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COMMENTS AND ADDENDA

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Variational Approach to the Calculation of the Dielectric Function of an Electron Gas: Exchange and Collisions

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In a recent work of Woo and Jha, the exchange correlations in a uniform electron gas were calculated. They ignored the Coulomb correlations completely. To describe the physical properties of an electron gas at metallic densities, we propose a variational method to calculate the dielectric function which takes into account the local-field corrections due to both Coulomb and exchange holes.

To consider electron correlations at metallic densities, various attempts[1] have been made to improve upon the high-density ($r_s \ll 1$) Lindhard dielectric function which corresponds to the random-phase approximation (RPA) or the self-consistent Hartree approximation. In the language of the diagrammatic perturbation theory,[2] the RPA is equivalent to the approximation in which the proper polarization part is replaced by a bare bubble (with the Hartree self-energy in the single-particle Green's function) in calculating the effective interaction. It neglects local-field corrections associated with both exchange and Coulomb holes. These become increasingly important for large momentum transfers ($q \sim k_F$, $\hbar k_F$ is the Fermi momentum). Since the pair distribution function is given by

$$g(r) = 1 + \frac{1}{n}\int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot\vec{r}} \times\left[\frac{-\hbar q^2}{2\pi e^2 n}\int_0^\infty \frac{d\omega}{2\pi}\,\mathrm{Im}\left(\frac{1}{\epsilon(q,\omega)}\right) - 1\right] , \quad (1)$$

the RPA gives unphysical results at metallic densities ($2 < r_s < 6$) for this function at short distances.[1] Although the phenomenological approach of Singwi *et al.*[1] to account for short-range correlations gives acceptable results for $g(r)$, a proper justification for this approach in terms of the many-body theory is lacking. The effect of exchange interaction in the proper polarization part can be calculated by summing up all (exchange) ladder diagrams (Fig. 1) self-consistently, in which the single-particle Green's function contains the Hartree-Fock self-energy with a statically screened Coulomb interaction. Langreth[3] proposed to use a simple variational solution of the resulting integral equation for the proper polarization part. By solving this integral equation numerically, Woo and Jha[4] have shown that the simple variational solution gives the dielectric function which is extremely close to the correct numerical solution. But the summation of exchange-ladder graphs is not enough to obtain sensible results for $g(r) = 0$ at metallic densities, since this leaves out the detailed correlations produced by interparticle collisions (t-matrix graphs).

The success of the variational solution in calculating the exchange effects, as shown by Woo and Jha, immediately suggests that one should use a similar approach to sum both collision and exchange graphs simultaneously [Figs. 2(a) and 2(b)]. We show in this note that it is indeed possible to obtain a simple variational solution for this problem. On physical grounds, our solution

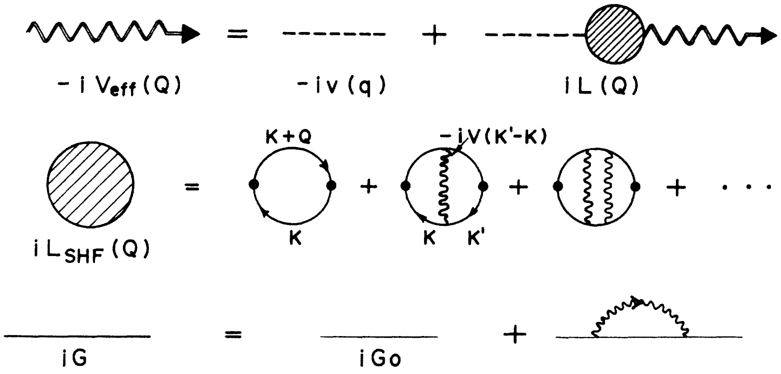

FIG. 1. Definition of proper polarization part and the summation of exchange-ladder diagrams.

is expected to give much more sensible results at metallic densities.

From Fig. 1, one finds that the dielectric function $\epsilon(Q)$ is given in terms of the proper polarization part $L(Q)$ by the relation

$$\epsilon(Q)=\frac{v_q}{V_{\rm eff}(Q)}=1-v_qL(Q),\quad v_q=\frac{4\pi e^2}{q^2} \tag{2}$$

where Q stands for the four-momenta $(q, \hbar\omega)$. In obtaining $L(Q)$ we want to keep both the exchange-ladder graphs and Coulomb collision graphs. The interaction V in these graphs has to be the self-consistent effective interaction, which depends on both $\vec{q}$ and ω. However, since screening of the Coulomb interaction is most important for $\omega = 0$ and q small, we assume it to be the statically screened Coulomb interaction[3, 4]

$$V(Q)=V(\vec{q})=4\pi e^2/(q^2+q_s^2)\,, \tag{3}$$

where q_s^{-1} is the Fermi-Thomas screening length. In the spirit of the self-consistent Hartree-Fock theory we may also assume that the single-particle propagator in polarization graphs is given by

$$G(K)=G(\vec{k},\epsilon)=[\epsilon-E_k+i\delta_k]^{-1}\,, \tag{4}$$

$$E_k=\frac{\hbar^2k^2}{2m}+\Sigma(\vec{k})=\frac{\hbar^2k^2}{2m}-\int\frac{d^3k'}{(2\pi)^3}V(|k-k'|)f(E_{k'})\,, \tag{5}$$

where $f(E)$ is the Fermi function at $T=0\,^\circ$K.

If we limit ourselves to the lowest-order contribution to collisions, from Fig. 2(a) we obtain the integral equation[5]

$$\mathcal{L}(K,Q)=l(K,Q)-l(K,Q)\textstyle\sum_{K'}Y_Q(K,K')\,\mathcal{L}(K',Q)\,,$$

$$l(K,Q)\equiv -iG(K)\,G(K+Q)\,, \tag{6}$$

$$Y_Q(K,K')\equiv V(K-K') - 2i\textstyle\sum_{K''}G(K+K''+\frac{1}{2}Q)\,[G(K'+K''+\frac{1}{2}Q) + G(K'-K''+\frac{1}{2}Q)]\,V(\frac{1}{2}Q-K'')\,V(\frac{1}{2}Q+K'')\,, \tag{7}$$

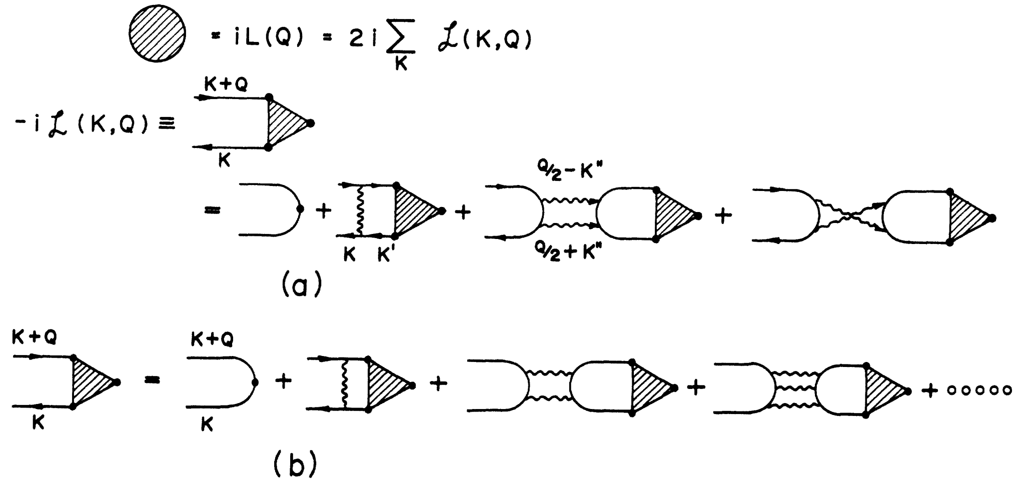

FIG. 2. (a) Diagrams with collision contributions to the lowest order, in addition to exchange. (b) Diagrams with collisions described by t-matrix ladder diagrams, in addition to exchange.

where

$$\sum_K \text{ implies } \int \frac{d^3k}{(2\pi)^3} \int \frac{d\epsilon}{(2\pi)} .$$

For $l(K,Q) \neq 0$, let us define the vertex function

$$\Lambda(K,Q) = \mathcal{L}(K,Q)/l(K,Q) ; \tag{8}$$

then

$$\Lambda(K,Q) = 1 - \sum_{K'} Y_Q(K,K')\, l(K',Q)\, \Lambda(K',Q) . \tag{9}$$

Since $Y_Q(K,K') = Y_Q(K',K)$, the appropriate variational functional $F(\Lambda(K,Q))$ is

$$F(\Lambda(K,Q)) = -\sum_{K,K'} \Lambda(K,Q)\, l(K,Q)\, Y_Q(K,K') \times l(K',Q)\, \Lambda(K',Q) + 2\sum_K l(K,Q)\, \Lambda(K,Q) - \sum_K l(K,Q)\, \Lambda^2(K,Q) , \tag{10}$$

because $[\delta F/\delta(\Lambda(K,Q))] = 0$ implies Eq. (9). If we take the trial function $\Lambda(K,Q)$ to be $\tilde{\Lambda}(Q)$, constant in K, we find

$$\tilde{\Lambda}(Q) = \frac{\sum_K l(K,Q)}{\sum_K l(K,Q) + \sum_{KK'} l(K,Q)\, Y_Q(K,K')\, l(K',Q)} , \tag{11}$$

which leads to

$$L(Q) = 2\sum_K \mathcal{L}(K,Q) = \tilde{\Lambda}(Q)\, 2\sum_K l(K,Q) . \tag{12}$$

Note that in RPA, $\tilde{\Lambda}(Q)$ is 1, so that

$$L_{\text{RPA}}(Q) = 2\sum_K l(K,Q) = 2\int \frac{d^3k}{(2\pi)^3} \frac{f(E_{k+q}) - f(E_k)}{(E_{k+q} - E_k - \hbar\omega - i\delta\, \text{sgn}\omega)} , \tag{13}$$

where in E_k, defined by Eq. (5), $\Sigma(\vec{k})$ has to be put equal to zero.

In the contribution to the proper polarization part we can also consider collisions to higher orders in V by summing the ladder diagrams (t matrix) as shown in Fig. 2(b). This would become necessary at lower densities. In this case, we find

$$\mathcal{L}(K,Q) = l(K,Q) - l(K,Q) \sum_{K'} Z_Q(K,K')\, \mathcal{L}(K',Q) , \tag{14}$$

$$Z_Q(K,K') = V(K-K') - 2S(K,K',Q) , \tag{15}$$

$$S(K,K',Q) = T(K,K',Q) - V(Q) , \tag{16}$$

$$T(K,K',Q) = V(Q) + \sum_{Q'} g(K,K',Q') \times V(Q-Q')\, T(K,K',Q') , \tag{17}$$

$$g(K,K',Q) = iG(K+Q)\, G(K'+Q) . \tag{18}$$

The new integral equation (14) is similar to Eq. (6). However, we have to solve first the t-matrix equation (17) to find $Z_Q(K,K')$. The appropriate variational functional to solve (17) is given by

$$F(T(Q)) = \sum_{QQ'} T(Q)\, g(Q)\, V(Q-Q')\, g(Q')\, T(Q') + 2\sum_Q g(Q)\, V(Q)\, T(Q) - \sum_Q g(Q)\, T^2(Q) , \tag{19}$$

where the K and K' dependence of $g(K,K',Q)$ and $T(K,K',Q)$ has been suppressed. As a trial function if we choose $T(K,K',Q) = V(Q)\, t(K,K')$, it leads to

$$S(K,K',Q) = V(Q) \times \frac{\sum_{QQ'} V(Q) g(Q) V(Q-Q') g(Q') V(Q')}{\sum_Q V^2(Q) g(Q) - \sum_{QQ'} V(Q) g(Q) V(Q-Q') g(Q') V(Q')} . \tag{20}$$

The approximate $Z_Q(K,K')$ thus obtained can now be used in Eq. (14). The variational solution of this equation gives

$$L(Q) = 2\sum_K \mathcal{L}(K,Q) = \tilde{\Lambda}_T(Q)\, 2\sum_K l(K,Q) , \qquad \tilde{\Lambda}_T(Q) = \frac{\sum_K l(K,Q)}{\sum_K l(K,Q) + \sum_{KK'} l(K,Q)\, Z_Q(K,K')\, l(K',Q)} \tag{21}$$

We are thus able to obtain analytic expressions to calculate the effect of exchange and Coulomb holes not only to the lowest order in collisions, but to all orders by finding the t matrix. However, solution (11) obtained to the lowest order in collisions is perhaps better in the sense of conserving approximations discussed by Baym and Kadanoff.[6] We may note that after the screening of the long-range part of the Coulomb interaction has been taken into account, the electron gas at metallic densities would behave like a low-density system since the average distance between particles is larger than the range of the screened interaction. In this sense our solution (11) should be sufficiently accurate at metallic densities.

One important question which one would like to ask is whether our variational approach gives an acceptable solution to integral equations. Since $\sum_\epsilon l(\vec{k}, \epsilon; Q)$, for $\omega = 0$, is proportional to $\delta(k - k_F)$ as $\vec{q} \to 0$, Eq. (6) or Eq. (14) can be solved exactly in this limit, if one neglects collisions.[3] One can verify that this leads after summation over $\vec{k}$ to the same L or ϵ as the variational solution. Similarly, we can show that for $\omega = 0$ and $\vec{q} \to \infty$, variational solutions (12) or (21) give the same L or ϵ as would be obtained by solving these integral equations exactly in this limit. Moreover, the numerical work of Ref. 4 gives us confidence to believe that the variational method provides a good approximation to calculate electron correlations at metallic densities.

[1] D. Pines, ***Elementary Excitations in Solids*** (Benjamin, New York, 1964), Chap. 3; K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. B 1, 1044 (1970), and other references in this paper.

[2] J. Hubbard, Proc. Roy. Soc. (London) A239, 267 (1957).

[3] D. C. Langreth, Phys. Rev. 181, 753 (1969).

[4] J. W. F. Woo and S. S. Jha, Phys. Rev. B 3, 87 (1971).

[5] To make contact with earlier calculations, let us point out that in RPA, $\mathfrak{L}(K, Q)$ is just $l(K, Q)$ with the self-energy $\Sigma(\vec{k}) = 0$, and in the self-consistent Hartree-Fock calculation of Woo and Jha, $\mathfrak{L}$ is obtained from Eq. (6) by replacing $Y_{\vec{Q}}(K, K')$, given by Eq. (7), by its first term $V(|\vec{k} - \vec{k}'|)$.

[6] G. Baym and L. P. Kadanoff, Phys. Rev. 124, 287 (1961).

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ERRATA

Comments on Effects of Electron-Electron Interactions on Nuclear Spin-Lattice Relaxation Times in Aluminum, F. Y. Fradin and T. J. Rowland [Phys. Rev. B 3, 1781 (1971)]. Some lines of this article were misplaced during the page makeup procedure.

(i) The last three lines in the second column of p. 1781 "··· the apparent values of δ found in a number of experiments on aluminum are considerably greater than 2^{10}" should appear at the end of the text on p. 1782.

(ii) The first four lines at the top of p. 1782 "of magnetization ··· measured by Pifer[5]" should be omitted, since they belong to the following paper.

Comments on Effects of Electron-Electron Interactions on Nuclear Spin-Lattice Relaxation Times in Aluminum—A Reply, D. P. Tunstall and D. Brown [Phys. Rev. B 3, 1783 (1971)]. Some lines of this article were erroneously inserted in the preceding article during the page makeup procedure. The paragraph preceding the *note added in proof* should read:

The value of δ that FR quote as measured by their technique, 2.65, as compared to our value of 2.15, is more worrying. It seems to us, from our arguments in the preceding paragraph, that the size of the quadrupole bath in thermal contact with the dipolar bath in the FR measurements will vary (a) during a single measurement, a fixed H_1, of magnetization against time and (b) with the amplitude of H_1, due to the mixing effect of the presence of H_1. As further support for our value we may note the value of $\delta = 2.07$ measured by Pifer.[5]