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Application of the Third Moment to the Electric and Magnetic Response Function

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The third frequency moments of the electric and magnetic response functions of a homogeneous electron gas are shown to reflect the short-time (or high-frequency) motion of an electron relative to its correlation hole. It is found that the relaxation of the local correlation hole effects the magnetic response much more strongly than the electric response, particularly for long wavelengths. Available models for these response functions are found to miss this particular aspect and, therefore, they cannot be valid both for low and high frequencies. An interpolation model, which in a more proper way includes the relaxation of the correlation hole, is used for some illustrative numerical calculations. It leads to damping of the long-wavelength plasmons in good agreement with earlier calculations based on diagram techniques and including multiple particle-hole excitations.

I. INTRODUCTION

In recent years considerable progress has been made in calculating transport properties of classical as well as quantum liquids.[1–4] Difficulties due to the strong interactions have been partially circumvented by formulating the theories so as to satisfy certain exactly calculable sum rules. In this paper we shall be concerned mainly with the electron liquid, although our conclusions have implications for other systems as well. Most treatments of the density and spin-density response of the electron liquid have been concerned with improving upon the random-phase approximation (RPA) by correcting the Hartree self-consistent field for effects due to strong short-range correlations.[5–11] So, for instance, Hubbard[5] very early introduced a correction the the RPA dielectric function arising from the Pauli-exchange hole and this has been generalized to include both the exchange and Coulomb holes in a self-consistent way.[7,8] Later developments along this line have led particularly to improved results for the long-wavelength low-frequency response.[9–11]

The response properties of a degenerate homogeneous electron liquid under external disturbances have provided the basic model for the behavior of valence electrons in metals. The main features, such as the perfect screening of charges at large distance and long-wavelength plasma oscillations, follow from general properties of the density response, or of the related dielectric function $\epsilon(\vec{q}, \omega)$, and do not depend on its detailed form.[12] More specific knowledge of the q dependence for low frequency is needed, for example, in the calculation of phonon-dispersion curves in simple metals. However, different choices of $\epsilon(\vec{q}, 0)$ together with the ion-electron pseudopotential $V(\vec{q})$ have led to essentially the same dispersion curves.[13] The correlation energy involves an integration of $\epsilon(\vec{q}, \omega)$ over $\vec{q}$ and ω and is insensitive to its detailed form.[11] The pair-correlation function $g(\vec{r})$ also requires a full knowledge of $\epsilon(\vec{q}, \omega)$ and is fairly sensitive to the q dependence[11] but again involves an integration over frequency. Optical properties provide, in principle, a more detailed test on the frequency dependence of $\epsilon(\vec{q}, \omega)$ but only after band-structure effects have been sorted out.[14] Therefore, we have at present no stringent tests of the detailed form of either the density or spin-density response functions. The strongest requirements on the various models have been that they should satisfy certain exactly known sum rules, in particular, the compressibility sum rule and the one giving the static-pair-correlation functions, including the requirement that the latter should be positive for all distances. No existing model satisfies these requirements exactly although a recent model of Vashishta and Singwi[11] comes rather close to doing so.

It was recently noted by one of the authors (B.G.) that the third moment of the spin-density response function has a singular q dependence in the long-wavelength limit as compared with the full density response function.[15] This difference between the two response functions is not contained in any theoretical model known to us. Knowing that the odd positive low-order moments are connected with the high-frequency response functions, one may guess that they do not directly have any large effect in determining the low-frequency response. However, they do indicate that the available models are not appropriate to describe the high-frequency response, particularly not the magnetic response. The first moment, or f-sum rule, is connected with particle-number conservation and is satisfied by any model which gives free-particle behavior in the high-frequency limit. The third moment has not been used until recently and its physical content has not been investigated before.

The purpose of this paper is to clarify the significance of the third moment. It is shown why conventional mean-field theories miss an essential aspect of the dynamics contained in the third moment. The singular behavior in the long-wavelength magnetic response is a direct consequence of the Coulomb correlation hole following each electron and of its dynamics. It is the short-time motion of this correlation hole relative to its electron which is not handled properly in available models. What is said here for electrons is equally valid for particles with short-range interactions.

The outline of this paper is as follow: In Sec. II a derivation of the third moment is given and its physical implications are discussed in some detail. In Sec. III we analyze the mean-field theories and show why they all disagree with the third moment. A recent momentum-dependent modification of the conventional mean-field theories of the dielectric response by Toigo and Woodruff[16] is discussed in Sec. IV and is shown to be a high-frequency approximation closely related to the third moment. Extending their treatment to the spin-density response leads to a zero value for the static spin susceptibility, confirming that the method is basically suited to high frequencies only. Section V contains a brief discussion of the Landau theory of Fermi liquids in relation to sum-rule arguments.[17] Finally, in Sec. VI we present results from some numerical calculations.

II. THIRD MOMENTS OF PARTIAL DENSITY RESPONSE FUNCTIONS

A. Neutral System

We start with a brief summary of some well known relations which we need for the following discussion. Let us consider a weak external disturbance V acting on our system and coupled directly to a dynamical variable A through a term $H' = VA$ in the Hamiltonian. The retarded response of a variable B is then, according to linear-response theory, given by[18]

$$\chi_{BA}(t) = (i\hbar)^{-1}\langle[B(t),\ A(0)]\rangle\,\theta(t) \equiv 2i\chi''_{BA}(t)\theta(t)\ , \tag{2.1}$$

where [ ] is an ordinary commutar and $\langle\ \rangle$ means averaging over an equilibrium ensemble with no external disturbance present. For brevity we have also introduced the notation $\chi''_{BA}(t)$. In Fourier space we get

$$\chi_{BA}(\omega) = \int_{-\infty}^{\infty} \chi_{BA}(t)e^{i\omega t}\,dt = \int_{-\infty}^{\infty} \frac{\chi''_{BA}(\omega')}{\omega' - \omega - i0^+}\ \frac{d\omega'}{\pi}\ , \tag{2.2}$$

and from this follows the asymptotic expansion

$$\chi_{BA}(\omega) \sim \sum_{l=0}^{\infty} \frac{M_{l,BA}}{\omega^{l+1}}\ , \tag{2.3}$$

where the coefficients are the moments of $\chi''_{BA}(\omega)$,

$$M_{l,BA} = -\int_{-\infty}^{\infty} \omega^l\,\chi''_{BA}(\omega)\,\frac{d\omega}{\pi} = i^l \left\langle \frac{1}{\hbar}\left[\frac{d^l}{dt^l}\ B(t), A(0)\right]\right\rangle_{t=0}\ . \tag{2.4}$$

The Taylor expansion of $\chi''_{BA}(t)$ is

$$\chi_{BA}(t) = \theta(t)\sum_{l=0}^{\infty} \frac{M_{l,BA}t^l}{i^{l+1}l\,!}\ . \tag{2.5}$$

This shows that the low-order moments are related to the short-time and correspondingly high-frequency behavior of the response function. These low-order moments are often easily evaluated and Eqs. (2.3) and (2.5), therefore, provide us with some useful exact statements concerning the response of the system. The case of interest to us is when A and B stand for the number densities $n_\sigma(\vec{r}, t)$ for particles of spin index $\sigma = \pm 1$; $\sigma = +1$ for spin up and -1 for spin down. The corresponding response functions

$$\chi_{\sigma\sigma'}(\vec{r}, \vec{r}\,';\ t) = (i\hbar)^{-1}\langle[n_\sigma(\vec{r}, t),\ n_{\sigma'}(\vec{r}\,', 0)\,]\rangle\,\theta(t) \tag{2.6}$$

depend only on the difference $\vec{r} - \vec{r}\,'$, and their spatial Fourier transforms can, therefore, be written as

$$\chi_{\sigma\sigma'}(\vec{q}, t) = (i\hbar\Omega)^{-1}\langle\,[\,n_\sigma(\vec{q}, t),\ n_{\sigma'}(-\vec{q}, 0)\,]\rangle\,\theta(t)\ , \tag{2.7}$$

Ω being the total volume of the system. We introduce separate notations for the full density and the spin-density response functions $[s_z(\vec{r}) \equiv n_\uparrow(\vec{r}) - n_\downarrow(\vec{r})]$;

$$\chi_{nn} = \sum_{\sigma\sigma'} \chi_{\sigma\sigma'}\ , \tag{2.8}$$

$$\chi_{zz} \equiv \chi_{s_z s_z} = \sum_{\sigma\sigma'} \sigma\sigma'\chi_{\sigma\sigma'}\ . \tag{2.9}$$

The even moments of these retarded response functions are zero and this holds true also for the magnetized state.[19]

The three lowest even moments of the density *correlation* function $S(\vec{q}, \omega)$ were first used by Yvon[20] for classical fluids[21] to estimate the frequency dispersion of short-wavelength density fluctuations. He showed that the fourth moment of $S(\vec{q}, \omega)$ could be calculated from the static-pair-correlation function $g(\vec{r})$ and the interatomic potential. DeGennes applied later the same moments together with approximate forms for $S(\vec{q}, \omega)$ to calculate inelastic-neutron-scattering cross sections.[22] Recent work[2] on the scattering function in liquids has been rather close to Yvon's idea of high-frequency collective motions. Related developments of semiempirical scattering functions using moment relations[1] have also been based on the continued fraction representation of Mori.[23]

The application of Eq. (2.4) to $\chi_{\sigma\sigma'}(\vec{r}, \vec{r}'; t)$ is simplified somewhat by transferring time derivatives from B to A and using the continuity equation

$$\dot{n}_\sigma = -\vec{\nabla}\cdot\vec{J}_\sigma \; (\equiv \nabla^\alpha J^\alpha_\sigma) , \tag{2.10}$$

$\vec{J}_\sigma$ being the current densities. The first moment is easily evaluated and gives

$$M_{1,\sigma\sigma'}(\vec{r}, \vec{r}') = -(i/\hbar)\nabla^\alpha_r \langle [J^\alpha_\sigma(\vec{r}), \; n_{\sigma'}(\vec{r}')]\rangle = m^{-1}\delta_{\sigma\sigma'}\vec{\nabla}_r\cdot\vec{\nabla}_{r'}(\delta(\vec{r}-\vec{r}')\langle n_\sigma(\vec{r})\rangle) , \tag{2.11}$$

where m is the mass of the particle. In deriving Eq. (2.11) we have used the operator relation

$$[J^\alpha_\sigma(\vec{r}), \; n_{\sigma'}(\vec{r}')] = (i\hbar/m) n_\sigma(\vec{r})\nabla^\alpha_{r'}\delta(\vec{r}-\vec{r}')\delta_{\sigma\sigma'} . \tag{2.12}$$

For a uniform system Eq. (2.11) gives us in Fourier space the familiar f-sum rule

$$M_{1,\sigma\sigma'}(\vec{q}) = \delta_{\sigma\sigma'} n_\sigma q^2/m , \tag{2.13}$$

where n_σ is the equilibrium density.

The third moment is evaluated similarly from the expression

$$M_3(1,2) = (i/\hbar)\nabla^\alpha_1\nabla^\beta_2\langle[\dot{J}^\alpha(1), \; J^\beta(2)]\rangle = M^T_3(1,2) + M^P_3(1,2) , \tag{2.14}$$

where here $1 = (\vec{r}, \sigma)$ and $2 = (\vec{r}', \sigma')$, and the convention of summing over repeated Cartesian indices is used. The two parts M^T_3 and M^P_3 come from the kinetic and potential terms, respectively, in the equation of motion for the current-density operator[9]:

$$m\dot{J}^\alpha(1) = -\nabla^\beta_1 T^{\alpha\beta}(1) - \int \nabla^\alpha_1 v(r_{13})[n(1)n(3)]' d(3) . \tag{2.15}$$

Here $T^{\alpha\beta}$ is the kinetic part of the stress tensor in operator form, $v(r)$ is the interaction potential, and $d(3) = \sum_{\sigma_3} d\vec{r}_3$ means summation over the spin index and integration over space. The prime in the integrand means that the self-force term should be removed, and this will be understood, even when the prime is omitted. We give the explicit form in ordinary space of M^P_3 only because it is helpful in visualizing the short-time response. The full expression for $M_{3,\sigma\sigma'}(\vec{q})$ will be given afterwards. Inserting the potential term of Eq. (2.15) into Eq. (2.14) yields

$$\begin{aligned} M^P_3(1,2) &= (i\hbar m)^{-1}\nabla^\alpha_1\nabla^\beta_2\int d(3)\nabla^\alpha_1 v(r_{13})\langle[n(1)n(3), \; J^\beta(2)]\rangle \\ &= (i\hbar m)^{-1}\nabla^\alpha_1\nabla^\beta_1\int d(3)\nabla^\alpha_1 v(r_{13})\{\langle[n(1), \; J^\beta(2)]n(3)\rangle + \langle n(1)[n(3), \; J^\beta(2)]\rangle\} \\ &= m^{-2}\nabla^\alpha_1\nabla^\beta_2\{\nabla^\beta_1\delta(1,2)\int d(3)\nabla^\alpha_1 v(r_{13})\langle n(2)n(3)\rangle + \nabla^\alpha_1\nabla^\beta_1 v(r_{12})\langle n(1)n(2)\rangle\} . \end{aligned} \tag{2.16}$$

By considering an external vector field coupled to the particle current operator, we get a simple physical interpretation of the commutator in the first line of the equation above, namely, it gives the instantaneous response of the equal time density correlation function $\langle n(1)n(3)\rangle$. The second line tells us that this can be viewed as arising from separate responses from the particles at sites r_1 and r_3, taking into account the spatial correlation of the two particles. So, for instance, the particle at r_1 sits in the correlation hole of its surrounding particles while responding to the external vector field.

In Fourier space the full third moment takes the following from

$$M_{3,\sigma\sigma'}(\vec{q}) = n_\sigma\delta_{\sigma\sigma'}(q^2/m)^2\{\langle p^2/m\rangle_\sigma + \hbar^2 q^2/4m\} + m^{-2}\vec{q}\cdot\overleftrightarrow{F}_{\sigma\sigma'}(\vec{q})\cdot\vec{q} , \tag{2.17}$$

where $\langle p^2\rangle_\sigma$ is the true mean square momentum of particles of spin σ with the effects of the interaction included.[24] The first term is the kinetic part M^T_3. The potential part M^P_3 is the term containing the tensor

$$\overleftrightarrow{F}_{\sigma\sigma'}(\vec{q}) = \delta_{\sigma\sigma'}\overleftrightarrow{T}_\sigma(0) - \overleftrightarrow{T}_{\sigma\sigma'}(\vec{q}), \tag{2.18}$$

with

$$T^{\alpha\beta}_{\sigma\sigma'}(\vec{q}) = \int d\vec{r}\, e^{i\vec{q}\cdot\vec{r}}\langle n_\sigma(0)n_{\sigma'}(\vec{r})\rangle\nabla^\alpha\nabla^\beta v(\vec{r}) \tag{2.19}$$

and

$$T^{\alpha\beta}_\sigma(\vec{q}) = \sum_{\sigma''} T^{\alpha\beta}_{\sigma\sigma''}(\vec{q}) . \tag{2.20}$$

Let us now consider χ_{nn} and χ_{zz} and their moments. From Eq. (2.13) follows

$$M_{1,nn}(\vec{q}) = M_{1,zz}(\vec{q}) = nq^2/m \quad (n = n_\uparrow + n_\downarrow). \tag{2.21}$$

Correspondingly the third moments are given by

$$M^T_{3,nn}(\vec{q}) = M^T_{3,zz}(\vec{q}) = n(q^2/m)^2\{\langle p^2/m\rangle + \hbar^2 q^2/4m\} , \tag{2.22}$$

and further

$$M^P_{3,nn}(\vec{q}) = m^{-2}\vec{q}\cdot[\overleftrightarrow{T}(0) - \overleftrightarrow{T}(\vec{q})]\cdot\vec{q} \tag{2.23a}$$

$$= (n^2q^2/m^2)\int d\vec{r}[(\hat{q}\cdot\nabla)^2 v(r)](1 - e^{i\vec{q}\cdot\vec{r}})g(\vec{r}) , \tag{2.23b}$$

and

$$M^P_{3,zz}(\vec{q}) = m^{-2}\vec{q}\cdot[\overleftrightarrow{T}(0) - \sum_{\sigma\sigma'} \sigma\sigma' \overleftrightarrow{T}_{\sigma\sigma'}(\vec{q})]\cdot\vec{q} \qquad (2.24a)$$

$$= (n^2q^2/m^2)\int d\vec{r}\,[(\hat{q}\cdot\vec{\nabla})^2 v(r)]\{(1 - e^{i\vec{q}\cdot\vec{r}})\tilde{g}(\vec{r}) + 4f_\uparrow f_\downarrow g_{\uparrow\downarrow}(\vec{r})\} . \qquad (2.24b)$$

Here $\overleftrightarrow{T}(0) = \sum_\sigma \overleftrightarrow{T}_\sigma(0)$, $f_\sigma = n_\sigma/n$ and $\hat{q}$ is the unit vector along $\vec{q}$. The various pair-correlation functions entering in the equations above are

$$n^2 g(\vec{r}) = \langle n(0)\,n(\vec{r})\rangle - n\delta(\vec{r}) ,$$

$$n_\uparrow n_\downarrow g_{\uparrow\downarrow}(\vec{r}) = n_\uparrow n_\downarrow g_{\downarrow\uparrow}(\vec{r}) = \langle n_\uparrow(0) n_\downarrow(\vec{r})\rangle , \qquad (2.25)$$

$$n^2\tilde{g}(\vec{r}) = \langle s_z(0)\,s_z(\vec{r})\rangle - n\delta(\vec{r}) ,$$

where the effect of the prime in Eq. (2.15) is shown explicitly. In the paramagnetic case $\tilde{g} = \frac{1}{2}(g_{\uparrow\uparrow} - g_{\uparrow\downarrow})$.

The expression for $M_{3,nn}$ is familiar and it was first derived by Yvon for a classical fluid,[20] in which case the curly bracket in Eq. (2.22) becomes $3k_BT/m$. Puff[3] appears to be the first to use the quantum-mechanical form of $M_{3,nn}$, whereas the corresponding expression for $M_{3,zz}$ was given more recently.[15,17] We note from Eqs. (2.22)–(2.24) that, for small values of q,

$$M_{3,nn}(\vec{q}) \propto q^4 \quad\text{and}\quad M_{3,zz}(\vec{q}) \propto q^2 . \qquad (2.26)$$

The reason for the difference in the small-q forms of χ_{zz} and χ_{nn} lies in the last term of Eq. (2.24b), containing $g_{\uparrow\downarrow}(\vec{r})$. It will be referred to in the following as the *singular part* of $M_{3,zz}$. Its appearance depends on the existence of a correlation hole around a particle due to the particle interaction and it would, therefore, not appear in the Hartree-Fock approximation.

The difference between $M_{3,nn}$ and $M_{3,zz}$ has an analog in the motion of a diatomic lattice. There the 6×6 dynamical matrix contains 3×3 submatrices of the same form as in Eq. (2.18) with σ now referring to the two sublattices, and

$$T^{\alpha\beta}_{\sigma\sigma'}(\vec{q}) = -\sum_{R\neq 0}\nabla^\alpha\nabla^\beta v_{\sigma\sigma'}(\vec{R}_{\sigma\sigma'})\,e^{i\vec{q}\cdot\vec{R}_{\sigma\sigma'}} , \qquad (2.27)$$

where the summation runs over the lattice vectors $\vec{R}_{\sigma\sigma'}$. The first term in Eq. (2.18) now determines the Einstein frequency of the atom σ and it represents the motion of a single atom while the other atoms are held fixed on their lattice sites. For small values of $\vec{q}$ and considering acoustic modes, the two sublattices move in phase and the square of the phonon frequency is determined from the combination $[\overleftrightarrow{T}(0) - \overleftrightarrow{T}(\vec{q})]$ analogous to that appearing in $M^P_{3,nn}(\vec{q})$. For the optical modes the sublattices move out of phase and a matrix combination like that for $M_{3,zz}$ gives a finite optical frequency for $\vec{q}=0$. Relative to the acoustic modes, the optical modes give a singular contribution of order q^{-2} to the third moment of the displacement response function.

A spin-independent driving force moves the up- and down-spin systems in the same direction, as in acoustic mode motion, while a magnetic field along the z axis drives them in opposite directions. Thus the form of the moments in Eq. (2.17) is characteristic of a two-component system.

B. Charged Systems

In order to include a neutralizing positive background, we replace $n_{\sigma_3}(\vec{r}_3)$ in Eq. (2.15) by $n_{\sigma_3}(\vec{r}_3) - n_{\sigma_3}$. This has the effect of changing g_σ to $(g_\sigma - 1)$ in $\overleftrightarrow{T}_\sigma(0)$ while leaving $\overleftrightarrow{T}_{\sigma\sigma'}(\vec{q})$ unchanged. We may write

$$M^P_{3,\sigma\sigma'}(\vec{q}) = m^{-2}\vec{q}\cdot[\delta_{\sigma\sigma'}\overleftrightarrow{\Gamma}_\sigma(0) - \overleftrightarrow{\Gamma}_{\sigma\sigma'}(\vec{q})]\cdot\vec{q} + m^{-2}n_\sigma n_{\sigma'}q^4 v(\vec{q}) , \qquad (2.28)$$

where $\overleftrightarrow{\Gamma}_{\sigma\sigma'}$ is obtained from $\overleftrightarrow{T}_{\sigma\sigma'}$ by replacing $g_{\sigma\sigma'}$ by $g_{\sigma\sigma'} - 1$; in this way separating out the Hartree term which appears as the last term of the equation. The integrals contained in $\overleftrightarrow{\Gamma}$ now converge at large r. For χ_{nn} and χ_{zz} we have[25]

$$M^P_{3,nn}(\vec{q}) = nq^2\omega_p^2/m + \bar{M}^P_{3,nn}(\vec{q}) \qquad (2.29)$$

and

$$M^P_{3,zz}(\vec{q}) = (nq^2/m)\{(f_\uparrow - f_\downarrow)^2\omega_p^2 + \omega_s^2\} + \bar{M}^P_{3,zz}(\vec{q}) , \qquad (2.30)$$

where $\bar{M}^P_{3,nn}$ is obtained from Eq. (2.23b) by changing g to $g-1$. $\bar{M}^P_{3,zz}$ is given by Eq. (2.24b) with the $g_{\uparrow\downarrow}$ term removed and $\tilde{g}(\vec{r})$ replaced by $\tilde{g}(\vec{r}) - \tilde{g}(\infty)$, where $g(\infty) = (f_\uparrow - f_\downarrow)^2$. Both $\bar{M}^P_{3,nn}$ and $\bar{M}^P_{3,zz}$ are proportional to q^4 for $q \to 0$. Relative to these the first terms in Eqs. (2.29) and (2.30) are singular and the two terms proportional to ω_p^2, $\omega_p = (4\pi ne^2/m)^{1/2}$ being the plasma frequency, come from the long-range Hartree field. The first one is connected with ordinary plasma oscillations and the second with the coupling of charge and spin-density oscillations, which only occurs if $f_\uparrow \neq f_\downarrow$.[26] The remaining singular term in Eq. (2.30) is proportional to

$$\omega_s^2 = (4f_\uparrow f_\downarrow/3m)\int d\vec{r}\,\nabla^2 v(\vec{r})\,[g_{\uparrow\downarrow}(r) - 1]$$

$$= 4f_\uparrow f_\downarrow[1 - g_{\uparrow\downarrow}(0)]\,\tfrac{1}{3}\omega_p^2 , \qquad (2.31)$$

and it depends on the short range correlations. It gives the "Einstein" frequency of, say, a spin-up particle moving in a *rigid* correlation hole of down-spin particles.

From these low-order moments alone we cannot determine whether there exists a fairly well defined "optical" spin mode at some frequency ω_s or whether such a motion is heavily damped. Neither could we tell that undamped plasmons exist at small

$\vec{q}$ without additional consideration such as conservation of the total internal momentum of the electron system. However, the momentum is not conserved for the up and down spin electrons separately and the situation for spin-density oscillations is, therefore, different from that for the full density oscillations. Since at metallic densities $\omega_s \sim \frac{1}{2}\omega_p$, an "optical" spin mode is probably overdamped because the correlation hole does not remain rigid. The possibility of an absorption maximum in the high-frequency spin susceptibility is not ruled out.

III. COMPARISON WITH LOCAL MEAN-FIELD THEORIES

Various mean-field models for the dielectric response[7,9–11,27] and for the spin-density response[8,9,28] of a system are based first on the assumption that a single particle responds as does a free-particle to some effective field. This means

$$\delta\langle n_\sigma(\vec{q},\ \omega)\rangle = \chi^{(0)}(\vec{q},\ \omega)\, v_\sigma^{\text{eff}}(\vec{q},\ \omega), \tag{3.1}$$

where $\chi^{(0)}$ is the free-particle response function. The second assumption is that the effective field contains an induced part proportional to the induced density of the surrounding particles. We may separate out the Hartree effective field and write

$$V_\sigma^{\text{eff}}(\vec{q},\ \omega) = V_\sigma^{H}(\vec{q},\ \omega) - v(q)\sum_{\sigma'} G_{\sigma\sigma'}(\vec{q},\ \omega) \times \delta\langle n_{\sigma'},(\vec{q},\ \omega)\rangle, \tag{3.2}$$

where the quantities $G_{\sigma\sigma'}(\vec{q},\ \omega)$ are the local field factors. For the paramagnetic state the resulting expressions for $\chi_{zz}(\vec{q},\ \omega)$ and for the screened density response function $\chi_{sc}(\vec{q},\ \omega) = \chi_{nn}(\vec{q},\ \omega)\,\epsilon(\vec{q},\ \omega)$, $\epsilon(\vec{q},\ \omega)$ being the dielectric function, are very similar since neither response function involves the long-range interaction of charge fluctuations. We get

$$\chi_{sc}(\vec{q},\ \omega) = \chi^{(0)}(\vec{q},\ \omega)\,[1 + v(q)\,G_+(\vec{q},\ \omega)\,\chi^{(0)}(\vec{q},\ \omega)]^{-1} \tag{3.3a}$$

and

$$\chi_{zz}(\vec{q},\ \omega) = \chi^{(0)}(\vec{q},\ \omega)\,[1 + v(q)\,G_-(\vec{q},\ \omega)\,\chi^{(0)}(\vec{q},\ \omega)]^{-1}, \tag{3.3b}$$

where

$$G_\pm(\vec{q},\ \omega) = \tfrac{1}{2}\,[G_{\uparrow\uparrow}(\vec{q},\ \omega) \pm G_{\uparrow\downarrow}(\vec{q},\ \omega)]\,. \tag{3.4}$$

This gives for both χ_{sc} and χ_{zz} the asymptotic expansion

$$\chi \sim \frac{nq^2}{m\omega^2} + \frac{1}{\omega^4}\left[M_3^{(0)}(\vec{q}) - \left(\frac{nq^2}{m}\right)^2 v(\vec{q})\,G_\pm(\vec{q},\ \infty)\right] + \cdots\ , \tag{3.5}$$

where $nq^2/m\omega^2$ comes from the first moment of $\chi^{(0)}(\vec{q},\ \omega)$, and $M_3^{(0)}(\vec{q})$ is the corresponding third moment and is proportional to q^4 [cf. Eq. (2.22)].

Local field factors $G_\pm(\vec{q})$, which do not depend on ω, cannot describe properly the short time response which goes into the third moments. This deficiency shows up clearly in the spin-density response. To get the singular q^2 term in Eq. (2.30) requires that $v(\vec{q})\,G_-(\vec{q})$ vary as q^{-2} for small q. Since $\chi^{(0)}(\vec{q},\ 0) \to -mp_F/\pi^2\hbar^3$ as $q\to 0$, the static spin susceptibility $\lim_{\vec{q}\to 0}\chi_{zz}(\vec{q},\ 0)$ would then be zero. Modifications of Eq. (3.3a) have been proposed in which $\chi^{(0)}(\vec{q},\ \omega)$ is replaced by a different single-particle response function.[4] If this single-particle response function has physical meaning, it should be used in Eq. (3.3b) also and the effect is to change $M_3^{(0)}(\vec{q})$ in Eq. (3.5). The difference between $v(\vec{q})\,G_-(\vec{q})$ and $v(\vec{q})\,G_+(\vec{q})$ must still be singular in order to reproduce the difference in the third moments and the difficulty above with the static susceptibility will remain.

The third moments of χ_{nn} and χ_{sc} differ just by the plasma term in Eq. (2.29). Therefore, the moment for the screened density response is proportional to q^4 for small q, owing to the cancellation of the singular "Einstein" term $\overleftrightarrow{\Gamma}(0)$ via the particular combination $[\overleftrightarrow{\Gamma}(0) - \overleftrightarrow{\Gamma}(\vec{q})]$ which occurs in Eq. (2.29) as a results of translation invariance of the whole system. The cancellation is not complete in Eq. (2.30) for the spin-density response, the remainder being the term with $\omega_s^2 = [1 - g_{\uparrow\downarrow}(0)] \times \frac{1}{3}\omega_p^2$. However, as discussed below, present mean field models give $G_\pm(\vec{q},\ \omega) \propto q^2$ as $q\to 0$, which is qualitatively correct for χ_{sc} only. One may ask, therefore, why the "Einstein" term seems to cancel out in both response functions.

Let us consider the simplest local-field model,[7,8] which corresponds to the replacement

$$\langle n(1)n(3)\rangle \to \langle n(1)\rangle\,\langle n(3)\rangle\, g^{eq}(1,\ 3) \tag{3.6}$$

in the equation for the mean current density in the presence of an external disturbance [see Eq. (2.15)]. In Eq. (2.16) it is equivalent to replacing the commutator term by

$$\langle [n(1)n_3 + n_1 n(3),\ J^\beta(2)]\rangle\, g^{eq}(1,\ 3) = -\,(i\hbar/m)\,[\nabla_1^\alpha\,\delta(1,\ 2) + \nabla_3^\beta\,\delta(3,\ 2)] \times n_1 n_3\, g^{eq}(1,\ 3),$$

where $n_1 = n_{\sigma_1}$, and $n_3 = n_{\sigma_3}$. This gives

$$M_3^P(1,\ 2) = m^{-2}\,\nabla_1^\alpha\nabla_1^\beta\{\nabla_1^\beta\,\delta(1,\ 2)\int d(3)\,\nabla_1^\alpha v(r_{13}) \times\langle n(1)n(3)\rangle + \nabla_1^\beta[\nabla_1^\alpha v(r_{12})\,\langle n(1)n(2)\rangle]\}\ , \tag{3.7}$$

and it differs from Eq. (2.16) in two respects. (a) The coordinate 2 is replaced by 1 in the integral and the integral now vanishes, making the "Einstein" term disappear. Physically it means that particle 1 is always kept at the center of its correlation hole. (b) In the second term of Eq. (3.7) the pair-correlation function is also differentiated, unlike in Eq. (2.16). The extra term $-\nabla_1^\alpha v(r_{12}) \times \nabla_2^\beta g(1, 2) n_{\sigma_1} n_{\sigma_2}$ represents a displacement of $g(1, 2)$ with particle 2 when the latter is moved. These two features show that, in making the approximation in Eq. (3.6), one ignores the finite relaxation time of the correlation hole. This results in a frequency-independent local-field factor $G_{\sigma\sigma'}(\vec{q})$ in Eqs. (3.3) and (3.5) with

$$v(\vec{q}) G_{\sigma\sigma'}(\vec{q}) = q^{-2} \int d\vec{r} e^{i\vec{q}\cdot\vec{r}} [-i\vec{q}\cdot\vec{\nabla} v(r)] [g_{\sigma\sigma'}(\vec{r}) - 1], \tag{3.8}$$

which is finite for $q = 0$.

It is interesting to compare the form of the integral above with the corresponding integral in Eq. (2.19) which appears in the third moment. We first notice that the coefficient of the ω^{-4} term in Eq. (3.5) is the third moment in the local field theory. Comparing with Eq. (2.28) and noticing that the "Einstein" term for the local field vanishes, we find that $G_{\sigma\sigma'}(\vec{q})$ has replaced $[\hat{q}\cdot \overleftrightarrow{\Gamma}_{\sigma\sigma'}(\vec{q})\cdot\hat{q}]$ except for a constant factor. The former is proportional to q^2 at small q while the latter goes to a finite value. This means that in the local-field theory all the partial moments go as q^4 whereas, in the exact moments, this is true only for the full density response and is the result of cancellations between the two terms in Eq. (2.28).

The translational invariance at small q is retained (3.7) even though its "Einstein" term has vanished. The explanation lies in remarks (a) and (b) above. It may also be phrased as follows: Each electron carries with it a rigid, symmetric correlation hole and the force on a particular electron arises from a displacement of other such *quasiparticles*. At equilibrium their density is uniform and a rigid displacement of all spin-up particles, for instance, will not create any force on the spin-down particles. This is the reason for the absence of a singular term in $M_{3,zz}$.

A similar assessment can be made of the theory of Ichimaru[29] which takes into consideration the effects of triplet correlations in $\langle n(1)n(2)\rangle$ but uses a static approximation for the triplet function. This has the effect of replacing the interparticle potential $v(r)$ by a screened one $\tilde{v}(\vec{r}) = \int d\vec{r}'\, v(\vec{r}+\vec{r}') \times s(\vec{r})$, where $s(\vec{r}) = \delta(\vec{r}) + n[g(\vec{r}) - 1]$.

There are various generalizations of the *Ansatz* in Eq. (3.6). We may write generally

$$\delta\langle n(1, t) n(3, t)\rangle = \int_{-\infty}^{t} dt' \int d(4)\, Q(1, 3, 4; t-t') \times \delta\langle n(4, t')\rangle, \tag{3.9}$$

where $Q(1, 3, 4; t-t')$ is the retarded response function of the equal time correlation function to a change in the local density. As before 1, 3 and 4 stand for both space and spin coordinates. This leads in general to a frequency-dependent local-field factor in Eq. (3.3), namely,

$$v(\vec{q}) G_{\sigma\sigma'}(\vec{q}, \omega) = -\frac{1}{q^2} \int \frac{d\vec{q}'}{(2\pi)^3} (\vec{q}\cdot\vec{q}') v(\vec{q}') \times \left(\sum_{\sigma''} \frac{1}{n_{\sigma''}} \overline{Q}_{\sigma\sigma''\sigma'} (\tfrac{1}{2}\vec{q} - \vec{q}', \vec{q}; \omega) \right), \tag{3.10}$$

where $Q(\vec{k}, \vec{q}; \omega)$ is the Fourier transform of $Q(\vec{r}_1, \vec{r}_3, \vec{r}_4; t-t')$ with respect to the variables $\vec{r}_3 - \vec{r}_1$, $\frac{1}{2}(\vec{r}_3 + \vec{r}_1) - \vec{r}_4$, and $(t-t')$, respectively. $\overline{Q}(\vec{k}, \vec{q}; \omega)$ is the corresponding quantity with the Hartree term $n_1\delta(3, 4)\delta(t-t')$ removed. Equation (3.10) differs from Eq. (3.8) in having the term in large parentheses replaced by $S_{\sigma\sigma'}(\vec{q}-\vec{q}') - 1$, which is the Fourier transform of $g_{\sigma\sigma'} - 1$. In order to get the correct third moments the term in large parentheses must, for $\omega\to\infty$, go as q^{-2} for small q. For $\omega\to 0$, on the other hand, this singular behavior must disappear in order to get a finite static spin susceptibility. Interpreting $\overline{Q}(1, 3, 4; t)$ as the response of the short-range pair correlation to a change in the local density does not immediately suggest such a singular behavior.

The *Ansatz* in Eq. (3.6) corresponds to choosing

$$Q(1, 3, 4; t) = \delta(t) g_{eg}(1, 3) [n_3\delta(1, 4) + n_1\delta(3, 4)]. \tag{3.11}$$

Vashishta and Singwi[11] have modified this to allow for the dependence of $g(r)$ on the density. This adds to Q a term

$$Q'(1, 3, 4; t) = n_1 n_3 \delta(t)\, \delta(\vec{R}(1, 3) - \vec{r}_4) \times \frac{\partial g^{eq}(1, 3; n)}{\partial n}, \tag{3.12}$$

where $\vec{R}(1, 3)$ is a somewhat arbitrarily chosen point at which to evaluate the density change in g. Their procedure seems to be well suited to get the static properties of the electron gas, like the static compressibility and the static pair-correlation function. In order to get the proper high-frequency response it is, however, essential to consider the response of the pair-correlation function to be noninstantaneous.

We conclude this section by making the remark that a local mean-field approach, where the effective potential acting on a particular particle depends only on the induced local mean density, does not seem suitable for handling high-frequency responses, not even if the local field factor $G_{\sigma\sigma'}(\vec{q}, \omega)$ is assumed to be frequency dependent, unless one is willing to let $G_{\sigma\sigma'}(\vec{q}, \omega)$ have a singular q dependence for small $\vec{q}$. It does not conveniently describe the short time *self-motion* of a particle relative to its correlation hole, and would therefore not give the "Einstein" term entering in the third moment. This will give an incorrect description of the transition from the high- to low-frequency response, particularly for the spin-response function.

IV. METHOD OF TOIGO AND WOODRUFF

In the theories discussed in Sec. III the interaction term in the appropriate equation of motion was factored into a local-field factor times $\delta\langle n(\vec{q}, \omega)\rangle$, where the local-field factor was assumed independent of the momenta of the electrons. Recently Toigo and Woodruff[16] have made a generalization in this respect by introducing a momentum-dependent local field factoring in the equation of motion for the individual component $n_{\vec{p}}(\vec{q}) = a^{\dagger}_{\vec{p}-\vec{q}/2}a_{\vec{p}+\vec{q}/2}$ of the density operator

$$n(\vec{q}) = \int e^{-i\vec{q}\cdot\vec{r}} n(\vec{r})\, d\vec{r} = \sum_{\vec{p}} n_{\vec{p}}(\vec{q}) . \tag{4.1}$$

They obtained an expression for the screened density response function of the form

$$\chi_{sc}(\vec{q}, \omega) = \chi^{(0)}(\vec{q}, \omega)/[1 - \overline{P}(\vec{q}, \omega)] , \tag{4.2}$$

where

$$\overline{P}(\vec{q}, \omega) = 2\sum_{\vec{p}} \frac{\overline{A}_{\vec{p}}(\vec{q})}{\omega - \vec{p}\cdot\vec{q}/m} , \tag{4.3}$$

and $\chi^{(0)}$ is, as before, the free-particle response function. The quantity $\overline{A}_{\vec{p}}(\vec{q})$ can be written in the form

$$\overline{A}_{\vec{p}}(\vec{q}) = (n^{(0)}_{\vec{p}+\vec{q}/2} - n^{(0)}_{\vec{p}-\vec{q}/2})\ v(\vec{q}) G_{\vec{p}}(\vec{q}) , \tag{4.4}$$

where $n^{(0)}_{\vec{p}}$ is the free-particle Fermi function and the $\vec{p}$-dependent local-field factor $G_{\vec{p}}(\vec{q})$ is given later in Eq. (4.35). The factor two in Eq. (4.3) comes from summing over the two spin states. If $G_{\vec{p}}(\vec{q})$ were independent of $\vec{p}$, we would recover the static local-field model discussed in Sec. III. Equation (4.2) can be brought into the form of Eq. (3.3a) by defining

$$v(\vec{q}) G_+(\vec{q}, \omega) \equiv -\overline{P}(\vec{q}, \omega)/\chi^{(0)}(\vec{q}, \omega) , \tag{4.5}$$

and it thus implies a frequency dependence in the local field factor G_+. Since any function of $\vec{q}$ and ω can be written in the form of Eq. (3.3a), thereby defining $G_+(\vec{q}, \omega)$, the frequency-dependent $G_+(\vec{q}, \omega)$ introduced via Eq. (4.5) does not necessarily mean an improvement in $\chi_{sc}(\vec{q}, \omega)$. For instance, it can be seen from Eqs. (4.3–4.5) that $\mathrm{Im}\overline{P}(\vec{q}, \omega)$ and $\mathrm{Im}\chi^{(0)}(\vec{q}, \omega)$ are nonzero in precisely the same region of $(\vec{q}, \omega)$, namely, for $\omega < m^{-1} q\,|p_F \pm \frac{1}{2} q\,|$, and the same holds for $\mathrm{Im}G_+(\vec{q},\omega)$ and for $\chi_{sc}(\vec{q}, \omega)$ itself. Therefore, the frequency dependence of the local-field factor in this case does not lead to any damping of long-wavelength plasmons. In this respect it does not lead to any improvement of the previous static local-field models.

In this section we will discuss some of the physical implications of the Toigo-Woodruff (TW) method. It will be shown that the procedure for determining $\overline{A}_{\vec{p}}(\vec{q})$ would satisfy the third moment if it were carried out exactly. On the other hand, there is no guarantee that the zeroth moment will be well satisfied (cf. Refs. 7–9 and 11), i.e., that

$$-\frac{\hbar}{n}\int_0^{\infty} \chi''_{nn}(\vec{q}, \omega)\frac{d\omega}{\pi} = S(\vec{q}) = 1 + n\int e^{-i\vec{q}\cdot\vec{r}}[g(\vec{r}) - 1]\, d\vec{r} . \tag{4.6}$$

The basic difference from the procedure in the above mentioned references seems to be that the latter use the zeroth moment to determine the local field factor, whereas TW use a quantity closely related to the third moment.

We shall extend the TW method to a spin- and $\vec{p}$-dependent local-field factorization, introducing a quantity $A_{\vec{p}\sigma\sigma'}(\vec{q})$ in such a way as to give the correct third moments $M_{3,\sigma\sigma'}(\vec{q})$ for the partial density response functions.[30] This local-field factor is appropriate for short times and it is assumed to hold approximately for all times. One consequence of this turns out to be that the singularity in $M_{3,zz}(\vec{q})$ at small q persists down to zero frequency and the resulting static spin susceptibility is zero. At the end of this section we will also show that some of the approximations made by TW in evaluating $\overline{A}_{\vec{p}}(\vec{q})$ of Eq. (4.4) can be avoided, with the result that the unperturbed occupation numbers $n^{(0)}_{\vec{p}}$ are replaced by the true average values $\langle n_{\vec{p}}\rangle$. This leads to somewhat less satisfactory values for the static compressibility than those obtained using $n^{(0)}_{\vec{p}}$. For the spin susceptibility the same approximation loses entirely the dominant q^2 term for small q and, therefore, violates the third moment.

Following Toigo and Woodruff, we start with the function

$$\chi_{\vec{p}\sigma}(\vec{q}, \sigma'; t) = (i\hbar)^{-1}\langle[n_{\vec{p}\sigma}(\vec{q}, t), n_{\sigma'}(-\vec{q}, 0)]\rangle\theta(t), \tag{4.7}$$

which gives the response of the density component $\langle a^{\dagger}_{\vec{p}-\vec{q}/2,\sigma}\, a_{\vec{p}+\vec{q}/2,\sigma}\rangle$ to an external spin-dependent potential $V_{\sigma'}(\vec{q}, t)$. In terms of $\chi_{\vec{p}\sigma}(\vec{q}, \sigma'; t)$ the partial density response functions are

$$\chi_{\sigma\sigma'}(\vec{q}, t) = \sum_{\vec{p}} \chi_{\vec{p}\sigma}(\vec{q}, \sigma'; t), \tag{4.8}$$

and, with the help of the continuity equation, the third moments can be written

$$M_{3,\sigma\sigma'}(\vec{q}) = -i\sum_{\vec{p}} \frac{\vec{q}\cdot\vec{p}}{m}\, \ddot{\chi}_{\vec{p}\sigma}(\vec{q}, \sigma'; 0+). \tag{4.9}$$

The equation of motion for $\chi_{\vec{p}\sigma}(\vec{q}, \sigma'; t)$ is

$$\left(i\frac{\partial}{\partial t} - \frac{\vec{p}\cdot\vec{q}}{m}\right)\chi_{\vec{p}\sigma}(\vec{q}, \sigma'; t) = \Omega^{-1}\delta_{\sigma\sigma'}\delta(t) \times\langle n_{\vec{p}-\vec{q}/2,\sigma} - n_{\vec{p}+\vec{q}/2,\sigma}\rangle + \Omega^{-1}{\sum_{\vec{k},\sigma''}}' v(\vec{k})\,\chi_{\vec{p}\sigma}(\vec{k}, \sigma'', \vec{q}, \sigma'; t) , \tag{4.10}$$

where $\sum'_{\vec{k}}$ means omitting $\vec{k} = 0$, and

$$\chi_{\vec{p}\sigma}(\vec{k},\sigma'',\vec{q},\sigma';t)\equiv(i\hbar\Omega)^{-1}\theta(t)$$
$$\times\langle[:(a^\dagger_{\vec{p}-\vec{q}/2,\sigma}(t)\,a_{\vec{p}-\vec{k}+\vec{q}/2,\sigma}(t)$$
$$-a^\dagger_{\vec{p}+\vec{k}-\vec{q}/2,\sigma}(t)\,a_{\vec{p}+\vec{q}/2,\sigma}(t))n_{\sigma''}(\vec{k},t):,\;n_{\sigma'}(-\vec{q},0)]\rangle\;, \tag{4.11}$$

where $:(\cdots):$ denotes normal ordering of the operators inside, that is, with the creation operators to the left. The last term in Eq. (4.10), which arises from the interaction between the particles, vanishes for $t=0^+$ [31] and we get the following initial values:

$$\chi_{\vec{p}\sigma}(\vec{q},\sigma';0^+)=-i\Omega^{-1}\delta_{\sigma\sigma'}\langle n_{\vec{p}-\vec{q}/2,\sigma}-n_{\vec{p}+\vec{q}/2,\sigma}\rangle\;;$$
$$\dot{\chi}_{\vec{p}\sigma}(\vec{q},\sigma';0^+)=-i(\vec{p}\cdot\vec{q}/m)\,\chi_{\vec{p}\sigma}(\vec{q},\sigma';0^+);$$
$$\ddot{\chi}_{\vec{p}\sigma}(\vec{q},\sigma';0^+)=-i(\vec{p}\cdot\vec{q}/m)\,\dot{\chi}_{\vec{p}\sigma}(\vec{q},\sigma';0^+)$$
$$-i\Omega^{-1}\sum_{\vec{k},\sigma''}v(\vec{k})\,\dot{\chi}_{\vec{p}\sigma}(\vec{k},\sigma'',\vec{q},\sigma';0^+)\;. \tag{4.12}$$

Inserting these in Eq. (4.9) yields

$$M_{3,\sigma\sigma'}(\vec{q})=\Omega^{-1}\delta_{\sigma\sigma'}\sum_{\vec{p}}\left(\frac{\vec{p}\cdot\vec{q}}{m}\right)^3\langle n_{\vec{p}-\vec{q}/2,\sigma}-n_{\vec{p}+\vec{q}/2,\sigma}\rangle$$
$$-\Omega^{-1}\sum_{\vec{p},\vec{k},\sigma''}\frac{\vec{p}\cdot\vec{q}}{m}\,v(\vec{k})\,\dot{\chi}_{\vec{p}\sigma}(\vec{k},\sigma'',\vec{q},\sigma';0^+)\;. \tag{4.13}$$

The first line of Eq. (4.13) is readily seen to agree with the kinetic part $M^T_{3,\sigma\sigma'}$ in Eq. (2.17), and by following the procedure in the Appendix it can be verified directly that the second line gives $M_{3,\sigma\sigma'}$.

Toigo and Woodruff considered only the total density response in the paramagnetic state to an ordinary spin-independent external potential and so summed Eq. (4.10) over σ'. They were particularly concerned with finding an appropriate approximation for the interaction term

$$\Omega^{-1}\sum_{\vec{k},\sigma',\sigma''}v(\vec{k})\,\chi_{\vec{p}\sigma}(\vec{k},\sigma'',\vec{q},\sigma';t)\;, \tag{4.14}$$

which they replaced by the approximate form

$$A_{\vec{p}}(\vec{q})\,\chi_{nn}(\vec{q},t)\,. \tag{4.15}$$

To determine $A_{\vec{p}}(\vec{q})$ they chose the condition that the first frequency moments of the two expressions should agree. This means equating the first-time derivatives at $t=0$, i.e.,

$$\Omega^{-1}\sum_{\vec{k},\sigma',\sigma''}v(\vec{k})\,\dot{\chi}_{\vec{p},\sigma}(\vec{k},\sigma'',\vec{q},\sigma';0^+)=A_{\vec{p}}(\vec{q})\,\dot{\chi}_{nn}(\vec{q},0^+). \tag{4.16}$$

Referring to Eq. (4.13) makes it clear that this approximation would give the correct value for the third moment of the density response function, provided the left hand side of Eq. (4.16) were evaluated exactly. The quantities in Eqs. (4.14) and (4.15) both have the initial value zero and they have, by condition (4.16), the same first time derivatives for $t=0^+$. The basic approximation of *TW* is to assume them equal for all times.

When Eq. (4.10) is summed over σ,σ' and the expression (4.15) is inserted, the resulting equation is easily solved for χ_{nn} and χ_{sc}. The expressions so obtained are

$$\chi_{nn}(\vec{q},\omega)=\chi^{(f)}(\vec{q},\omega)/[1-P(\vec{q},\omega)]\;; \tag{4.17}$$

$$\chi_{sc}(\vec{q},\omega)=\chi^{(f)}(\vec{q},\omega)/[1-\overline{P}(\vec{q},\omega)], \tag{4.18}$$

where

$$\chi^{(f)}(\vec{q},\omega)=2\Omega^{-1}\sum_{\vec{p}}\frac{\langle n_{\vec{p}-\vec{q}/2}-n_{\vec{p}+\vec{q}/2}\rangle}{\omega-\vec{p}\cdot\vec{q}/m} \tag{4.19}$$

is the density response function for a system of *noninteracting* particles with the same momentum distribution as in the interacting system, and

$$P(\vec{q},\omega)=2\sum_{\vec{p}}\frac{A_{\vec{p}}(\vec{q})}{\omega-\vec{p}\cdot\vec{q}/m} \tag{4.20}$$

$$\equiv\overline{P}(\vec{q},\omega)+v(\vec{q})\,\chi^{(f)}(\vec{q},\omega)\;\;. \tag{4.21}$$

Equation (4.21) can be written in the form of Eq. (4.3) by defining

$$\overline{A}_{\vec{p}}(\vec{q})=A_{\vec{p}}(\vec{q})-\Omega^{-1}\langle n_{\vec{p}-\vec{q}/2}-n_{\vec{p}+\vec{q}/2}\rangle\,v(\vec{q})\;. \tag{4.22}$$

The subtracted term is the RPA or Hartree field. Equation (4.18) differs from TW's results, given in Eq. (4.2), by having $\chi^{(f)}$, which contains the true mean occupation numbers $\langle n_{\vec{p}}\rangle$, in place of $\chi^{(0)}$ which contains $n^{(0)}_{\vec{p}}$.

The same method can be applied to the partial density response functions. The last term in Eq. (4.10) is now replaced by the approximate form

$$\sum_{\sigma''}A_{\vec{p}\sigma\sigma''}(\vec{q})\,\chi_{\sigma''\sigma'}(\vec{q},t)\;\;, \tag{4.23}$$

where, in analogy to Eq. (4.16), the coefficients $A_{\vec{p}\sigma\sigma'}(\vec{q})$ are determined from the condition

$$\Omega^{-1}\sum_{\vec{k},\sigma''}v(\vec{k})\,\dot{\chi}_{\vec{p}\sigma}(\vec{k},\sigma'',\vec{q},\sigma';0^+)$$
$$=\sum_{\sigma''}A_{\vec{p}\sigma\sigma''}(\vec{q})\,\dot{\chi}_{\sigma''\sigma'}(\vec{q},0^+)$$
$$=A_{\vec{p}\sigma\sigma'}(\vec{q})\,n_\sigma q^2/m\,. \tag{4.24}$$

The evaluation of the left-hand side of Eq. (4.24) is discussed in the Appendix. The RPA term comes from the $\vec{k}=\vec{q}$ term in Eq. (4.24) and it can be split off from the rest by introducing new coefficients $\overline{A}_{\vec{p}\sigma\sigma'}(\vec{q})$ as in Eq. (4.22)

$$\overline{A}_{\vec{p}\sigma\sigma'}(q)=A_{\vec{p}\sigma\sigma'}(q)-\Omega^{-1}\langle n_{\vec{p}-\vec{q}/2,\sigma}-n_{\vec{p}+\vec{q}/2,\sigma}\rangle\,v(\vec{q})\;\;. \tag{4.25}$$

Equation (4.13) shows as before that the approximation in Eq. (4.23) together with Eq. (4.24) would guarantee the correct third partial moments $M_{3,\sigma\sigma'}(\vec{q})$, if the left-hand side of Eq. (4.24) were evaluated exactly. The resulting equation for $\chi_{\sigma\sigma'}$ is

$$\chi_{\sigma\sigma'}(\vec{q},\omega)=\delta_{\sigma\sigma'}\chi_{\sigma}^{(f)}(\vec{q},\omega)+\sum_{\sigma''}[\overline{P}_{\sigma\sigma''}(\vec{q},\omega)+v(\vec{q})\chi_{\sigma}^{(f)}(\vec{q},\omega)]\chi_{\sigma''\sigma'}(\vec{q},\omega)\ , \qquad (4.26)$$

where

$$\chi_{\sigma}^{(f)}(\vec{q},\omega)=\Omega^{-1}\sum_{\vec{p}}\left[\frac{\langle n_{\vec{p}-\vec{q}/2,\sigma}-n_{\vec{p}+\vec{q}/2,\sigma}\rangle}{\omega-\vec{p}\cdot\vec{q}/m}\right] \qquad (4.27)$$

and

$$\overline{P}_{\sigma\sigma'}(\vec{q},\omega)=\sum_{\vec{p}}\frac{\overline{A}_{\vec{p}\sigma\sigma'}(\vec{q})}{\omega-\vec{p}\cdot\vec{q}/m}\quad . \qquad (4.28)$$

Equation (4.26) is a 2×2 matrix equation in the indices σ, σ'. For the paramagnetic state the forms of the screened density response and the spin-density response obtained from it are similar to those in Eqs. (3.3), namely,

$$\chi_{sc}=\chi^{(f)}(1-\overline{P}_{+})^{-1}\ \text{ and }\ \chi_{zz}=\chi^{(f)}(1-\overline{P}_{-})^{-1}\ , \qquad (4.29)$$

where

$$\overline{P}_{\pm}(\vec{q},\omega)=\overline{P}_{\uparrow\uparrow}(\vec{q},\omega)\pm\overline{P}_{\uparrow\downarrow}(\vec{q},\omega)\ . \qquad (4.30)$$

Let us first consider the spin-response function. For $\omega=0$ we have, from Eq. (4.28),

$$\overline{P}_{-}(\vec{q},0)=-\sum_{\vec{p}}\left(\frac{\vec{p}\cdot\vec{q}}{m}\right)^{-1}[\overline{A}_{\vec{p}\uparrow\uparrow}(\vec{q})-\overline{A}_{\vec{p}\uparrow\downarrow}(\vec{q})]\ . \qquad (4.31)$$

This is to be compared with the corresponding expression for the third moment:

$$M_{3,zz}^{P}(\vec{q})=\frac{nq^2}{m}\sum_{\vec{p}}\frac{\vec{p}\cdot\vec{q}}{m}[\overline{A}_{\vec{p}\uparrow\uparrow}(\vec{q})-\overline{A}_{\vec{p}\uparrow\downarrow}(\vec{q})]\ . \qquad (4.32)$$

Since $M_{3,zz}^{P}(\vec{q})$ is proportional to q^2 for small q, the sum in Eq. (4.32) has a nonzero limit for $\vec{q}=0$. Correspondingly $\overline{P}(\vec{q},0)$ is proportional to q^{-2} so that the $\vec{q}=0$ static spin susceptibility is zero. The similar structure of Eqs. (4.31) and (4.32) shows clearly that the reason for this unphysical result is that the $\vec{p}$-dependent local field approximation in Eq. (4.23) forces the same type of structure on the short- and long-time behavior of the interaction between a particle and its surroundings.

Since $\overline{M}_{3,nn}^{P}(\vec{q})$ $[=M_{3,sc}^{P}(\vec{q})$; cf. Eq. (2.29)] is proportional to q^4 for small q, $\overline{P}_{+}(\vec{q},0)$ has a finite limit for $\vec{q}=0$. On comparing Eqs. (4.16) and (4.24) one sees that

$$\overline{A}_{\vec{p}\uparrow\uparrow}(\vec{q})+\overline{A}_{\vec{p}\uparrow\downarrow}(\vec{q})=2\overline{A}_{\vec{p}}(\vec{q})\ , \qquad (4.33)$$

so that $\overline{P}_{+}(\vec{q},\omega)$ is the same as $\overline{P}(\vec{q},\omega)$ in Eq. (4.21). This means that the same density response is obtained from the TW approximation in Eq. (4.15) as from the spin-dependent local field in Eq. (4.23). If the exact expression for $\overline{A}_{\vec{p}\sigma\sigma'}(\vec{q})$, which is given in Eqs. (A4)–(A6) of the Appendix, is evaluated by making the additional factorization approximation,

$$\langle a_1^\dagger a_2^\dagger a_3 a_4\rangle\cong\langle a_1^\dagger a_4\rangle\langle a_2^\dagger a_3\rangle-\langle a_1^\dagger a_3\rangle\langle a_2^\dagger a_4\rangle\ , \qquad (4.34)$$

the result is

$$\overline{A}_{\vec{p}}(\vec{q})\cong\langle n_{\vec{p}-\vec{q}/2}-n_{\vec{p}+\vec{q}/2}\rangle(nq^2\Omega)^{-1}\times\sum_{\vec{k}}v(\vec{k})(\vec{q}\cdot\vec{k})\langle n_{\vec{p}+\vec{k}-\vec{q}/2}-n_{\vec{p}+\vec{k}+\vec{q}/2}\rangle\ . \qquad (4.35)$$

This is precisely the form obtained by Toigo and Woodruff, who used the same factorization as above. However, at an earlier stage they made an approximation in evaluating the left-hand side of Eq. (4.16), using only the Hamiltonian for a noninteracting system. This means that $\langle n_{\vec{p}}\rangle$ is replaced by the Fermi function $n_{\vec{p}}^{(0)}$ in Eq. (4.35). The replacement of $\langle n_{\vec{p}}\rangle$ by $n_{\vec{p}}^{(0)}$ in both $\chi^{(f)}$ and P_{+} in Eq. (4.29) can have a significant numerical effect on χ_{sc}. Consider the static compressibility ratio

$$\frac{\kappa_0}{\kappa}=\lim_{q\to 0}\frac{\chi^{(0)}(\vec{q},0)}{\chi_{sc}(\vec{q},0)}\ . \qquad (4.36)$$

From Eqs. (4.28)–(4.29) and (4.35) we get after some algebra

$$\kappa_0/\kappa=(1-\tfrac{1}{4}\rho^2\lambda)/\rho\ , \qquad (4.37)$$

where

$$\rho=-\frac{1}{p_F}\int_0^\infty\frac{d\langle n_p\rangle}{dp}\,p\,dp\le 1\ ,$$

and $\lambda=k_{\mathrm{TF}}^2/p_F^2=0.663r_s$, k_{TF} being the Thomas-Fermi wave vector. Setting $\langle n_p\rangle=n_p^{(0)}$ gives $\rho=1$ and

$$\kappa_0/\kappa=1-\tfrac{1}{4}\lambda\ , \qquad (4.38)$$

the result obtained by Toigo and Woodruff; and this is also the result obtained from differentiating the Hartree-Fock energy. This value is slightly higher than the best values obtained when the correlation energy is included. The effect of ρ in Eq. (4.37) is to raise the value of κ_0/κ. For example, for $r_s=5$, ρ is estimated[32] to be 0.92 and $\kappa_0/\kappa=1.9\ \kappa_0/\kappa_{\mathrm{TW}}$. Therefore, the static properties are not as well reproduced as it might appear from Ref. 16(a), when a more consistent evaluation of the approximation in Eqs. (4.15) and (4.16) is made. This is not unreasonable since the TW procedure is based on satisfying the equation of motion at short times. This is opposite to the Vashishta-Singwi procedure,[11] which is based on a long-time approximation. Similarly, following TW for spin susceptibility gives the value obtained from differentiating the Hartree-Fock energy with respect to the magnetization.[33] The factorization in

Eq. (4.34), therefore, gives a result which contradicts the exact property of $\bar{P}_{-}(\vec{q}, 0)$ in Eq. (4.31).

The factorization (4.34) evidently has some relation to the Hartree-Fock picture. It leads to local field coefficients $\bar{A}_{\vec{p}\sigma\sigma'}(\vec{q})$ which vanish for antiparallel spins (see Appendix). Also the third moment $M^{P}_{3,\sigma\sigma'}(\vec{q})$ is given by Eq. (2.18) where now the density correlation function in Eq. (2.19) has the Hartree-Fock factored form

$$\langle n_\sigma(0) n_{\sigma'}(\vec{r})\rangle = n_\sigma n_{\sigma'}\, g_{\sigma\sigma'}(\vec{r})\,,$$
$$= n_\sigma n_{\sigma'} - \delta_{\sigma\sigma'}\,|\langle \psi^\dagger_\sigma(0)\psi_\sigma(\vec{r})\rangle|^2\,. \qquad (4.39)$$

The Fourier transform of $\lambda_{\sigma\sigma'}(r) = g_{\sigma\sigma'}(r) - 1$ is

$$\lambda_{\sigma\sigma'}(q) = -\frac{2}{n_\sigma^2}\,\delta_{\sigma\sigma'}\int \frac{d\vec{p}}{(2\pi)^3}\,\langle n_{\vec{p}\sigma}\rangle\langle n_{\vec{p}+\vec{q},\sigma'}\rangle\,, \qquad (4.40)$$

which corresponds precisely to the exchange hole for noninteracting particles with the momentum distribution $\langle n_{\vec{p}\sigma}\rangle$. The short-time pair correlations which are contained in Eq. (4.35) or Eqs. (A7)–(A8) are therefore due just to the exchange hole. Here, this approximation is made, of course, at a different stage in the calculation from what is done in the ordinary Hartree-Fock approximation for the density response functions. There Eq. (4.34) would be applied directly to the interaction term on the second line of Eq. (4.10). The latter approximation is usually called the generalized RPA and, like the RPA, it is still a weak coupling theory and would presumably give a poor prediction of short-range correlations.[34]

The long-time density response predicted by Eq. (4.35) must include some adjustment of the exchange hole to the change in local density. This follows from the facts that Eqs. (4.37) and (4.38) have the same structure and that by differentiating E_{HF} one explicitly includes the density dependence to the exchange hole. This is also consistent with the observation in Ref. 11 that using $g^{\mathrm{HF}}(\vec{r})$ in the density-dependent local field of Eqs. (3.11) and (3.12) also gives the Hartree-Fock value of the static compressibility.

V. REMARKS ON THE LANDAU FERMI-LIQUID THEORY

The different high-frequency behavior of the density and spin-density response at long wavelength raises the question of whether the domain of validity of the Landau theory of Fermi liquids may be different for density and spin-density fluctuations. Safir and Widom[17] have suggested that the Landau theory may not be applicable to spin-density fluctuations. In this section we make a more conservative restatement of the implications of the sum rules for the Landau theory.

This theory assumes that for sufficiently small q and ω the response is dominated by single quasiparticle and quasi-hole-pair excitations and coherent superposition of these. The quasiparticles and quasiholes interact through static $f_{\vec{p}\vec{p}'}$ parameters. In this sense it is similar to the mean-field theories discussed above. The response of the internal structure of a quasiparticle is not considered. Such response would correspond actually to multipair excitations.

TABLE I. Matrix elements, excitation energies, and sum-rule contributions to $S_{\sigma\sigma}(\vec{q}, \omega)$ in the long-wavelength limit. The values in parentheses refer to $S_{nn}(\vec{q}, \omega)$ The table also applies to $S_{zz}(\vec{q}, \omega)$ if $n_\sigma(\vec{q})$ is replaced by $S_z(\vec{q})$ in the first column. $\bar{\omega}$ is an average excitation frequency for multipair states of zero total momentum, and s is the velocity of the collective mode if it exists.

	Single pair	Collective mode	Multipair Translation invariance	Multipair No transl. invariance
$\langle m\,\vert\, n_\sigma(\vec{q})\,\vert\, 0\rangle$	1	$q^{1/2}$	$q(q^2)$	q
ω_{m0}	qv_F	qs	$\bar{\omega}$	$\bar{\omega}$
Pauli principle restriction	q/p_F	...	...	...
$\sum_m \vert\langle m\,\vert\, n_\sigma(\vec{q})\,\vert\, 0\rangle\vert^2(\omega_{m0})^l$	q^{l+1}	q^{l+1}	$q^2(q^4)$	q^2
$l=-1, 0, 1, \cdots$				

In support of the above assumptions, Pines and Nozières have given a table of the contribution at small q from different kinds of excitations to the low-order moments of the dynamic density correlation function $S_{nn}(\vec{q}, \omega)$ for a system of neutral fermions.[35] At zero temperature this quantity is equal to $-\chi''_{nn}(\vec{q}, \omega)/\pi$ for $\omega > 0$ and is zero for $\omega < 0$. Therefore, the odd moments of S_{nn} and χ_{nn} are the same but S_{nn} has even moments also.

Their table would be different for the partial density correlation functions and for the spin-density correlation function S_{zz}. To show this we list in Table I the corresponding contributions to the positive moments of $S_{\sigma\sigma}(\vec{q}, \omega)$, the density correlation function for particles of the same spin σ, again for neutral fermions. This particular component is similar to S_{nn} in that it is non-negative and is related to the response function $\chi_{\sigma\sigma}$ in the same way as S_{nn} is to χ_{nn}. Table I applies to S_{zz} also.

Multipair excitations contribute to the order q^2 to the moments of $S_{\sigma\sigma}$ whereas they contribute to order q^4 to the moments of S_{nn} and, therefore, are significant only in the third and higher moments. The difference lies in the matrix elements

$$\langle m|\,n_\sigma(\vec{q})|\,0\rangle = \vec{q}\cdot\langle m|\,\vec{J}_\sigma(\vec{q})|\,0\rangle/\omega_{m0}\,, \qquad (5.1)$$

where $|0\rangle$ and $|m\rangle$ are the ground state and some excited state, respectively, and $\hbar\omega_{m0}$ is the excitation energy. For a multipair state $|m\rangle$ it follows from conservation of total momentum that

$\langle m|\vec{J}(\vec{q})|0\rangle \to 0$ as $\vec{q}\to 0$.[35] On the other hand, the momenta $\vec{P}_\sigma = m\vec{J}_\sigma(0)$ of the separate spin densities are not conserved so that $\langle m|\vec{J}_\sigma(0)|0\rangle \neq 0$. [In Table I of Ref. 17 it seems to have been assumed that multipair excitations contribute in the same way to both S_{nn} and S_{zz}, which is evidently not the case. Their table, if right, would imply that $M_{3,zz}(\vec{q})$ would have to go as q^4 for small q instead of q^2 as found.] Table I shows that the f-sum rule ($l=1$) for S_{nn} is exhausted by single-pair excitations and coherent superpositions of these (collective modes), whereas this is not true for S_{zz}. This is brought out by the Landau theory itself, which predicts, for $\omega/qk_F \gg 1$,

$$\chi_{nn}(\vec{q},\omega)\sim nq^2/m\omega^2\ , \quad \chi_{zz}(\vec{q},\omega)\sim nq^2/m^*\omega^2\ , \tag{5.2}$$

m^* being the effective mass. The correct asymptotic form of χ_{zz} is $nq^2/m\omega^2$ [recall Eqs. (2.3)–(2.4)], and the difference between this and that in Eq. (5.2) has to come from multipair excitations.

The role of momentum conservation in differentiating between χ_{nn} and χ_{zz} is connected of course with the different ways the up- and down-spin subsystems move under the influence of a spin-independent and a spin-dependent external disturbance, as described in Sec. II. In the spin response there is a net rate of momentum transfer between the subsystems and at the same time there occurs a dynamic adjustment of the correlation hole of particles with opposite spins, when the two subsystems move relative to each other. This dynamical effect is not taken into account in the Landau theory and it shows up in the f-sum rule for the spin response function. The above remarks are already contained in the work of Leggett.[36]

Table I and the table in Ref. 35 say nothing directly about the domain of validity of the assumption of the Landau theory. This is because they do not show where or how the transition from high- to low-frequency behavior occurs. The fact that the Landau-theory excitations exhaust the f sum for S_{nn} for a pure Fermion system with no external interactions is really a special case and does not apply, for example, to S_{nn} for ^{3}He-^{4}He mixtures nor to electrons in metals.

VI. NUMERICAL CALCULATIONS

We are at present unable to suggest a more proper model for the electric and magnetic response functions, which would be consistent with the third moments and also be valid for low frequencies. Nevertheless, we would like to have some idea of the changes to be expected from such a model and for this reason we shall consider a simple interpolation scheme. We assume a frequency-dependent local-field factor of the following form

$$G_\pm(\vec{q},\omega) = G_\pm(\vec{q},\infty) + \xi(\omega)[G_\pm(\vec{q},0) - G_\pm(\vec{q},\infty)]\ , \tag{6.1}$$

where $\xi(\omega)$ is a certain relaxation function, and $G_\pm(\vec{q},\infty)$ and $G_\pm(\vec{q},0)$ are the limiting values of the local field factors. We choose

$$\xi(\omega) = (1 - i\omega\tau)^{-1} \tag{6.2}$$

with $\tau \sim 1/\omega_p$.

Comparing Eq. (3.5) with the moment expansion suggests taking

$$\begin{aligned} G_+(\vec{q},\infty) &= -(m/nq^2\omega_p^2)M^P_{3,nn}(\vec{q})\ ,\\ G_-(\vec{q},\infty) &= -(m/nq^2\omega_p^2)M^P_{3,zz}(\vec{q})\ . \end{aligned} \tag{6.3}$$

The kinetic part $[M_3^T(\vec{q}) - M_3^{(0)}(\vec{q})]$ is not included in the local field factor. It would give $G\propto q^2$ for large q and this would lead to a divergence in the pair-correlation functions for $r\to 0$. We argue that this contribution to the moment should instead be connected with a modification of $\chi^{(0)}(\vec{q},\omega)$ as, for example, in the appearance of $\chi^{(f)}(\vec{q},\omega)$ in the Toigo-Woodrull procedure.

For $G_+(\vec{q},0)$ we adopt the expression given by Vashista and Singwi,[11]

$$G_+(\vec{q},0) = \left(1 + an\frac{\partial}{\partial n}\right)G^I(\vec{q})\ , \tag{6.4}$$

where $a\approx\frac{2}{3}$ and $G^I(\vec{q})$ is given by Eq. (3.8) with $g_{\sigma\sigma'}(r)$ replaced by $g(r)$. This expression seems to give a good description of the low-frequency response. For $G_-(\vec{q},0)$ we use the semiempirical formula

$$G_-(\vec{q},0) = \gamma_-^0(q/p_F)^2 I(q)/I(0)\ , \tag{6.5}$$

where $I(q)/I(0)$ is taken from the calculation in Ref. (9) and γ_-^0 is chosen to give the long-wavelength static susceptibility.[37] In Ref. 38 an expression of the form of Eq. (6.5) is shown to lead to reasonable values of the Korringa constant and nuclear-spin-relaxation rate in alkali metals.

For small q the expressions (6.3)–(6.5) reduce to

$$\begin{aligned} &G_+(\vec{q},\infty)\to\gamma_+^\infty(q/p_F)^2\ , && G_+(\vec{q},0)\to\gamma_+^0(q/p_F)^2\ ,\\ &G_-(\vec{q},\infty)\to -\tfrac{1}{3}[1-g_{\uparrow\downarrow}(0)]\ , && G_-(\vec{q},0)\to\gamma_-^0(q/p_F)^2\ , \end{aligned} \tag{6.6}$$

where

$$\gamma_+^\infty = \frac{-1}{5p_F}\int_0^\infty [S(k)-1]\,dk$$

and

$$\gamma_+^0 = \tfrac{5}{2}p_F^2\left(1 + an\frac{\partial}{\partial n}\right)p_F^{-2}\gamma_+^\infty$$

are the same as $\frac{2}{5}\bar{\gamma}$ and γ in Tables I and III respectively, of Ref. 11, while

TABLE II. Values of the coefficients γ_+^∞, γ_+^0, and γ_-^0 for various r_s.

r_s	1	2	3	4	5	6
γ_+^∞	0.18	0.20	0.20	0.22	0.22	0.23
γ_+^0	0.24	0.26	0.27	0.28	0.29	0.30
γ_-^0	0.20	0.17	0.16	0.14	0.13	0.12
$\gamma_+^0-\gamma_+^\infty$	0.06	0.06	0.07	0.07	0.08	0.08

$$\gamma_-^\infty=\frac{-1}{5p_F}\int_0^\infty [\tilde{S}(k)-1]\,dk\,.$$

These coefficients are listed in Table II for different values of r_s.

For large q some simple calculations give

$$\begin{aligned} &G_+(\vec{q},\infty)\to\tfrac{2}{3}[1-\tfrac{1}{2}g_{\uparrow\downarrow}(0)],\\ &G_-(\vec{q},\infty)\to-\tfrac{1}{3}[1-2g_{\uparrow\downarrow}(0)],\\ &G_+(\vec{q},0)\to\left(1+an\frac{\partial}{\partial n}\right)[1-\tfrac{1}{2}g_{\uparrow\downarrow}(0)],\\ &G_-(\vec{q},0)\sim-\tilde{g}(0)=\tfrac{1}{2}g_{\uparrow\downarrow}(0)\,, \end{aligned} \tag{6.7}$$

where we have put $g_{\uparrow\uparrow}(0)=0$. From Eqs. (6.6), (6.7), and the fact that $g_{\uparrow\downarrow}(0)\approx 0$ for $r_s>4$, we may expect that $G_-(\vec{q},\infty)$ will be close to the value $-\frac{1}{3}$ for all q.

A. Dielectric Response

We notice that $G_+(\vec{q},\infty)$ is not very different from $G_+(\vec{q},0)$ which was used by Vashishta and Singwi. Both G's are proportional to $(q/p_F)^2$ for small q and the proportionality factors differ by about 30%. Their asymptotic values at larger q differ by roughly the same amount. Therefore, we do not expect large changes in the dielectic response and it is difficult to know whether or not the frequency dependence in Eq. (2.1) leads to an improvement without carrying out more extensive calculations.

However, there is one significant change. Owing to the relaxation effects built into the interpolation (6.1), plasma waves are now damped at long wavelength. The plasma dispersion becomes

$$\omega=\omega_p[1+\alpha(q/p_F)^2+\cdots]\;, \tag{6.8}$$

with

$$\mathrm{Re}\,\alpha=\mathrm{Re}\,\alpha_{\mathrm{RPA}}-\tfrac{1}{2}\gamma_+^0+\tfrac{1}{2}(\gamma_+^0-\gamma_+^\infty)\frac{(\omega_p\tau)^2}{1+(\omega_p\tau)^2}\,, \tag{6.9a}$$

$$\mathrm{Im}\,\alpha=-\tfrac{1}{2}(\gamma_+^0-\gamma_+^\infty)\frac{\omega_p\tau}{1+(\omega_p\tau)^2}\,. \tag{6.9b}$$

The dispersion curve is somewhat closer to the RPA value than that given by Vashishta and Singwi, but the change is small. For $\tau\sim\omega_p^{-1}$ the values of $-\mathrm{Im}\,\alpha$ are 0.015 and 0.017 for Al and Na, respectively, in good agreement with the plasmon damping rates calculated by Hasegawa and Watabe[39] and by DuBois and Kivelson.[40] ($-\mathrm{Im}\,\alpha$ is the same as $\frac{1}{2}b$ in Table III of Ref. 39.) They used diagram techniques and included multiple electron-hole excitations, which corresponds in our language to including the relaxation of the local field. The numerical agreement suggests that, for small q at least, the relaxation time is of order ω_p^{-1}. The above calculated values of the plasmon damping are significantly smaller then experimental values[41–43] and damping mechanisms involving the lattice appear to dominate.[40,44] The neglect in our calculation of the kinetic contribution to the third moment can have a significant effect on the values of α. How it should affect the plasmon damping is not clear, in view of the remark below Eq. (6.3). Since the change in M_3^T is accounted for by using $\chi^{(f)}(\vec{q},\omega)$, its effect on the plasmon frequency can be estimated by replacing $\langle v^2\rangle^{(0)}$ in α_{RPA} by $\langle v^2\rangle$. The increase in $\mathrm{Re}\,\alpha$ cancels most of the γ-term contribution in (6.9a) and gives a dispersion curve much closer to the RPA curve.

B. Magnetic Response

The major change will enter in the magnetic response, where the two limiting local field factors are very different. For the static response we get the same result as in Ref. 9, except for the adjustment of the long-wavelength limit. With a static local field factor, as in Ref. 9, the spectral function, $\mathrm{Im}\chi_{zz}$, vanishes where $\mathrm{Im}\chi^{(0)}$ does and for long wavelengths this happens for $\omega>qv_F$. In our extrapolation model, on the other hand, this is not true and for small wave vectors we have approximately $(\omega>qv_F)$

$$\mathrm{Im}\chi_{zz}(q,\omega)=-\frac{nq^2}{m\omega_s^2}\,\frac{1}{\omega\tau} \tag{6.10}$$

for $\omega\ll 1/\tau$ and $\omega_s\tau$ small, and

$$\mathrm{Im}\chi_{zz}(q,\omega)=-\frac{nq^2}{m\omega_s^2}\,\frac{1/\omega\tau}{[(\omega/\omega_s)^2-1]^2+(1/\omega\tau)^2} \tag{6.11}$$

for $\omega\gg 1/\tau$. Thus, for $\omega_s\tau>1$ we get a resonance peak around $\omega=\omega_s$ $(\approx\omega_p/\sqrt{3})$. In Fig. 1 is shown as an illustration the spectral function for $q=0.2p_F$ and with $\tau=1/\omega_p$. The result is compared with that obtained from the model in Ref. 9. The two curves differ significantly but the difference would decrease as we go to larger wave vectors. We recall that

$$\chi_{zz}(\vec{q},0)=\frac{1}{\pi}\int_0^\infty \mathrm{Im}\chi_{zz}(\vec{q},\omega)\,\frac{d\omega}{\omega}\,, \tag{6.12}$$

and this means that the two curves give the same value for the integral above. Figure 2 shows the spectral function for $q=0.1p_F$ and with $\tau=1/\omega_p$ and

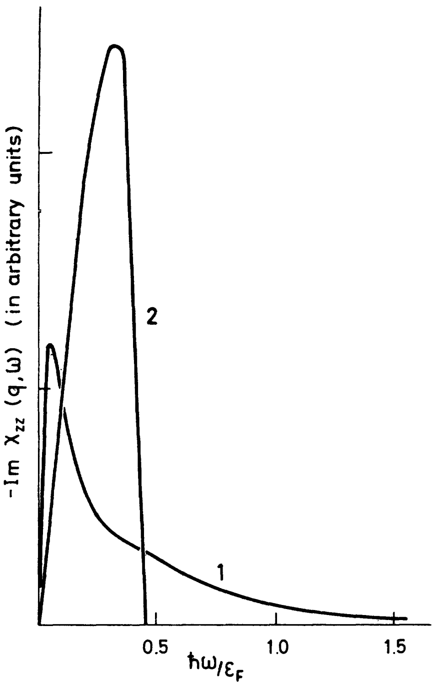

FIG. 1. Magnetic spectral function $\mathrm{Im}\chi_{zz}(\vec{q}, \omega)$ for $q = 0.2p_F$ and $r_s = 4$ with the frequency-dependent local-field factor $G_-(\vec{q}, \omega)$ (curve 1) and with the frequency-independent one $G_-(\vec{q}, 0)$ (curve 2).

$\tau = 2/\omega_p$. In the latter case we see the beginning of a resonance peak.

An important test of the accuracy of the response functions is obtained through the static pair-correlation functions $g_{\uparrow\uparrow}(r)$ and $g_{\uparrow\downarrow}(r)$. We have found them sensitive to the detailed form of the local field factor and to the choice of τ. At present there is no clear indication that our extrapolation scheme would remedy the existing defects in the pair-correlation functions, as shown in Ref. (9). Our calculation gives a significant change in the magnetic response, whereas the change in the dielectric response is much less pronounced. A basic remaining problem is to understand in more detail how the relaxation of the local field actually occurs.

ACKNOWLEDGMENT

We would like to thank M. Olle Gunnarsson for carrying out some of the numerical calculations.

APPENDIX: EVALUATION OF $A_{\vec{p}\sigma\sigma'}(\vec{q})$

The time derivative on the left-hand side of Eq. (4.16) can be evaluated by differentiating Eq. (4.11), transferring the time derivative over to $n_{\sigma'}(-\vec{q}, 0)$ and finally using the continuity equation. This gives

$$\dot{\chi}_{\vec{p}\sigma}(\vec{k}, \sigma'', \vec{q}, \sigma'; 0^+) = (i\hbar\Omega)^{-1}$$

$$\times\langle [:\cdots:, -i\vec{q}\cdot\vec{J}_{\sigma'}(-\vec{q})]\rangle, \quad \text{(A1)}$$

where

$$\vec{J}_{\sigma'}(-\vec{q}) = \sum_{\vec{p}'} \frac{\vec{p}'}{m} a^\dagger_{\vec{p}'+\vec{q}/2,\sigma'} a_{\vec{p}'-\vec{q}/2,\sigma'} . \quad \text{(A2)}$$

The commutators in Eq. (A1) are readily evaluated with the help of the following relations:

$$[a_{\vec{p}+\vec{q}/2,\sigma}, \vec{q}\cdot\vec{J}_{\sigma'}(-\vec{q})] = \delta_{\sigma\sigma'}(\vec{q}\cdot\vec{p}/m)\, a_{\vec{p}-\vec{q}/2,\sigma},$$

$$[a^\dagger_{\vec{p}-\vec{q}/2,\sigma}, \vec{q}\cdot\vec{J}_{\sigma'}(-\vec{q})] = -\delta_{\sigma\sigma'}(\vec{q}\cdot\vec{p}/m)\, a^\dagger_{\vec{p}+\vec{q}/2,\sigma},$$

$$[n_{\sigma''}(\vec{k}), \vec{q}\cdot\vec{J}_{\sigma'}(-\vec{q})] = \delta_{\sigma''\sigma'}(\vec{q}\cdot\vec{k}/m) n_{\sigma'}(\vec{k}-\vec{q}).$$

The resulting form of the condition (4.24), after inserting the above, is

$$(n_{\sigma'} q^2/m) A_{\vec{p}\sigma\sigma'}(\vec{q}) = \delta_{\sigma\sigma'} B_{\vec{p}\sigma}(\vec{q}) + C_{\vec{p}\sigma\sigma'}(\vec{q}), \quad \text{(A3)}$$

where

$$B_{\vec{p}\sigma}(\vec{q}) = -(m\Omega^2)^{-1} \sum_{\vec{k}\neq 0} v(\vec{k}) \langle :([\vec{p}\cdot\vec{q}\,] a^\dagger_{\vec{p}+\vec{q}/2,\sigma} a_{\vec{p}-\vec{k}+\vec{q}/2,\sigma}$$

$$- [(\vec{p}-\vec{k})\cdot\vec{q}\,] a^\dagger_{\vec{p}-\vec{q}/2,\sigma} a_{\vec{p}-\vec{k}-\vec{q}/2,\sigma}$$

$$- \text{corresponding terms with } \vec{p} \to \vec{p}+\vec{k})\, n(\vec{k}) :\rangle, \quad \text{(A4)}$$

and

$$C_{\vec{p}\sigma\sigma'}(\vec{q}) = m n_{\sigma'} \Omega^{-1} q^2 v(\vec{q}) \langle n_{\vec{p}-\vec{q}/2,\sigma} - n_{\vec{p}+\vec{q}/2,\sigma}\rangle + \overline{C}_{\vec{p}\sigma\sigma'}(\vec{q}), \quad \text{(A5)}$$

with

$$\overline{C}_{\vec{p}\sigma\sigma'}(\vec{q}) = (m\Omega^2)^{-1} \sum_{\vec{k}\neq 0, \vec{q}} \vec{k}\cdot\vec{q}\, v(\vec{k}) \langle :(a^\dagger_{\vec{p}-\vec{q}/2,\sigma} a_{\vec{p}-\vec{k}-\vec{q}/2,\sigma}$$

$$- a^\dagger_{\vec{p}+\vec{k}-\vec{q}/2,\sigma} a_{\vec{p}+\vec{q}/2,\sigma}) n_{\sigma'}(\vec{k}-\vec{q}) :\rangle . \quad \text{(A6)}$$

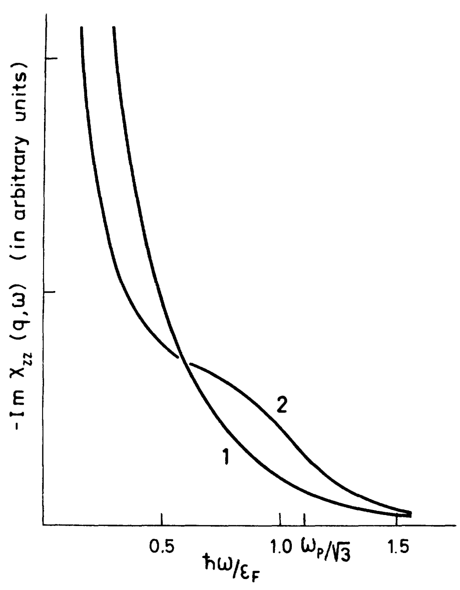

FIG. 2. Magnetic spectral function $\mathrm{Im}\chi_{zz}(\vec{q}, \omega)$ for $q = 0.1p_F$ and $r_s = 4$ with the frequency-dependent local-field factor $G_-(\vec{q}, \omega)$ and $\tau = 1/\omega_p$ (curve 1) and $\tau = 2/\omega_p$ (curve 2).

The first term in Eq. (A5) is the RPA term and it corresponds to $\vec{k}=\vec{q}$, which is removed from the sum in Eq. (A6).

To check that the last term in Eq. (4.13) is the same as $M^{P}_{3,\sigma\sigma'}(\vec{q})$ in Eq. (2.17) is mainly a question of reproducing $\langle n_\sigma(0)\, n_{\sigma'}(\vec{r})\rangle$ in Eq. (2.19). The procedure for doing this will be indicated without giving the detailed steps. From Eqs. (4.13) and (4.24) we notice that what is required is to multiply Eq. (A3) with $(\vec{p}\cdot\vec{q})$ and then sum over $\vec{p}$. We also notice that both $A_{\vec{p}\sigma}(\vec{q})$ and $\overline{C}_{\vec{p}\sigma\sigma'}(\vec{q})$ in Eqs. (A4) and (A6) are of the form $\sum_{\vec{k}}[F(\vec{p},\vec{k})-F(\vec{p}+\vec{k},\vec{k})]$. This means that after performing the summation over $\vec{p}$ we obtain an expression of the form $\sum_{\vec{k}}(\vec{q}\cdot\vec{k})\times[\sum_{\vec{p}}F(\vec{p},\vec{k})]$, where the last factor contains the required density correlation function. An explicit evaluation of the sum leads to $M^{P}_{3,\sigma\sigma'}(\vec{q})$ in Eq. (2.17).

Applying the factorization approximation (4.34) to the expression in Eqs. (A4) and (A6) yields

$$B_{\vec{p}\sigma}(\vec{q}) = -(m\Omega^2)^{-1}\sum_{\vec{k}\neq 0} v(\vec{k})(\vec{k}\cdot\vec{q}) \times\left(\langle n_{\vec{p}+\vec{q}/2,\sigma}\rangle\langle n_{\vec{p}+\vec{k}+\vec{q}/2,\sigma}\rangle + \langle n_{\vec{p}-\vec{q}/2,\sigma}\rangle\langle n_{\vec{p}+\vec{k}-\vec{q}/2,\sigma}\rangle\right) \tag{A7}$$

and

$$\overline{C}_{\vec{p}\sigma\sigma'}(\vec{q}) = (m\Omega^2)^{-1}\delta_{\sigma\sigma'}\sum_{\vec{k}\neq 0,\vec{q}} v(\vec{k})(\vec{k}\cdot\vec{q})\left(\langle n_{\vec{p}+\vec{q}/2,\sigma}\rangle \times\langle n_{\vec{p}+\vec{k}-\vec{q}/2,\sigma}\rangle + \langle n_{\vec{p}-\vec{q}/2,\sigma}\rangle\langle n_{\vec{p}+\vec{k}+\vec{q}/2,\sigma}\rangle\right). \tag{A8}$$

Equation (4.35) follows directly from the above two equations. In this approximation $\overline{A}_{\vec{p}\uparrow\downarrow}(\vec{q})=0$, so that the whole local field comes from parallel spins, as the ordinary exchange potential.

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[17]E. Safir and A. Widom [J. Low Temp. Phys. **6**, 397 (1972)] have also noted the singular q dependence of the third moment of the spin response but interpret it as indicating a possible breakdown of the Landau theory.

[18]See, for example, P. C. Martin, *Measurement and Correlation Functions* (Gordon and Breach, New York, 1968).

[19]This follows from the general relation $\chi_{AB}''(t) = -\chi''_{BA}(-t)$ combined with the inversion transformation $A,B \rightarrow A',B'$. From $n_\sigma(\vec{r}) \rightarrow n_\sigma(-\vec{r})$ it follows that $\chi''_{\sigma\sigma'}(\vec{r},t) = -\chi''_{\sigma'\sigma}(\vec{r},-t)$ and similarly with $\vec{r}$ replaced by $\vec{q}$. Therefore, χ''_{nn} and χ''_{zz} are odd functions of t or ω. They are negative for $\omega>0$.

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[21]In the classical limit, i.e., at temperatures $k_B T \gg \hbar\omega_{av}$, where ω_{av} is a typical excitation frequency involved, $\langle \omega^{l+1}\rangle_{BA} = k_B T M_{l,BA}$, where $\langle\omega^{l+1}\rangle_{BA}$ is the $(l+1)$ frequency moment of the classical correlation function $\langle B(t)A\rangle^{cl}$.

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[24]The mean square momentum is really $3\langle(\vec{q}\cdot\vec{p})^2\rangle$. As long as spin-orbit forces are negligible the Hamiltonian is separately invariant under rotations of space and spin coordinates. The momentum distribution is then isotropic even when the spins are magnetized, except for diamagnetism.

[25]Equation (2.29) seems to have been derived first by K. N. Pathak and K. S. Singwi for application to $\epsilon(q,\omega)$ [in Proceedings of the Symposium in Nuclear and Solid State Physics, Mudurai, India, 1970 (unpublished)].

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[30]We remark here that expressions like Eqs. (4.2) and (3.3) automatically satisfy the first moment as long as $[v(\vec{q})G(\vec{q},\infty)]$ or the quantities $A_{\vec{p}}(\vec{q})$ are bounded. As is seen in Eq. (3.5), this moment is determined entirely by the form of $\chi^{(0)}(\vec{q},\omega)$ at high frequency. Therefore, the remark in TW(c) below Eq. (3.23) is puzzling in that it appears to relate $G(\vec{q},\omega)$ to the numerical accuracy of the f sum. $\chi^{(f)}(\vec{q},\omega)$ in Eq. (4.19) also

approaches $nq^2/m\omega^2$ at high frequency so that the f sum is satisfied by the response functions in this section.

[31]This follows from the fact the $\chi_{\vec{p}\sigma}(\vec{q},\sigma';t)$ in Eq. (4.7) is the response to an external perturbation acting on the *density*. No new internal forces are produced until there has been time for an induced change in the density. To see this formally, take the time derivative Eq. (4.10) and compare with the equation of motion of the quantity $(i\hbar)^{-1}\langle[\dot{n}_{\vec{p}}(\vec{q},t), n(-\vec{q})]\rangle\,\theta(t)$ $= -(\vec{q}/\hbar)\cdot\langle[n_{\vec{p}}(\vec{q},t), J(-\vec{q})]\rangle\,\theta(t)$. The two resulting equations differ by a term $\delta(t)[\Sigma'_{\vec{k}}\nu(k)\,\chi_{\vec{p}\sigma}(\vec{k},\sigma',\vec{p},\sigma';0^+)]$, which must, therefore, be equal to zero.

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