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New self-consistent quasistatic approximation for screening and plasma dispersion in the electron gas

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A new self-consistent quasistatic screening approach is proposed for studying the properties of an interacting electron gas. The compressibility divergence and the ferromagnetic instability found in the static unscreened Hartree-Fock approximation are nonexistent in this scheme. A better fit to the experimental data on the plasma dispersion relation than the existing calculations for free-electron metals is obtained.

Recently there has been considerable interest in calculating the longitudinal dielectric response function of the homogeneous electron gas in the time-dependent Hartree-Fock theory. In this scheme one goes beyond the random-phase approximation (RPA) by including the exchange-ladder diagrams for the proper polarization part. The resulting integral equation for the polarization or the irreducible vertex function has been solved variationally.[1,2] Woo and Jha[3] have solved this integral equation exactly by numerical methods, and find close agreement with the variational solution. In all these calculations a statically screened Coulomb interaction of the Yukawa form, $4\pi e^2/(q^2+\xi^2 k_F^2)$, for the effective two-particle interaction in the momentum space, treating ξ^2 as an undetermined parameter, is used. ξ^2 is assumed to be either zero or to have the Fermi-Thomas value, for purposes of simplicity. This procedure is not self-consistent since the final expression for the dielectric function leads to a value different from the starting value for the screening parameter.

In this paper we also use the static effective two-particle interaction as the starting point, but we determine its form in the $\omega=0$, $\vec{q}\to 0$ limit self-consistently, taking care not to be in any real conflict with the Ward identity. In this sense, our theory may be termed "quasistatic." This leads to a new self-consistent screening parameter ξ^2 as a function of r_s [in terms of the electron density n and Bohr radius a_0, $r_s=(\frac{3}{4}\pi n a_0^3)^{-1/3}$]. We obtain an expression for the compressibility of the electron gas as a function of r_s. The so-called compressibility divergence in the unscreened Hartree-Fock approximation is found to be suppressed in this scheme. The integral equation for the irreducible vertex function is solved variationally to determine the plasma dispersion, and it is found that this leads to good agreement with the experimental results for the plasma dispersion relation in various metals.

In an earlier work, Garrison, Morrison, and Wong[4(a)] have proposed a similar method to compute ξ^2 self-consistently. However, they have ignored the vertex renormalization,[1] which must accompany the mass renormalization, even though they are consistent with the Ward identity. This implies that their results are inconsistent within the time-dependent Hartree-Fock scheme. This work has been critically examined by Rajagopal and Mahanti.[4(b)]

Recently, Singwi and collaborators[5] have developed a successful ansatz to study the effects of electron correlations in a consistent fashion. There seems to be no obvious relation of their approach to known schemes of the many-body theory, even though there are some investigations with this in view published recently.[6]

In terms of the single-particle propagator $G(K)$, self-energy $\Sigma(K)$, proper vertex function $\Lambda(K, Q)$, the Coulomb interaction $v(\vec{q})=4\pi e^2/q^2$, and the unperturbed energy $\mathcal{E}_{\vec{k}}=\hbar^2k^2/2m$, the dynamical self-consistent dielectric function $\epsilon(Q)$ can be obtained in a shielded time-dependent Hartree-Fock theory by solving the set of equations

$$\begin{aligned}
G^{-1}(K) &= \mathcal{E}-\mathcal{E}_{\vec{k}}-\Sigma(K),\\
\Sigma(K) &= i\sum_Q G(K-Q)\, v(\vec{q})/\epsilon(Q),\\
\Lambda(K, Q) &= 1+i\sum_{K'} G(K')\, G(K'+Q)\\
&\quad\times\Lambda(K', Q)(\vec{K}-\vec{K}')\,[\epsilon(K-K')]^{-1}\\
\epsilon(Q) &= 1+2iv(\vec{q})\sum_K G(K)\, G(K+Q)\,\Delta(K, Q),
\end{aligned} \tag{1}$$

where K, Q, etc., stand for four momenta $(\vec{K}, \mathcal{E})$, $(\vec{q}, \hbar\omega)$, etc. Instead of solving this dynamical problem exactly, we assume that the quasistatic dielectric function in the long-wavelength limit may be obtained from the above set of equations by replacing $\epsilon(Q)$ in Σ and Λ by its static value $\epsilon(\vec{q}, 0)$. In this approximation, the dielectric function is given by

$$\epsilon(Q) = 1 - 2v(\vec{q}) \sum_{\vec{k}} M(\vec{k}, Q)\, \lambda(\vec{k}, Q), \tag{2}$$

$$\lambda(\vec{k}, Q) = -[(\mathcal{E}_{\vec{k}+\vec{q}} - \mathcal{E}_{\vec{k}} - \hbar\omega)/(E_{\vec{k}+\vec{q}} - E_{\vec{k}} - \hbar\omega)]\, \Lambda(\vec{k}, Q),$$

$$E_{\vec{k}} = \mathcal{E}_{\vec{k}} - \sum_{\vec{k}} V(\vec{k} - \vec{k}')\, n_{\vec{k}'},$$

$$M(\vec{k}, Q) = (n_{\vec{k}} - n_{\vec{k}+\vec{q}})/\Delta\mathcal{E}(\vec{k}, Q),$$

$$\Delta\mathcal{E}(\vec{k}, Q) \equiv \mathcal{E}_{\vec{k}+\vec{q}} - \mathcal{E}_{\vec{k}} - \hbar\omega - i\delta$$

$$V(\vec{k} - \vec{k}') = v(\vec{k} - \vec{k}')/\epsilon(\vec{k} - \vec{k}', 0), \tag{3}$$

where $n_{\vec{k}}$'s are the usual Fermi functions. The integral equation obeyed by $\lambda(\vec{k}, Q)$ is[1]

$$\lambda(\vec{k}) = -1 + \int V(\vec{k} - \vec{k}')\, M(\vec{k}') \times \left(\lambda(\vec{k}') - \frac{\Delta\mathcal{E}(\vec{k}')}{\Delta\mathcal{E}(\vec{k})}\, \lambda(\vec{k}) \right) \frac{d^3k'}{(2\pi)^3},$$

where we have suppressed the $\vec{q}$, ω dependences. The proper vertex function Λ must obey the Ward identity[7]

$$\lim_{q\to 0} \lim_{\omega\to 0} \Lambda(\vec{k}, Q) = 1 - \frac{\partial\Sigma(\vec{k}, E_{\vec{k}})}{\partial E_{\vec{k}}} = \frac{1}{Z_{\vec{k}}}. \tag{5}$$

Here $Z_{\vec{k}}$ is the wave-function renormalization[7] and must be such that $0 < Z_{\vec{k}} \le 1$. We require in the foregoing analysis only the value of (5) evaluated at $k = k_F$. One notes at once that it would be inconsistent with the variational solutions[1] if one takes our static model literally, since one would then have $Z_{\vec{k}} = 1$ for all $\vec{k}$. We therefore *suggest* that we should employ (5) as *defining* the renormalization $Z_{\vec{k}'}$, *with values of* $Z_{\vec{k}}$ *close to unity as a criterion for the validity of our approximation.* It is in this sense that our theory incorporates some of the dynamical aspects, and thus is a "quasistatic" scheme. The statically screened interaction $V(\vec{q})$ in the above equations is given by

$$V(\vec{q}) = \frac{v(\vec{q})}{\epsilon(\vec{q}, 0)} = \frac{4\pi e^2}{q^2 + k_F^2 \xi^2 W(q)}, \quad W(q=0) = 1, \tag{6}$$

where $W(q)$ is expected to be a slowly decreasing function of q. Equation (4) can be solved exactly[1] in the $\omega = 0$, $\vec{q} \to 0$ limit, after replacing $W(q)$ by its long-wavelength limit, namely unity. This is justified since the integral in Eq. (4) is dominated by the small $|\vec{k} - \vec{k}'|$ regions. We thus obtain

$$\lim_{\vec{q}\to 0} \epsilon(\vec{q}, 0) = \frac{1}{q^2}\left(q^2 + \frac{(4\alpha r_s/\pi)\, k_F^2}{1 - (\alpha r_s/\pi)\, S(\xi^2)} \right), \qquad S(\xi^2) = 1 - (\xi^2/4)\ln(1 + 4/\xi^2), \tag{7}$$

where

$$\alpha = (4/9\pi)^{1/3}.$$

For self-consistency, therefore, we demand

$$\xi^2 = \frac{(4\alpha r_s/\pi)}{1 - (\alpha r_s/\pi)\, S(\xi^2)}. \tag{8}$$

In doing this, we have taken care to introduce the mass, wave function, and vertex renormalizations. A direct calculation of $\Lambda(k_F, 0)$ using the exact solution of (4), coupled with the self-consistency condition (8), leads to the result

$$Z_{k_F} = 1/[1 + \tfrac{1}{8}\xi^2 \ln(1 + 4/\xi^2)]. \tag{5'}$$

The screening parameter can be numerically determined from Eq. (8) for different r_s. This should be contrasted with the corresponding result of Ref. 4. We have verified that for r_s between 1 and 6 (relevant to simple metals), the self-consistent value of $(\xi^2/4)$ varies monotonically from 0.19 to 1.33. Also, we find that $\frac{2}{3} \le Z_{k_F} \le 1$ for all r_s. One would thus expect this theory to be quite reliable in the sense that $Z_{k_F} \simeq 1$, $\partial\Sigma/\partial E_{k_F} \simeq 0$ for r_s in the range 1–3, and not too good for larger r_s. Note that in RPA, $\xi^2_{\mathrm{RPA}} = q^2_{\mathrm{FT}}/k_F^2 = 4\alpha r_s/\pi$. The compressibility ratio of the free and interacting electron gas is[7]

$$\frac{\kappa_F}{\kappa} = \lim_{q\to 0} \frac{(4\alpha r_s/\pi)}{[\epsilon(\vec{q}, 0) - 1]\, q^2} = \frac{\xi^2_{\mathrm{RPA}}}{\xi^2}. \tag{9}$$

The ratio is plotted as a function of r_s in Fig. 1. This is compared with the result obtained in Hubbard,[8] Vasishta and Singwi (VS),[5] and the static Hartree-Fock theories.[6] The divergence in κ/κ_F obtained in all these theories, including that of Ref. 4, is seen to be nonexistent in our scheme. This is consistent with the present experimental situation, and shows that the correlations tend to

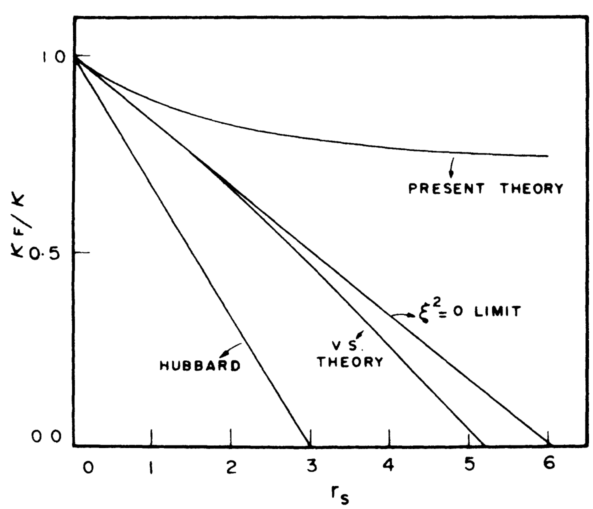

FIG. 1. Compressibility ratio κ_F/κ in various theories (see text). In our scheme, this is also the ratio $\chi_{Pauli}/\chi_{zz}(0, 0)$ for the static paramagnetic spin susceptibility.

wash out the Hartree-Fock enhancement as they do in various other physical problems of interest. The calculation of the paramagnetic spin susceptibility χ_{zz} of the electron gas[1] in our scheme is very similar to that of the dielectric susceptibility, and we get $\chi_{zz}(0, 0)/\chi_{\text{PAULI}} = \kappa/\kappa_F$. This is a consequence of our approximation scheme. Because of this relationship, it appears that the ferromagnetic instability does not exist in this approach [see Refs. 1 and 4(b)].

The collective plasma mode in the electron gas can be found either as the zero of the real part of the dielectric function or as the pole of the real part of the reducible polarization part $\sum_{\vec{k}} M(\vec{k})\lambda(\vec{k})/\epsilon(Q)$. The best k-independent variational solution of Eq. (4) for λ is[1]

$$\lambda(\vec{q}, \omega) = -\frac{M(\vec{q}, \omega)}{M(\vec{q}, \omega) - J(\vec{q}, \omega)}, \tag{10}$$

where

$$M(\vec{q}, \omega) = \int \frac{d^3k}{(2\pi)^3} M(\mathrm{k}, Q) \tag{11}$$

and

$$J(\vec{q}, \omega) = \iint \frac{d^3k}{(2\pi)^3} \frac{d^3k'}{(2\pi)^3} V(\vec{k} - \vec{k}') \times M(\vec{k}, Q) M(\vec{k}', Q)\left(1 - \frac{\Delta\mathcal{E}(\vec{k}', Q)}{\Delta\mathcal{E}(\vec{k}, Q)}\right). \tag{12}$$

From Eq. (1), we therefore find that the plasma mode is determined by

$$\mathrm{Re}\left[1 + 2vM(\vec{q}, \omega)\ (\vec{q}, \omega)\left(1 + \frac{J(\vec{q}, \omega)}{M(\vec{q}, \omega)}\right)\right] = 0. \tag{13}$$

Assuming $V(q) = 4\pi e^2/(q^2 + \xi^2 k_F^2)$, the functions involved in Eq. (13) can be expanded in powers of qv_f/ω, in the plasma range of frequencies. The various integrals can be performed[1] by using associated Legendre functions and spherical harmonics for the expansion of the interaction $V(|\vec{k} - \vec{k}|)$. This leads to the plasma dispersion relation

$$1 - (\omega_p^2/\omega^2)\left[1 + \tfrac{9}{5}(q/q_{\mathrm{FT}})^2 - \tfrac{3}{20}(q/k_F)^2 P(\xi^2)\right] = 0, \tag{14}$$

where

$$P(\xi^2) = (1 - \xi^2) + \tfrac{1}{4}\xi^2(1 + \xi^2)\ln(1 + 4/\xi^2) \tag{15}$$

If the plasma frequency is written

$$\omega_p(q) = \omega_p(0) + \beta q^2, \tag{16}$$

a quantity of great interest is the ratio $\beta/\beta_{\mathrm{RPA}}$, where β_{RPA} is determined from Eqs. (14) and (16) by putting $P(\xi^2) = 0$. In our calculation we get

$$\frac{\beta}{\beta_{\mathrm{RPA}}} = 1 - \frac{\alpha r_s}{3\pi} P(\xi^2). \tag{17}$$

Using the self-consistent value of ξ^2 determined earlier, we plot this ratio for various r_s's in Fig. 2. This appears to fit the experimental data remarkably well. It is gratifying to note that the free-electron metals like Al and Na give the best fit. For comparison we have plotted the results of VS[5] theory and the $\xi^2 = 0$ limit of (16). In the $\xi^2 = 0$ limit, $P(\xi^2) = 1$. This particular case was considered earlier by Rajagopal, Rath, and Kimball (RRK).[6]

Although we have obtained very interesting results as a consequence of our self-consistent quasistatic screening approach, we would have liked to use a more realistic variation of $W(q)$ in Eqs. (4) and (6) than to replace it by its long-wavelength value. However, as explained earlier, the error introduced due to this in obtaining the long-wavelength limit of $\epsilon(\vec{q}, 0)$ is expected to be extremely small.

A complete theory would necessarily involve complications of dynamical nature and would make Eq. (5) an identity, as well as make the computations more involved. The approach presented here is one where the approximations are consistent with the basic requirements of many-body theory but still retain the ease with which all the calculations can be performed. It is in this sense that this approach seems to be complimentary to the Vasishta and Singwi[5] result. A closer relationship with his scheme could perhaps be inferred when we compute the dynamical dielectric function in our scheme.

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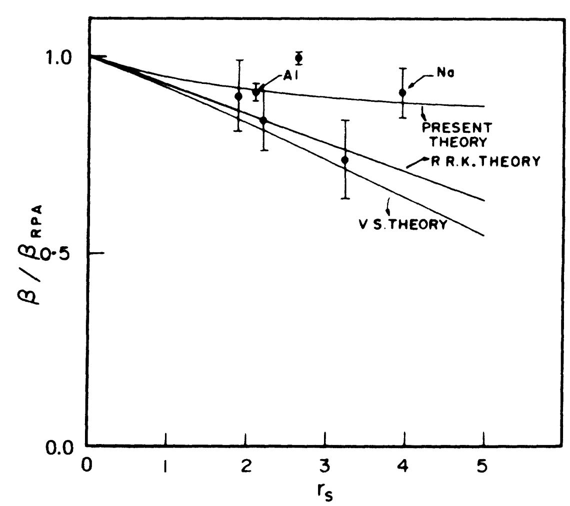

FIG. 2. Plasma dispersion parameter $\beta/\beta_{\mathrm{RPA}}$ in various theories (see text). Experimental results (Ref. 9) for Be, Al, Sb, Mg, Li, and Na in order of increasing r_s are also shown.

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