Thermodynamic limits of the local field corrections in a spin-polarized electron system

D. C. Marinescu and I. Tifrea
Department of Physics, Clemson University, Clemson South Carolina 29634
(Received 19 September 2001; published 12 February 2002)

In a spin-polarized electron gas, the effect of the exchange (x) and correlation (c) interactions can be incorporated into the dynamic response functions through spin-dependent local-field corrections $G_\sigma^{x,c}(\omega,\vec{q})$. We obtain the zero-frequency and long-wavelength limits of $G_\sigma^{x,c}(\omega,\vec{q})$ by analyzing the connection between the macroscopic response function and the thermodynamic parameters of the system.

DOI: 10.1103/PhysRevB.65.113201 PACS number(s): 72.25.−b, 71.10.−w

The introduction of frequency- and wave-vector-dependent local-field corrections is motivated by the necessity of obtaining a more realistic picture of the effective electron-electron interaction. Generally, the local field corrections $G^{x,c}(\vec{q},\omega)$ describe the deviation from the average electron density considered in the random-phase approximation (RPA) induced by the short-range Coulomb interaction through exchange (x) and correlations (c). Their knowledge is very important in estimating system parameters that are influenced by the interaction, such as response functions and effective mass, and obtaining better and better approximations has been a continuous effort in condensed-matter theory.[1]

An important view of this old problem appears in the context of spin-dependent interaction in itinerant magnetic systems with a high degree of spin polarization. This description is appropriate for dilute magnetic semiconductor systems, where high values of the effective electron gyromagnetic factor γ^* facilitate a large Zeeman splitting and consequently, a large magnetic polarization even at low values of an external magnetic field. The possibility of using these materials for spin-dependent applications hinges on the ability to distinguish between the spin states, a goal that can be achieved by understanding the difference in the electron-electron interaction among electrons of different spins.

A basic model for such a system is a spin-polarized electron gas (SPEG) under the effect of a static magnetic field that lifts the spin degeneracy and induces an equilibrium polarization. In this situation, it is expected that local-field corrections are functions of the spin degree of freedom as the short-range Coulomb interaction is spin dependent. In the present work, the system of interest is a SPEG of density n versus a positive background to assure charge neutrality, polarized by a dc magnetic field $B\hat{z}$ that creates a spin imbalance $\zeta=(n_\uparrow-n_\downarrow)/n$. ζ is considered a continuous function of B, and can take any value between -1 and 1. Conclusions based on the simple model outlined above—an electron gas in the presence of a static, external magnetic field—can also be important for a situation in which the polarization is a results of a self-consistent magnetic field, given that the many-body interaction will be the same, independent of the nature of the magnetic field.

The inclusion of spin-dependent local-field corrections in the effective potential experienced by an electron of spin $\vec{\sigma}$ in the presence of an electromagnetic field—an electric potential $\varphi(\vec{q},\omega)$ and a magnetic induction $\vec{b}(\vec{q},\omega)$—can be obtained by generalizing the classical work of Kukkonen and Overhauser.[2] This approach simply showcases the different interaction undergone by the up- and down-spins in the magnetic system on account of the Pauli exclusion principle. Following Ref. 3 we write the self-consistent, one-particle, effective interaction potential in the presence of the external field:

$$\mathcal{V}_\sigma=-e\varphi(\vec{q},\omega)+\gamma^*\vec{\sigma}\cdot\vec{b}(\vec{q},\omega)+v(\vec{q})\times\left\{[1-G_\sigma^+(\vec{q},\omega)]\Delta n(\vec{q},\omega)+\frac{1}{\gamma^*}\vec{\sigma}\cdot\Delta\vec{m}(\vec{q},\omega)G_\sigma^-(\vec{q},\omega)\right\}. \tag{1}$$

Here $\Delta n(\vec{q},\omega)$ and $\Delta\vec{m}(\vec{q},\omega)$ are the electron density and magnetic fluctuations. G_σ^+ represents the sum of the interactions experienced by an electron of spin σ. These are composed of exchange with spins σ and of correlations with both σ and $\overline{\sigma}$. G_σ^- is the difference between same-spin interaction (correlations and exchange with other spins σ), and opposite-spin interaction (correlations with $\overline{\sigma}$). Same-spin correlations are usually neglected on account of the Pauli principle that diminishes the concentration of same-spin electrons around a given spin. $v(q)$ is the Fourier transform of the Coulomb interaction, equal to $2\pi e^2/q$ in two dimensions and to $4\pi e^2/q^2$ in three dimensions.

In a linear approximation, the density fluctuations in each spin population are proportional to the corresponding effective potential, $\Delta n_\sigma=\Pi_{\sigma\sigma}\mathcal{V}_\sigma$, where the proportionality coefficients are appropriately defined polarization functions, given below. The total density fluctuation is $\Delta n=\Delta n_\uparrow+\Delta n_\downarrow$. A set of three equations, one for each direction, is needed to describe the magnetization. The longitudinal component, parallel to the $\hat{z}$ axis, is generated by $\Delta m_z=-\gamma^*(\Delta n_\uparrow-\Delta n_\downarrow)$. The transverse-induced magnetization arises from spin-flip processes determined by $b^\pm=b_x\pm ib_y$, the components of the ac magnetic field coupled to $\sigma^\mp=\sigma_x\mp\sigma_y$, and respectively the Pauli lowering and raising spin operators. To cover all possible cases, we define the generalized polarization functions

$$\Pi_{\sigma\sigma'}(\vec{q},\omega)=\frac{1}{L^d}\sum_k \frac{n_{\vec{k}-\vec{q}/2,\sigma}-n_{\vec{k}+\vec{q}/2,\sigma'}}{\hbar\omega-(\epsilon_{\vec{k}+\vec{q}/2,\sigma'}-\epsilon_{\vec{k}-\vec{q}/2,\sigma})}. \quad (2)$$

$\epsilon_{k,\sigma}=(\hbar^2k^2/2m^*)+\mathrm{sgn}(\sigma)\gamma^*B$ is the single-electron energy in the static magnetic field, and $n_{k,\sigma}$ is the single-electron occupation function, the usual Fermi distribution associated with energy $\epsilon_{k,\sigma}$. $V=L^d$, with $d=2$ and 3, is the ''volume'' of the system. Here, sgn(σ) is equal to $+1$ for up spin electrons and to -1 for down spins.

The knowledge of $G_\sigma(\vec{q},\omega)$, and especially its dependence on ζ, is very important in estimating the three different electron-electron interactions present in the system: up-up, up-down, and down-down. As in the unpolarized case, the exact ω and $\vec{q}$ dependences are very elusive, but attempts have been made to calculate the asymptotic values of the local factors at short wavelengths ($q\to\infty$) and large frequencies ($\omega\to\infty$) in both two[4] and three dimensions.[5]

The object of this paper is to analyze the asymptotic values of $G_\sigma(\vec{q},\omega)$ at the opposite end of the spectrum, at zero frequency and long wavelengths. In this limit, the response functions represent the response of the system to a static field which varies slowly in space, and can be connected with the thermodynamic parameters of the system, that are second-order derivatives of the total free energy in respect to the particle density and magnetization. It is important to note that this case corresponds to ω being set to zero before letting q vanish. For an unpolarized electron system, the limiting procedure outlined above generates a connection between the static, long-wavelength, charge susceptibility and the compressibility known as ''the compressibility sum rule.''[6] Our work will provide a generalization of this sum rule to include the case of off-diagonal magnetoelectric effects. From the appropriate sum rules we will derive the corresponding expressions of the local factors. We compare these results with the recent work of Ref. 4.

On account of the equilibrium magnetization, in the presence of an electromagnetic perturbation, a SPEG exhibits coupled particle and longitudinal spin-density fluctuations triggered by φ and b_z:

$$\Delta n=\chi_{ee}(-\mathrm{e}\varphi)+\chi_{em}b_z, \quad (3)$$

$$\Delta m_z=\chi_{me}(-\mathrm{e}\varphi)+\chi_{mm}b_z. \quad (4)$$

The spin-flip fluctuations induced by $b^{\pm}=b_x\pm ib_y$ give rise to

$$\Delta m^{\pm}=\chi^{\pm}b^{\pm}. \quad (5)$$

In Eqs. (3), (4), and (5), the ω and $\vec{q}$ dependence of all the quantities involved is understood. All six response functions χ can be derived by making use of Eq. (1) self-consistenly. Here we will quote only the main results that follow the detailed calculation presented in Refs. 3 and 5:

$$\chi_{ee}=\frac{1}{D}[\Pi_{\uparrow\uparrow}+\Pi_{\downarrow\downarrow}+2\Pi_{\uparrow\uparrow}\Pi_{\downarrow\downarrow}v(\vec{q})(G^-_{L,\uparrow}+G^-_{L,\downarrow})], \quad (6)$$

$$\chi_{em}=\frac{\gamma^*}{D}[\Pi_{\uparrow\uparrow}-\Pi_{\downarrow\downarrow}+2v(\vec{q})\Pi_{\uparrow\uparrow}\Pi_{\downarrow\downarrow}(G^-_{L,\downarrow}-G^-_{L,\uparrow})], \quad (7)$$

$$\chi_{me}=-\frac{\gamma^*}{D}[\Pi_{\uparrow\uparrow}-\Pi_{\downarrow\downarrow}+2v(\vec{q})\Pi_{\uparrow\uparrow}\Pi_{\downarrow\downarrow}(G^+_{\downarrow}-G^+_{\uparrow})], \quad (8)$$

$$\chi_{mm}=-\frac{(\gamma^*)^2}{D}[\Pi_{\uparrow\uparrow}+\Pi_{\downarrow\downarrow}-2v(\vec{q})\Pi_{\uparrow\uparrow}\Pi_{\downarrow\downarrow}(2-G^+_{\downarrow}-G^+_{\uparrow})], \quad (9)$$

where

$$2D=[1-2v(\vec{q})\Pi_{\uparrow\uparrow}(1-G^+_{\uparrow})][1+2v(\vec{q})\Pi_{\downarrow\downarrow}G^-_{L,\downarrow}]+[1-2v(\vec{q})\Pi_{\downarrow\downarrow}(1-G^+_{\downarrow})][1+2v(\vec{q})\Pi_{\uparrow\uparrow}G^-_{L,\downarrow}]. \quad (10)$$

The corresponding transverse susceptibilities are:

$$\chi^+=-\frac{2(\gamma^*)^2\Pi_{\downarrow\uparrow}}{1+2v(\vec{q})\Pi_{\downarrow\uparrow}G^-_{T,\uparrow}}, \quad (11)$$

$$\chi^-=-\frac{2(\gamma^*)^2\Pi_{\uparrow\downarrow}}{1+2v(\vec{q})\Pi_{\uparrow\downarrow}G^-_{T,\downarrow}}. \quad (12)$$

In the zero-frequency, long-wavelength limit the local-field behavior can be related to the static response functions of the system, as discussed in Refs. 7 and 8. By following the same argument, we obtain immediately that, for the up-spin, the transverse local-field factor is:

$$G^-_{T,\uparrow}=-\frac{(\gamma^*)^2}{v(q)}\left(\frac{1}{\chi^+}-\frac{1}{\chi_0^+}\right), \quad (13)$$

while, for the down-spin, $G^-_{T,\downarrow}(\zeta)=G^-_{T,\uparrow}(-\zeta)$. $\tilde{\chi}_0^-=-2(\gamma^*)^2\Pi_{\downarrow\uparrow}$ is the transverse magnetic susceptibility in the RPA.

In the longitudinal case, care needs to be exercised since the charge and magnetic response are coupled, i.e. both the electric potential and the $\hat{z}$ component of the ac magnetic field simultaneously induce density and spin variations. Let us first consider the situation in which only the electric potential is applied. Equation (4) indicates that the density fluctuation expected as a result of the scalar field is accompanied by a change in the magnetization of the system, Δm_z. This is easy to understand when one considers the effect of the perturbation on the local electron energies and implicitly on the electron occupation number. Since in equilibrium the system is described by a spin imbalance, the induced changes are different for up- and down-spins, resulting in a nonzero magnetization.

In the thermodynamic limit the aim is to connect the response functions with second-order derivatives of the free energy of the system. However, these derivatives are calculated when only one parameter of the system varies, while the others are kept constant. In the problem at hand, the correct way to relate the scalar field with the density fluctuation in the thermodynamic limit is by keeping the magnetization constant. This is possible when, in Eq. (4) $\Delta m_z = 0$, with the implication that in a SPEG, a magnetic field $b_z = -(\chi_{me}/\chi_{mm})(-\mathrm{e}\varphi)$ is induced by the scalar potential. Of course, this value needs to be introduced into Eq. (3), leading to:

$$\Delta n = \left(\chi_{ee} - \frac{\chi_{em}\chi_{me}}{\chi_{mm}} \right)(-\mathrm{e}\varphi). \tag{14}$$

The density fluctuation [Eq. (14)], gives rise to an additional pressure distribution ΔP, such that the corresponding pressure force ∇P balances the average external force per unit volume, $-n\nabla(-e\varphi)$. At zero frequency, the long-wavelength limit of Eq. (14) is then connected to the macroscopic compressibility of the electron system, K. Based on this argument we write

$$\lim_{q\to 0}\left(\chi_{ee} - \frac{\chi_{em}\chi_{me}}{\chi_{mm}} \right) = -n\left(\frac{\partial P}{\partial n}\right)^{-1}, \tag{15}$$

with $(\partial P/\partial n)^{-1} = nK$. We stress here that in all the quantities above, ω is first set to zero, and then q is allowed to approach zero. By introducing appropriate expressions for the susceptibilities from Eqs. (6)–(9), and performing the required elementary algebra, we obtain that

$$G_\uparrow^+ + G_\downarrow^+ = -\frac{2}{nv(q)}\left[\left(\frac{\partial P}{\partial n}\right) - \left(\frac{\partial P}{\partial n}\right)_0\right]. \tag{16}$$

$(\partial P/\partial n)_0^{-1} = nK_0$ is obtained from Eq. (14) in the RPA, when all G's are set equal to zero. The pressure of a SPEG is simply $P = -(\partial E/\partial V)$, where E is the total energy of the system.

The electric potential can also be related to the induced magnetization, when the density fluctuation is kept constant. From Eq. (3), the density fluctuation is zero under the application of an electric potential, when a longitudinal magnetic field $b_z = -(\chi_{em}/\chi_{ee})(-\mathrm{e}\varphi)$ is induced. By considering Eq. (4), we obtain the induced magnetization generated by φ in the absence of any charge fluctuations:

$$\Delta m_z = \left(\chi_{me} - \frac{\chi_{ee}\chi_{mm}}{\chi_{em}} \right)(-e\varphi). \tag{17}$$

The longitudinal magnetization, which arises only from different density fluctuations for opposite spins, modifies the pressure distribution in the system. Since the resulting pressure force has to balance the external force averaged per unit volume, $-n\nabla(-\mathrm{e}\varphi)$, the static, long-wavelength limit of Eq. (17) is

$$\lim_{q\to 0}\left(\chi_{me} - \frac{\chi_{ee}\chi_{mm}}{\chi_{em}} \right) = -n\left(\frac{\partial P}{\partial m_z}\right)^{-1}. \tag{18}$$

Again, by using Eqs. (6)–(9) we obtain,

$$G_\uparrow^- - G_\downarrow^- = \frac{2\gamma^*}{v(q)}\left[\left(\frac{\partial P}{\partial m_z}\right) - \left(\frac{\partial P}{\partial m_z}\right)_0\right]. \tag{19}$$

Similar arguments can be made when only the longitudinal component of the magnetic field is applied, b_z. To obtain the thermodynamic limit of the magnetic susceptibility, we require that no density fluctuations are allowed. This implies, from Eq. (3), that an electric potential is induced, $(-\mathrm{e}\varphi) = -(\chi_{em}/\chi_{ee})b_z$ that produces an additional magnetic fluctuation as in Eq. (4). The static limit of the total magnetization is the magnetic susceptibility of the system, $\chi = (\partial m_z/\partial b_z)$:

$$\lim_{q\to 0}\left(\chi_{mm} - \frac{\chi_{em}\chi_{me}}{\chi_{ee}} \right) = \left(\frac{\partial m_z}{\partial b_z}\right). \tag{20}$$

Thermodynamically, $b_z = [\partial F/\partial(L^d m_z)]$, since it is the conjugate variable of the volumic magnetization.

The density fluctuation associated with the longitudinal component of the magnetic field, obtained when the magnetic fluctuation is forced to be zero, is connected in the thermodynamic limit with $(\partial b_z/\partial n)$:

$$\lim_{q\to 0}\left(\chi_{em} - \frac{\chi_{ee}\chi_{mm}}{\chi_{me}} \right) = \left(\frac{\partial b_z}{\partial n}\right)^{-1}. \tag{21}$$

Upon considering Eqs. (6)–(9) in Eqs. (20) and (21), the following relations for the local field corrections, G_σ^-, are obtained:

$$G_\uparrow^- + G_\downarrow^- = -\frac{(\gamma^*)^2}{v(q)}\left[\left(\frac{\partial b_z}{\partial m_z}\right) - \left(\frac{\partial b_z}{\partial m_z}\right)_0\right], \tag{22}$$

$$G_\uparrow^+ - G_\downarrow^+ = \frac{2\gamma^*}{v(q)}\left[\left(\frac{\partial b_z}{\partial n}\right) - \left(\frac{\partial b_z}{\partial n}\right)_0\right]. \tag{23}$$

One can immediately write down the thermodynamic limit of the local-field corrections from Eqs. (16) and (23) and Eqs. (22) and (19), respectively. The results are

$$G_\sigma^+(q\to 0,0) = -\frac{1}{v(q)}\left\{\frac{1}{n}\left[\left(\frac{\partial P}{\partial n}\right) - \left(\frac{\partial P}{\partial n}\right)_0\right] - \mathrm{sgn}(\sigma)\gamma^*\left[\left(\frac{\partial b_z}{\partial n}\right) - \left(\frac{\partial b_z}{\partial n}\right)_0\right]\right\}. \tag{24}$$

$$G_\sigma^-(q\to 0,0) = -\frac{\gamma^*}{v(q)}\left\{\gamma^*\left[\left(\frac{\partial b_z}{\partial m_z}\right) - \left(\frac{\partial b_z}{\partial m_z}\right)_0\right] - \mathrm{sgn}(\sigma)\frac{1}{n}\left[\left(\frac{\partial P}{\partial m_z}\right) - \left(\frac{\partial P}{\partial m_z}\right)_0\right]\right\}. \tag{25}$$

These results can be particularized for two or three dimensions by calculating the appropriate thermodynamic coefficients. In all cases, the dependence on ζ is implicit in the thermodynamic coefficients, while that on q is the same as in the case of an unpolarized gas of the same dimensionality.

The thermodynamic limit of the local fields in a SPEG was recently analyzed in Ref. 4, with different results. To obtain the response functions of the system, the authors employed an equation-of-motion technique originally developed by Caccamo *et al.*[9] A careful examination of the latter reference leads one to believe that, in deriving the equations satisfied by the charge and spin fluctuations, the finite-frequency, short-wavelength limit of the polarization functions, $\Pi_{\sigma\sigma}(\vec{q},\omega)=n_\sigma q^2/m^*\omega^2$, was used, and the final results were given in this approximation. The above limit of the polarization function results from a power expansion, and is valid only when $\omega \gg q v_F$ (v_F is the Fermi velocity). Obviously, in this form one cannot take the limit $\omega\rightarrow 0$ for the static case. Using the same equations as a starting point in deriving the asymptotic expressions of the local-field corrections in the zero-frequency, long-wavelength limit is inappropriate. This, we think, is the origin of the discrepancy between the present results and those obtained in Ref. 4.

The general expressions for the local-field corrections, [Eqs. (24) and (25)], can be used to obtain analytical results in both two and three dimensions. To determine the thermodynamic parameters involved, we need only consider the total interaction energy of the system, since the kinetic-energy derivatives will simply cancel the RPA estimate of the same quantities. Including the exchange and correlation contributions alone, we write

$$E=V\sum_\sigma n_\sigma[-\alpha k_{F\sigma}+w_{c\sigma}(k_{F\sigma},k_{F\bar{\sigma}})], \tag{26}$$

where

$$k_{F\sigma}=2\sqrt{\pi}\left[\Gamma\left(\frac{d}{2}+1\right)n_\sigma\right]^{1/d}$$

is the Fermi wave vector for spin population σ, and $w_{c\sigma}$ is the spin-dependent correlation energy per particle considered function of both $k_{F\sigma}$ and $k_{F\bar{\sigma}}$. α is a constant equal to $3e^2/4\pi$ three dimensions, and to $4e^2/3\pi$ in two dimensions. By taking the appropriate derivatives of Eq. (26), we arrive at

$$G^+_\sigma(q\rightarrow 0,0)=\frac{\alpha(d+1)}{2v(q)nd^2}\sum_{\sigma'} k_{F\sigma'}\left[1+\frac{n}{2n_{\sigma'}}\times\text{sgn}(\sigma')\text{sgn}(\sigma)\right](1-s), \tag{27}$$

$$G^-_\sigma(q\rightarrow 0,0)=\frac{\alpha(d+1)}{2v(q)nd^2}\sum_{\sigma'}{}' k_{F\sigma'}\text{sgn}(\sigma')\text{sgn}(\sigma)\times\left[1+\frac{n}{2n_{\sigma'}}\text{sgn}(\sigma')\text{sgn}(\sigma)\right](1-s'). \tag{28}$$

Here s and s' stand for contributions from the correlation energy, that involve first and second-order derivatives of $w_{c\sigma}(k_{F\sigma},k_{F\bar{\sigma}})$ in with respect to $k_{F\sigma}$ and $k_{F\bar{\sigma}}$. For an unpolarized electron system $w_{c\sigma}(k_{F\sigma})$ is obtained numerically, but we are not aware of similar calculations being done for a SPEG.

We gratefully acknowledge support from the U.S. Department of Energy, Grant No. DE-FG02-01ER45897.

[1] A discussion of this problem can be found in the review by K. S. Singwi and M. P. Tosi, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic Press, New York 1981), Vol. 36, p. 117.
[2] C. A. Kukkonen and A. W. Overhauser, Phys. Rev. B **20**, 550 (1979).
[3] K. S. Yi and J. J. Quinn, Phys. Rev. B **54**, 13 398 (1996).
[4] Marco Polini and M. P. Tosi, Phys. Rev. B **63**, 045118 (2001).
[5] D. C. Marinescu and J. J. Quinn, Phys. Rev. B **56**, 1114 (1997).
[6] See, for example, Phillipe Noziéres and David Pines, *The Theory of Quantum Liquids* (Perseus Books, 1999), p. 104.
[7] A. W. Overhauser, Phys. Rev. B **3**, 1888 (1971).
[8] Giuseppe E. Santoro and Gabriele F. Giuliani, Phys. Rev. B **37**, 4813 (1988).
[9] C. Caccamo, G. Pizzimenti, and M. P. Tosi, Nuovo Cimento B **31**, 53 (1976).