single-particle frequency) and the replacement of ω by ε_λ means that the collective response is being driven "off-resonance," resulting in the shielding of the exchange terms. In the same way, in the superconducting case the correction will stem from an off-resonance excitation of a collective response to $C_\lambda*$ and $C_{-\lambda}$, the relevant modes being combinations of single-particles with the collective modes considered by Bardasis and Schrieffer.[18]

Finally we note that the present method resembles the Green's function method of Martin and Schwinger.[19] It also is closely related to the density matrix method of Ehrenreich and Cohen.[20] In fact, the results in the present paper can also be derived by writing down the equations for successive partial traces of the density matrix in an n representation, stopping at a particular stage and replacing elements like $(n_1 n_2 n_3 \cdots |\rho| n_1 n_2' n_3' \cdots)$ by $(n_1|\rho|n_1)(n_2 n_3 \cdots |\rho| n_2' n_3' \cdots)$. However, these authors carry their procedures only to the point reached by the ordinary random phase approximation.

APPENDIX

General Commutator with Contractions

In this Appendix, we exhibit a general formula for the commutator with the Hamiltonian of a product of creation and destruction operators, arbitrary except for the requirement that all indices shall be distinct (no contractions possible). In the resulting commutator, we make all possible contractions, that is, isolate all terms in which a $C*$ and a C have the same index and replace the operator product C_k*C_k by the number n_k. With the

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[19] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959).
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J. Goldstone and K. Gottfried, Nuovo cimento **13**, 849 (1959).

commutation and contraction operations performed, we find

$$[C(\mathbf{a}_1\cdots\mathbf{a}_M;\mathbf{b}_1\cdots\mathbf{b}_N),H]$$

$$=\{-\varepsilon(\mathbf{a}_1\cdots\mathbf{a}_M;\mathbf{b}_1\cdots\mathbf{b}_N)+\sum_\lambda n_\lambda[\sum_\lambda^M v(\lambda-\mathbf{a}_i)-\sum_j^N v(\lambda-\mathbf{b}_j)]+\sum_{i<j}^M (1-n\mathbf{a}_i-n\mathbf{a}_j)v(\mathbf{a}_i-\mathbf{a}_j)$$

$$-\sum_{i<j}^N{}' (1-n\mathbf{b}_i-n\mathbf{b}_j)v(\mathbf{b}_i-\mathbf{b}_j)\}C(\mathbf{a}_1\cdots\mathbf{a}_M;\mathbf{b}_1\cdots\mathbf{b}_N)-\sum_{\lambda_1\lambda_2\lambda_3\lambda_4} v(\lambda_1\lambda_2\lambda_3\lambda_4)$$

$$\times\{\sum_i^M \delta_{\lambda_3,\,\mathbf{a}_i}C(\mathbf{a}_1\cdots(\lambda_1)_i\cdots\mathbf{a}_M\lambda_2;\lambda_4\mathbf{b}_1\cdots\mathbf{b}_N)-\sum_j^N \delta_{\lambda_1,\,\mathbf{b}_j}C(\mathbf{a}_1\cdots\mathbf{a}_M\lambda_2;\lambda_4\mathbf{b}_1\cdots(\lambda_3)_j\cdots\mathbf{b}_N)$$

$$+[\sum_{i<j}^M \delta_{\lambda_3,\,\mathbf{a}_i}\delta_{\lambda_4,\,\mathbf{a}_j}(1-n\mathbf{a}_i-n\mathbf{a}_j)C(\mathbf{a}_1\cdots(\lambda_1)_i\cdots(\lambda_2)_j\cdots\mathbf{a}_M;\mathbf{b}_1\cdots\mathbf{b}_N)$$

$$-\sum_{i<j}^N \delta_{\lambda_1,\,\mathbf{b}_i}\delta_{\lambda_2,\,\mathbf{b}_j}(1-n\mathbf{b}_i-n\mathbf{b}_j)C(\mathbf{a}_1\cdots\mathbf{a}_M;\mathbf{b}_1\cdots(\lambda_3)_i\cdots(\lambda_4)_j\cdots\mathbf{b}_N)$$

$$-2\sum_i^M\sum_j^N \delta_{\lambda_1,\,\mathbf{b}_j}\delta_{\lambda_3,\,\mathbf{a}_i}(n\mathbf{a}_i-n\mathbf{b}_j)C(\mathbf{a}_1\cdots(\lambda_2)_i\cdots\mathbf{a}_M;\mathbf{b}_1\cdots(\lambda_4)_j\cdots\mathbf{b}_N)]\}$$

$$+2(-1)^M\sum_{i<j}^M\sum_k^N\sum_\lambda v(\mathbf{a}_i\mathbf{a}_j\lambda\mathbf{b}_k)(n\mathbf{b}_k(1-n\mathbf{a}_i-n\mathbf{a}_j)+n\mathbf{a}_in\mathbf{a}_j)C(\mathbf{a}_1\cdots(\lambda)_i\cdots(\ )_j\cdots\mathbf{a}_M;\mathbf{b}_1\cdots(\ )_k\cdots\mathbf{b}_N)$$

$$-2(-1)^M\sum_i^M\sum_{j<k}^N\sum_\lambda v(\mathbf{a}_i\lambda\mathbf{b}_j\mathbf{b}_k)(n\mathbf{a}_i(1-n\mathbf{b}_j-n\mathbf{b}_k)+n\mathbf{b}_jn\mathbf{b}_k)C(\mathbf{a}_1\cdots(\ )_i\cdots\mathbf{a}_M;\mathbf{b}_1\cdots(\ )_j\cdots(\lambda)_k\cdots\mathbf{b}_N)$$

$$-2\sum_{i<j}^M\sum_{k<l}^N v(\mathbf{a}_i\mathbf{a}_j\mathbf{b}_k\mathbf{b}_l)(n\mathbf{a}_in\mathbf{a}_j(1-n\mathbf{b}_k-n\mathbf{b}_l)-n\mathbf{b}_kn\mathbf{b}_l(1-n\mathbf{a}_i-n\mathbf{a}_j))$$

$$\times C(\mathbf{a}_1\cdots(\ )_i\cdots(\ )_j\cdots\mathbf{a}_M;\mathbf{b}_1\cdots(\ )_k\cdots(\ )_l\cdots\mathbf{b}_N)$$

$$-v(\lambda)A\{\sum_i^M C(\mathbf{a}_1\cdots(\mathbf{a}_i-\lambda)_i\cdots\mathbf{a}_M;\mathbf{b}_1\cdots\mathbf{b}_N)-\sum_j^N C(\mathbf{a}_1\cdots\mathbf{a}_M;\mathbf{b}_1\cdots(\mathbf{b}_j+\lambda)_j\cdots\mathbf{b}_N)$$

$$+(-1)^M\sum_i^M\sum_j^N \delta_{\mathbf{a}_i-\mathbf{b}_j,\,\lambda}(n\mathbf{a}_i-n\mathbf{b}_j)C(\mathbf{a}_1\cdots(\ )_i\cdots\mathbf{a}_M;\mathbf{b}_1\cdots(\ )_j\cdots\mathbf{b}_N)\}. \quad (A.1)$$

The notation $\cdots(\lambda)_i\cdots$, and $\cdots(\ )_i\cdots$, means: Replace $C\mathbf{b}_i$ by C_λ, and by $(-1)^i$, respectively.

It is of interest to note the three types of "reaction" terms in Eq. (A.1), which have been enclosed in square brackets. If an iterative solution for the corresponding integral equation is written down, and the iterations classified diagramatically, then these three sections of the kernel lead to three different types of diagrams. The first, involving the sum $i<j$ to M, produces only particle-particle scattering, the second ($i<j$ to N) only hole-hole scattering, and the third only particle-hole pair scattering. In the case of the Coulomb potential, we have seen that only the third type of term plays an important role, since it alone contains the dominant singularity for small momentum transfers.