Exact exchange and correlation corrections for large wave vectors

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We extend Niklasson's method in order to study the spin response of an electron liquid in a weak sinusoidal magnetic field. The many-body correction $G_-(\vec{q},\omega)$ caused by exchange and correlation is introduced to describe the correct wave-vector- and frequency-dependent spin susceptibility. The exact behavior of $G_-(\vec{q},\omega)$ in the large-q limit is related to the pair distribution function $g(\vec{r})$ at $r=0$. $G_-(\vec{q},\omega)\rightarrow[4g(0)-1]/3$, as $q\rightarrow\infty$. At metallic densities this value is negative, opposite in sign to the limit at small wave vector. Thus the spin susceptibility for large wave vectors is suppressed, rather than enhanced, by many-body effects.

I. INTRODUCTION

One of the goals of many-body physics is to obtain the *correct* wave-vector- and frequency-dependent dielectric function

$$\epsilon(\vec{q},\omega)=1-\frac{v(q)\Pi^0(\vec{q},\omega)}{1+G_+(\vec{q},\omega)v(q)\Pi^0(\vec{q},\omega)}\ , \tag{1}$$

and spin susceptibility

$$\chi(\vec{q},\omega)=-\frac{\mu_B^2\Pi^0(\vec{q},\omega)}{1+G_-(\vec{q},\omega)v(q)\Pi^0(\vec{q},\omega)}\ , \tag{2}$$

where $v(q)=4\pi e^2/q^2$ and μ_B is the Bohr magneton. $\Pi^0(\vec{q},\omega)$ is the Lindhard response function for the free-electron gas,

$$\Pi^0(\vec{q},\omega)=\frac{1}{\nu}\sum_{\vec{k},\sigma}\frac{n_{\vec{k}-\vec{q}/2,\sigma}-n_{\vec{k}+\vec{q}/2,\sigma}}{\hbar\omega-(\epsilon_{\vec{k}+\vec{q}/2}-\epsilon_{\vec{k}-\vec{q}/2})}\ , \tag{3}$$

with free-electron energy $\epsilon_k=\hbar^2k^2/2m$ and $n_{\vec{k},\sigma}$ being the occupation number for electrons with momentum $\hbar\vec{k}$ and spin σ. ν is the total volume of the system.

Equations (1) and (2) are considered as definitions of the wave-vector- and frequency-dependent many-body corrections $G_+(\vec{q},\omega)$ and $G_-(\vec{q},\omega)$; they are introduced to incorporate the many-body effects. The objective is to find the functions $G_+(\vec{q},\omega)$ and $G_-(\vec{q},\omega)$ so that $\epsilon(\vec{q},\omega)$ and $\chi(\vec{q},\omega)$ are exact.

It is a custom to divide many-body effects into exchange and correlation. The Hartree-Fock (HF) approximation takes care of exchange, while dynamical effects of the Coulomb repulsion not included in the HF approximation are defined as correlation. We introduce $G_x(\vec{q},\omega)$ for the exchange correction, and $G_c^p(\vec{q},\omega)$ and $G_c^a(\vec{q},\omega)$ for correlation corrections associated with parallel spins and antiparallel spins, respectively. The many-body corrections, $G_+(\vec{q},\omega)$ and $G_-(\vec{q},\omega)$, are then given by[1]

$$G_+(\vec{q},\omega)=G_x(\vec{q},\omega)+G_c^p(\vec{q},\omega)+G_c^a(\vec{q},\omega) \tag{4}$$

and

$$G_-(\vec{q},\omega)=G_x(\vec{q},\omega)+G_c^p(\vec{q},\omega)-G_c^a(\vec{q},\omega)\ . \tag{5}$$

From the above expressions we see that $G_+(\vec{q},\omega)$ is defined as the sum of parallel-spin and antiparallel-spin effects, whereas $G_-(\vec{q},\omega)$ is the difference of parallel-spin and antiparallel-spin effects. This is understandable. Density response depends on spin-symmetric properties, whereas spin response depends on spin-antisymmetric properties.

The struggle to find $G_+(\vec{q},\omega)$ and $G_-(\vec{q},\omega)$ has lasted more than a quarter of a century, ever since the pioneering work of Hubbard.[2] Further progress was due to Toigo and Woodruff,[3] Singwi and co-workers,[4,5] and countless others.[6] However, except for their quadratic dependence on q in the limit of small wave vectors, the precise expressions for $G_+(\vec{q},\omega)$ and $G_-(\vec{q},\omega)$ remain unknown. Knowledge of their exact behavior for large wave vectors is also important. Niklasson[7] used the equation-of-motion method to study the density response of the uniform electron liquid and found an exact condition on $G_+(\vec{q},\omega)$,

$$\lim_{q\rightarrow\infty} G_+(\vec{q},\omega)=\tfrac{2}{3}[1-g(0)]\ , \tag{6}$$

where $g(0)$ is the pair distribution function $g(\vec{r})$ at $r=0$.

To our knowledge, the analogous relation for $G_-(\vec{q},\omega)$ does not appear in the literature. It is the object of this paper to find this complementary result.

II. EXCHANGE CORRECTION

Parallel to Niklasson,[7] we apply weak sinusoidal magnetic fields to a system of N electrons with a uniform positive background. The Hamiltonian of the system consists of two parts: H_0 for the unperturbed system is

$$H_0=\sum_{\vec{k},\sigma}\epsilon_k a^\dagger_{\vec{k},\sigma}a_{\vec{k},\sigma}+\frac{1}{2\nu}\sum_{\vec{q}\neq0}v(q)\sum_{\vec{k},\sigma}\sum_{\vec{k}',\sigma'}a^\dagger_{\vec{k}-\vec{q}/2,\sigma}a^\dagger_{\vec{k}'+\vec{q}/2,\sigma'}\times a_{\vec{k}'-\vec{q}/2,\sigma'}a_{\vec{k}+\vec{q}/2,\sigma}\ , \tag{7}$$

where $a^{\dagger}_{\vec{k},\sigma}$ and $a_{\vec{k},\sigma}$ are creation and annihilation operators for an electron with momentum $\hbar\vec{k}$ and spin σ. The interaction Hamiltonian H_1 has the form

$$H_1(t)=\frac{1}{v}\sum_{\vec{q}}\mu_B B(-\vec{q},t)\times\sum_{\vec{k},\sigma}\mathrm{sgn}(\sigma)a^{+}_{\vec{k}-\vec{q}/2,\sigma}a_{\vec{k}+\vec{q}/2,\sigma}\,, \tag{8}$$

where $B(\vec{q},t)$ is the spatial Fourier transform of the magnetic field. The signum function is defined by

$$\mathrm{sgn}(\sigma)=\begin{cases}+1 & \text{if spin up}\\ -1 & \text{if spin down}\,.\end{cases} \tag{9}$$

We introduce the Wigner distribution function

$$f^{(1)}_{\vec{k},\sigma}(\vec{q},t)=\langle a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t)\rangle \tag{10}$$

to describe the density of the perturbed system. The induced density of electrons $\Delta n_\sigma(\vec{q},t)$ is then given by

$$\Delta n_\sigma(\vec{q},t)=\sum_{\vec{k}}\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},t)\,, \tag{11}$$

with $\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},t)$ being the perturbed part caused by the external field

$$\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},t)=f^{(1)}_{\vec{k},\sigma}(\vec{q},t)-\delta_{\vec{q},0}n_{\vec{k},\sigma}\,. \tag{12}$$

Evaluation of $\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},t)$ proceeds by considering the equation of motion, obtained from the commutator

$$[a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t),\ H_0+H_1(t)]\,. \tag{13}$$

Keeping only terms linear in the external field we obtain

$$\begin{aligned}i\hbar\frac{\partial}{\partial t}\langle a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t)\rangle={}&(\epsilon_{\vec{k}+\vec{q}/2}-\epsilon_{\vec{k}-\vec{q}/2})\langle a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t)\rangle\\&+\frac{1}{v}(n_{\vec{k}-\vec{q}/2,\sigma}-n_{\vec{k}+\vec{q}/2,\sigma})\{\mu_B B(\vec{q},t)\mathrm{sgn}(\sigma)+v(q)[\Delta n_\uparrow(\vec{q},t)+\Delta n_\downarrow(\vec{q},t)]\}\\&+\frac{1}{v}\sum_{\vec{q}\,'}v(\vec{q}\,')\sum_{\vec{k}',\sigma'}[\Delta f^{(2)}_{\vec{k}-\vec{q}\,'/2,\sigma;\vec{k}',\sigma'}(\vec{q}-\vec{q}\,',\vec{q}\,';t)\\&\qquad-\Delta f^{(2)}_{\vec{k}+\vec{q}\,'/2,\sigma;\vec{k}',\sigma'}(\vec{q}-\vec{q}\,',\vec{q}\,';t)]\,,\end{aligned} \tag{14}$$

The expression

$$\begin{aligned}\Delta f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}\,';t)={}&\langle a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a^{+}_{\vec{k}'-\vec{q}\,'/2,\sigma'}(t)a_{\vec{k}'+\vec{q}\,'/2,\sigma'}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t)\rangle\\&-\langle a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t)\rangle\langle a^{+}_{\vec{k}'-\vec{q}\,'/2,\sigma'}(t)a_{\vec{k}'+\vec{q}\,'/2,\sigma'}(t)\rangle-\delta_{\vec{q}+\vec{q}\,',0}f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q})\end{aligned} \tag{15}$$

is the perturbed part of the two-particle distribution function in the presence of the external potential, while the equilibrium part $f^{(2)}_{\vec{k}\sigma;\vec{k}',\sigma'}(\vec{q})$ is

$$\begin{aligned}f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q})={}&\langle 0|a^{+}_{\vec{k}-\vec{q}/2,\sigma}a^{+}_{\vec{k}'+\vec{q}/2,\sigma'}a_{\vec{k}'-\vec{q}/2,\sigma'}a_{\vec{k}+\vec{q}/2,\sigma}|0\rangle\\&-\langle 0|a^{+}_{\vec{k}-\vec{q}/2,\sigma}a_{\vec{k}+\vec{q}/2,\sigma}|0\rangle\langle 0|a_{\vec{k}'+\vec{q}/2,\sigma'}a_{\vec{k}'-\vec{q}/2,\sigma'}|0\rangle\,.\end{aligned} \tag{16}$$

We note that Eq. (14) is exact in the linear-response regime. Unfortunately, it is only a symbolic equation unless one knows the behavior of $\Delta f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}\,';t)$. The precise evaluation of Eq. (15) is even more hopeless. We are forced to make an approximation. The simplest one is the HF approximation: neglect correlation, i.e., two-particle expectations are decoupled as multiplications of one-particle expectations. Thus

$$\begin{aligned}&\langle a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a^{+}_{\vec{k}'-\vec{q}\,'/2,\sigma'}(t)a_{\vec{k}'+\vec{q}\,'/2,\sigma'}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t)\rangle\\&\quad\cong\langle a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t)\rangle\langle a^{+}_{\vec{k}'-\vec{q}\,'/2,\sigma'}(t)a_{\vec{k}'+\vec{q}\,'/2,\sigma'}(t)\rangle\\&\quad\quad-\delta_{\sigma,\sigma'}\langle a^{+}_{\vec{k}-\vec{q}/2,\sigma}(t)a_{\vec{k}'+\vec{q}\,'/2,\sigma}(t)\rangle\langle a^{+}_{\vec{k}'-\vec{q}\,'/2,\sigma}(t)a_{\vec{k}+\vec{q}/2,\sigma}(t)\rangle\,.\end{aligned} \tag{17}$$

The Fourier transform of Eq. (14) with respect to t can be reduced to

$$\begin{aligned}\hbar\omega\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},\omega)={}&(\epsilon_{\vec{k}+\vec{q}/2}-\epsilon_{\vec{k}-\vec{q}/2})\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},\omega)\\&+\frac{1}{v}(n_{\vec{k}-\vec{q}/2,\sigma}-n_{\vec{k}+\vec{q}/2,\sigma})\{\mu_B B(\vec{q},\omega)\mathrm{sgn}(\sigma)+v(q)[\Delta n_\uparrow(\vec{q},\omega)+\Delta n_\downarrow(\vec{q},\omega)]\}\\&+\frac{1}{v}\sum_{\vec{q}\,'}[v(\vec{k}-\vec{q}/2-\vec{q}\,')-v(\vec{k}+\vec{q}/2-\vec{q}\,')]n_{\vec{q}\,',\sigma}\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},\omega)\\&-\frac{1}{v}(n_{\vec{k}-\vec{q}/2,\sigma}-n_{\vec{k}+\vec{q}/2,\sigma})\sum_{\vec{q}\,'}v(\vec{q}\,')\Delta f^{(1)}_{\vec{k}-\vec{q}\,',\sigma}(\vec{q},\omega)\,,\end{aligned} \tag{18}$$

where we have made a trivial change of the summation variable so that the third term of the right-hand side has the form of an exchange energy, which leads to the well-known HF dispersion relation

$$\tilde{\epsilon}_{\vec{k}}=\epsilon_{\vec{k}}+E_x(\vec{k})=\frac{\hbar^2k^2}{2m}-\frac{1}{\nu}\sum_{\vec{k}'}v(\vec{k}-\vec{k}')n_{\vec{k}',\sigma} . \tag{19}$$

The fourth term then introduces a nonlocal exchange potential, i.e., the potential depends on the momentum of the electron,

$$V_x^\sigma(\vec{q},\omega;\vec{k})=-\sum_{\vec{q}'}v(\vec{q}')\Delta f^{(1)}_{\vec{k}-\vec{q}',\sigma}(\vec{q},\omega) . \tag{20}$$

What an electron with momentum $\hbar\vec{k}$ and spin σ experiences is

$$U^\sigma_{\text{eff}}(\vec{q},\omega;\vec{k})=\mu_B B(\vec{q},\omega)\text{sgn}(\sigma)+v(q)[\Delta n_\uparrow(\vec{q},\omega)+\Delta n_\downarrow(\vec{q},\omega)]+V_x^\sigma(\vec{q},\omega;\vec{k}) . \tag{21}$$

With this expression Eq. (18) can be rewritten as an integral equation for $\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},\omega)$,

$$\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},\omega)=\frac{1}{\nu}\frac{n_{\vec{k}-\vec{q}/2,\sigma}-n_{\vec{k}+\vec{q}/2,\sigma}}{\hbar\omega-(\tilde{\epsilon}_{\vec{k}+\vec{q}/2}-\tilde{\epsilon}_{\vec{k}-\vec{q}/2})}U^\sigma_{\text{eff}}(\vec{q},\omega;\vec{k}) . \tag{22}$$

The density response of electrons $\Delta n_\sigma(\vec{q},\omega)$ is then given by the solution of the above integral equation through Eq. (11).

Solving for the spin susceptibility, and noting that $G_c^p=G_c^a=0$ in the HF approximation, we obtain the following expression for the exchange correction $G_x(\vec{q},\omega)$:

$$G_x(\vec{q},\omega)=[v(q)\Pi^0(\vec{q},\omega)\Delta n_\sigma(\vec{q},\omega)]^{-1}\left\{\frac{1}{\nu}\sum_{\vec{k}}\frac{n_{\vec{k}-\vec{q}/2,\sigma}-n_{\vec{k}+\vec{q}/2,\sigma}}{\hbar\omega-(\epsilon_{\vec{k}+\vec{q}/2}-\epsilon_{\vec{k}-\vec{q}/2})}\sum_{\vec{q}'}v(\vec{q}')\Delta f^{(1)}_{\vec{k}-\vec{q}',\sigma}(\vec{q},\omega)\right.$$
$$\left.+\frac{1}{\nu}\sum_{\vec{k}}\frac{E_x(\vec{k}-\vec{q}/2)-E_x(\vec{k}+\vec{q}/2)}{\hbar\omega-(\epsilon_{\vec{k}+\vec{q}/2}-\epsilon_{\vec{k}-\vec{q}/2})}\Delta f^{(1)}_{\vec{k},\sigma}(\vec{q},\omega)\right\} . \tag{23}$$

The first explicit calculation of $G_x(\vec{q},\omega)$ within the time-dependent HF approximation was made by Devreese, Brosens, and Lemmens.[8]

III. CORRELATION CORRECTIONS

The full expression for $G_-(\vec{q},\omega)$ should be obtained from the original formula in Eq. (14) and the definition of the spin susceptiblity in Eq. (2). We first derive the magnetic moment of the system induced by the magnetic field:

$$M(\vec{q},\omega)=\mu_B[\Delta n_\downarrow(\vec{q},\omega)-\Delta n_\uparrow(\vec{q},\omega)] . \tag{24}$$

Using Eq. (14), we get after some transformations

$$M(\vec{q},\omega)=-\Pi^0(\vec{q},\omega)\mu_B^2B(\vec{q},\omega)+m(\vec{q},\omega) , \tag{25}$$

with $m(\vec{q},\omega)$ standing for the many-body corrections

$$m(\vec{q},\omega)=-\frac{\mu_B}{\nu}\sum_{\vec{q}'}v(\vec{q}')\sum_{\vec{k},\sigma}\sum_{\vec{k}',\sigma'}\left[\frac{1}{\hbar\omega-(\hbar^2/m)(\vec{k}+\vec{q}'/2)\cdot\vec{q}}-\frac{1}{\hbar\omega-(\hbar^2/m)(\vec{k}-\vec{q}'/2)\cdot\vec{q}}\right]\text{sgn}(\sigma)\Delta f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q}-\vec{q}',\vec{q}';\omega) . \tag{26}$$

According to the definition of the spin susceptibility and Eq. (2),

$$G_-(\vec{q},\omega)=-\frac{1}{v(q)\Pi^0(\vec{q},\omega)}\left[1+\frac{\mu_B^2\Pi^0(\vec{q},\omega)}{M(\vec{q},\omega)/B(\vec{q},\omega)}\right] . \tag{27}$$

Alternatively,

$$G_-(\vec{q},\omega)=-[v(q)\Pi^0(\vec{q},\omega)]^{-1}\frac{m(\vec{q},\omega)}{-\Pi^0(\vec{q},\omega)\mu_B^2B(\vec{q},\omega)+m(\vec{q},\omega)} . \tag{28}$$

The decoupling scheme for $\Delta f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}';\omega)$ in Eq. (17) shows that the HF approximation does not take care of correlation effects. We should carry the exact formalism one step further and study the equation of motion for

$\Delta f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}\,';\omega)$ in the presence of the external field.

Following Niklasson,[7] we obtain

$$\left[\hbar\omega-\frac{\hbar^2}{m}\vec{k}\cdot\vec{q}-\frac{\hbar^2}{m}\vec{k}\,'\cdot\vec{q}\,'\right]\Delta f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}\,';\omega)$$
$$=\frac{1}{\nu}[f^{(2)}_{\vec{k}-(\vec{q}+\vec{q}\,')/2,\sigma;\vec{k}',\sigma'}(-\vec{q}\,')-f^{(2)}_{\vec{k}+(\vec{q}+\vec{q}\,')/2,\sigma;\vec{k}',\sigma'}(-\vec{q}\,')]\mathrm{sgn}(\sigma)\mu_B B(\vec{q}+\vec{q}\,',\omega)$$
$$+\frac{1}{\nu}[f^{(2)}_{\vec{k}'-(\vec{q}\,'+\vec{q})/2,\sigma';\vec{k},\sigma}(-\vec{q})-f^{(2)}_{\vec{k}'+(\vec{q}\,'+\vec{q})/2,\sigma';\vec{k},\sigma}(-\vec{q})]\mathrm{sgn}(\sigma')\mu_B B(\vec{q}\,'+\vec{q},\omega)$$
$$+\bar{F}^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}\,';\omega)+\bar{F}^{m}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}\,';\omega)+\bar{F}^{m}_{\vec{k}'\sigma';\vec{k}\sigma}(\vec{q}\,',\vec{q};\omega)\;. \tag{29}$$

The first two terms on the right-hand side are just the Hartree terms; they describe how one electron interacts with an external magnetic field in the presence of another electron. The equilibrium parts of the two-particle correlation functions $f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q})$ are related to the pair distribution functions $g_{\sigma\sigma'}(\vec{r})$ by

$$\frac{1}{(N/2)^2}\sum_{\vec{q}}e^{i\vec{q}\cdot\vec{r}}\sum_{\vec{k}}\sum_{\vec{k}'}f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q})=2g_{\sigma\sigma'}(\vec{r})-1\;, \tag{30}$$

$g_{\sigma\sigma'}(\vec{r})$ being the probability that one spin-σ' electron is at $\vec{r}$ if the spin-σ electron is at $r=0$.

The other terms are the same as those of Niklasson.[7] The term $\bar{F}^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}\,';\omega)$ arises from the mutual interaction between the two electrons. As for the terms $\bar{F}^{m}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q},\vec{q}\,';\omega)$ and $\bar{F}^{m}_{\vec{k}'\sigma';\vec{k}\sigma}(\vec{q}\,',\vec{q};\omega)$ in Eq. (29), the many-body aspects of the interaction are displayed by considering that one particle interacts with all the surrounding particles in the presence of the other particle. Obviously they should contain the perturbed parts of the three-particle distribution functions. In the limit of large q or ω, these last three terms are of higher order in comparison with the Hartree terms. They are irrelevant to our final problem. Interested readers are referred to the original paper.[7]

IV. LIMIT OF LARGE q OR ω

As discussed in Sec. III, the equation of motion for two-particle distribution functions involves the three-particle distribution functions. This endless chain can be terminated only in the limit of large wave vector or frequency. At these limits the electrons behave like free particles. Terms that arise from the interaction of electrons with the external field dominate over those containing the Coulomb interaction between the electrons. Consequently we can neglect the last three terms in Eq. (29).

Inserting the large-q or -ω version of Eq. (29) into Eq. (26) and keeping the leading contributions, we obtain a simple but exact expression for $m(\vec{q},\omega)$ at large q or ω. After tedious but straightforward transformations similar to those of Niklasson,[7] we find

$$m(\vec{q},\omega)=\frac{v(q)\mu_B^2B(\vec{q},\omega)}{\nu^2}\left[\frac{\hbar^2q^2/m}{(\hbar\omega)^2-(\hbar^2q^2/2m)^2}\right]^2$$
$$\times\sum_{\vec{q}\,'}\left[\alpha(\vec{q},\omega)\frac{(\vec{q}\cdot\vec{q}\,')^2v(\vec{q}\,')}{q^4v(\vec{q})}\sum_{\vec{k},\sigma}\sum_{\vec{k}',\sigma'}f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q}\,')\right.$$
$$\left.-\left[\frac{\vec{q}\cdot(\vec{q}+\vec{q}\,')}{q^2}\right]^2\frac{v(\vec{q}+\vec{q}\,')}{v(\vec{q})}\sum_{\vec{k},\sigma}\sum_{\vec{k}',\sigma'}\mathrm{sgn}(\sigma)\mathrm{sgn}(\sigma')f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q}\,')\right]\;, \tag{31}$$

where

$$\alpha(\vec{q},\omega)=\frac{1}{2}\left[\left[\frac{\hbar\omega+(\hbar^2/2m)q^2}{\hbar\omega-(\hbar^2/2m)q^2}\right]^2+\left[\frac{\hbar\omega-(\hbar^2/2m)q^2}{\hbar\omega+(\hbar^2/2m)q^2}\right]^2\right]\;. \tag{32}$$

The Lindhard response function $\Pi^0(\vec{q},\omega)$ reduces to

$$\Pi^0(\vec{q},\omega)=\frac{n\hbar^2q^2/m}{(\hbar\omega)^2-(\hbar^2q^2/2m)^2}\;. \tag{33}$$

Now we are ready to discuss the asymptotic form of $G_-(\vec{q},\omega)$ given by Eq. (28). First we consider the case for which q is finite but ω tends to infinity. We obtain

$$\lim_{\omega\to\infty} G_-(\vec{q},\omega)=\frac{1}{N^2}\sum_{\vec{q}\,'}\left[\frac{(\vec{q}\cdot\vec{q}\,')^2}{q^2q'^2}\sum_{\vec{k},\sigma}\sum_{\vec{k}',\sigma'} f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q}\,')-\frac{[\vec{q}\cdot(\vec{q}+\vec{q}\,')]^2}{q^2(\vec{q}+\vec{q}\,')^2}\sum_{\vec{k},\sigma}\sum_{\vec{k}',\sigma'}\mathrm{sgn}(\sigma)\mathrm{sgn}(\sigma')f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q}\,')\right]. \tag{34}$$

In the opposite limit, when ω is finite but q tends to infinity, we obtain

$$\lim_{q\to\infty} G_-(\vec{q},\omega)=\frac{1}{N^2}\left[\sum_{\vec{q}\,'}\frac{(\vec{q}\cdot\vec{q}\,')^2}{q^2q'^2}\sum_{\vec{k},\sigma}\sum_{\vec{k}',\sigma'} f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q}\,')-\sum_{\vec{q}\,'}\sum_{\vec{k},\sigma}\sum_{\vec{k}',\sigma'}\mathrm{sgn}(\sigma)\mathrm{sgn}(\sigma')f^{(2)}_{\vec{k}\sigma;\vec{k}'\sigma'}(\vec{q}\,')\right]. \tag{35}$$

Using Eq. (30) we can express this result in terms of the pair distribution functions

$$\lim_{q\to\infty} G_-(\vec{q},\omega)=\tfrac{1}{4}\sum_{\vec{q}\,'}\frac{(\vec{q}\cdot\vec{q}\,')^2}{q^2q'^2}\int\frac{d^3\vec{r}}{v}e^{-i\vec{q}\,'\cdot\vec{r}}\times\sum_{\sigma,\sigma'}[2g_{\sigma\sigma'}(\vec{r})-1]-\tfrac{1}{4}\sum_{\sigma,\sigma'}[2g_{\sigma\sigma'}(0)-1]\mathrm{sgn}(\sigma)\mathrm{sgn}(\sigma'). \tag{36}$$

It can be shown that

$$\frac{1}{v}\sum_{\vec{q}\,'}\frac{(\vec{q}\cdot\vec{q}\,')^2}{q^2q'^2}e^{-i\vec{q}\,'\cdot\vec{r}}=\tfrac{1}{3}\delta(\vec{r}). \tag{37}$$

Hence,

$$\begin{aligned}\lim_{q\to\infty} G_-(\vec{q},\omega)&=\sum_{\sigma,\sigma'}[\mathrm{sgn}(\sigma)\mathrm{sgn}(\sigma')-\tfrac{1}{3}][\tfrac{1}{4}-\tfrac{1}{2}g_{\sigma\sigma'}(0)]\\&=\tfrac{2}{3}[g_{\uparrow\downarrow}(0)+g_{\downarrow\uparrow}(0)]\\&\quad-\tfrac{1}{3}[g_{\uparrow\uparrow}(0)+g_{\downarrow\downarrow}(0)]-\tfrac{1}{3}.\end{aligned} \tag{38}$$

The equilibrium pair distribution functions satisfy $g_{\uparrow\uparrow}(0)\equiv g_{\downarrow\downarrow}(0)\equiv 0$ and $g_{\uparrow\downarrow}(0)=g_{\downarrow\uparrow}(0)=g(0)$. Thereby we obtain the desired final result

$$\lim_{q\to\infty} G_-(\vec{q},\omega)=\tfrac{1}{3}[4g(0)-1]. \tag{39}$$

It is worthwhile to point out that when q tends to infinity, Eq. (23) has an analogous solutions for $G_x(\vec{q},\omega)$:

$$\lim_{q\to\infty} G_x(\vec{q},\omega)=\tfrac{1}{3}. \tag{40}$$

This relation has been derived by Geldart and Taylor[9] with a different method. In fact, this value is a special case of Eq. (39) by noting that $g(0)=\frac{1}{2}$ in the HF approximation.

The value of the pair distribution function $g(\vec{r})$ at $r=0$ depends on the electron density. Overhauser[10] derived an approximate formula

$$g(0)=32/(8+3r_s)^2, \tag{41}$$

where r_s is the equivalent sphere radius in Bohr units. This relation is in good agreement with recent calculations.[11] At metallic densities, $2<r_s<6$, $g(0)\sim 0.1$. Putting this value into Eq. (39), we find

$$\lim_{q\to\infty} G_-(\vec{q},\omega)\cong -0.2. \tag{42}$$

It is surprising to see a negative value for $G_-(\vec{q},\omega)$. It is well known that many-body corrections always enhance the spin susceptibility for small wave vectors. In view of the decomposition of $G_-(\vec{q},\omega)$ expressed by Eq. (5), the negative value means that, for large wave vectors, the correction due to antiparallel spins exceeds that due to parallel spins. Therefore, the spin susceptibility for large wave vectors is suppressed by correlation effects in excess of the enhancement caused by exchange.

Combining the results in Eqs. (6) and (39) along with the relations given by Eqs. (4) and (5), we also find the correlation corrections for parallel and antiparallel spin, respectively,

$$\lim_{q\to\infty} G_c^p(\vec{q},\omega)=-\tfrac{1}{6}[1-2g(0)] \tag{43}$$

and

$$\lim_{q\to\infty} G_c^a(\vec{q},\omega)=\tfrac{1}{2}[1-2g(0)]. \tag{44}$$

At metallic densities we have $G_c^p(\infty)\cong -0.13$ and $G_c^a(\infty)\cong 0.4$.

V. DISCUSSION

The exact asymptotic values of $G_+(\vec{q},\omega)$ and $G_-(\vec{q},\omega)$ are important because they offer guidance in constructing approximate expressions. For small q we know that

$$G_+(\vec{q},0)=(1+\alpha)\left[\frac{q}{2k_F}\right]^2 \tag{45}$$

and

$$G_-(\vec{q},0)=\beta\left[\frac{q}{2k_F}\right]^2. \tag{46}$$

k_F is the Fermi wave vector. The coefficient α is chosen to satisfy the compressibility relation.[12] In the metallic density regime $\alpha \cong 0.1$.[13] β is determined from the theoretical calculations of the spin susceptibility.[14,15] $\beta \cong 0.6$, a value which has been confirmed by experiments.[15]

Unfortunately, the construction of interpolation formulas to describe G_+ and G_- between the $q=0$ and $q=\infty$ limits is at present just a guess. We cite Fig. 1 of Utsumi and Ichimaru,[16] which displays the wide spectrum of current opinion regarding $G_+(\vec{q},0)$ near $q=2k_F$. Many-electron theory remains in its infancy.

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