Limits of the exchange-correlation local fields in the magnetic response of a spin-polarized electron gas

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We analyze the spin and charge susceptibilities of a spin-polarized electron gas subject to a weak space- and time-dependent field coupled to the electronic spins, with the main attention given to the case of space dimensionality $D=2$. Exchange and correlations enter the dynamic susceptibilities through spin-dependent local-field factors $G_\sigma^\pm(\mathbf{q},\omega)$. For an arbitrary degree of polarization, we determine the exact analytic expressions of $G_\sigma^\pm(\mathbf{q},\omega)$ in two limiting cases: (i) the limit of large wave number q at finite frequency ω, already considered in $D=3$ by D. C. Marinescu and J. J. Quinn [Phys. Rev. B **56**, 1114 (1997)]; and (ii) the static limit at small wave number. In the latter case, we obtain thermodynamic sum rules of general validity in both dimensionalities. Our work gives insight into many-body vertex corrections and basic information for calculations of the effects of the electron-electron interactions on physical properties.

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I. INTRODUCTION

An interacting electron gas (EG) on a uniform neutralizing background is used as the reference system in most realistic calculations of electronic structure in condensed-matter physics.[1] Understanding the many-body aspects of this model has attracted continued interest for many decades.[2] The EG, unlike systems of classical particles, behaves like a gas at high density and like a solid at low density.[3] At intermediate densities, the EG is in a fluid state with intermediate-to-strong electron-electron coupling and is accessible to approximate theories and to quantal simulation techniques.

A great deal of theoretical work has been devoted to the EG in the paramagnetic fluid state. Quantal simulation and experiment have been bringing to light the importance of spin polarization at strong coupling. Simulation studies[4,5] have revealed a continuous transition from the paramagnetic to the ferromagnetic state taking place in the three-dimensional (3D) fluid with increasing coupling strength, before a first-order transition into a ferromagnetic crystal occurs. Similar studies of the (2D) EG (Refs. 6–8) indicate a first-order transition to a ferromagnetic fluid state before crystallization. On the experimental side, one may recall that metallic conductivity in disordered 2D electron systems is suppressed through induction of spin polarization by an in-plane magnetic field[9,10] and that spontaneous spin polarization (''weak ferromagnetism'') has been observed in electron-doped calcium hexaboride.[11]

Exchange between parallel-spin electrons and correlations from the Coulomb repulsion, which induce a local decrease in the density of electrons of each spin orientation around each electron of given spin, are clearly crucial in such situations. These effects are embodied in the so-called local-field corrections in the expressions of the charge and spin susceptibilities of the EG,[12–14] or equivalently in the vertex corrections that account for the difference between the effective potential experienced by an electron and the mean-field value. Their evaluation determines the spin-dependent exchange-correlation hole, from which the quasiparticle self-energies and the effective electron-electron interactions can be calculated.[15–21]

The behavior of the local-field factors can be determined exactly in some limits, as was first shown in a number of studies referring to the EG in the paramagnetic state. Denoting by $G^+(q,\omega)$ and $G^-(q,\omega)$ the local-field factors for the charge and spin response in this state, the values of $G^+(q,0)$ and $G^-(q,0)$ at long wavelengths ($q\to 0$) determine the thermodynamic compressibility and magnetic susceptibility, respectively (see, e.g., Ref. 2). Kimball[22] and Niklasson[23] studied the charge response of the 3D EG in the limit of large wave number at finite frequency, showing that $G^+(q\to\infty,\omega)$ is determined by the value of the pair distribution function $g(r)$ at the origin ($r=0$). These results were extended to the spin response of the 3D EG by Zhu and Overhauser[24] and to the 2D EG by Santoro and Giuliani.[25] The same limiting behavior was studied for a spin-polarized 3D EG by Marinescu and Quinn.[26]

As is well known, the relevance of exchange and correlation increases as the dimensionality of the EG is lowered. In view of the evidence cited earlier in this section, it is useful and timely to give the exact expressions of the (spin-dependent) local-field factors $G_\sigma^\pm(\mathbf{q},\omega)$ at large and small wave number for a 2D EG with arbitrary spin polarization ζ. This is the main purpose of the present work. While available evidence[8] indicates that in 2D the ground state corresponds to $\zeta=0$ or $\zeta=1$ only, it remains to be understood why the states with $0<\zeta<1$ should lie at higher energy in this dimensionality. Furthermore, an equilibrium imbalance between the two spin polarizations can be induced by a static magnetic field $\mathbf{B}$, diamagnetic currents being absent if this field lies in the plane of the 2D EG. As remarked earlier, this is a configuration of active experimental interest. While in the following we shall work at arbitrary ζ without specifying the origin of such spin imbalance, our results are easily extended to the case $\mathbf{B}\neq\mathbf{0}$ by adding a Zeeman term in the unperturbed Hamiltonian.

The contents of the paper are described briefly as follows.

In Sec. II, we introduce the magnetic perturbation Hamiltonian from two alternative viewpoints and give the basic definitions of structural functions, response functions, and local-field factors. We proceed in Sec. III and in Appendix A to evaluate the large wave-number limit, while in Sec. IV we determine the local-field factors in the thermodynamic limit. We obtain thermodynamic sum rules through an extension of the virial theorem, which is proved in Appendix B. These sum rules are valid independently of the EG dimensionality. Finally, Sec. V reports our main conclusions.

II. LINEAR RESPONSE OF A SPIN-POLARIZED ELECTRON FLUID

We consider an EG in a fluid state with equilibrium spin densities $n_\uparrow$ and $n_\downarrow$, corresponding to a mean particle density $n=n_\uparrow+n_\downarrow$ and a spin polarization $\zeta=(n_\uparrow-n_\downarrow)/n$. The unperturbed Hamiltonian of the system is

$$\mathcal{H}_0=\sum_\sigma \int d\mathbf{r}\,\psi^\dagger_\sigma(\mathbf{r})\frac{p^2}{2m}\psi_\sigma(\mathbf{r}) + \frac{1}{2}\sum_{\sigma,\sigma'}\int d\mathbf{r}\int d\mathbf{r}'\,\psi^\dagger_\sigma(\mathbf{r})\psi^\dagger_{\sigma'}(\mathbf{r}') \times v(|\mathbf{r}-\mathbf{r}'|)\psi_{\sigma'}(\mathbf{r}')\psi_\sigma(\mathbf{r}), \tag{1}$$

where $v(r)=e^2/r$ is the Coulomb interaction potential and $\psi_\sigma(\mathbf{r})$, $\psi^\dagger_\sigma(\mathbf{r})$ are the Schrödinger field operators obeying canonical anticommutation relations. We have omitted a constant term due to the neutralizing background, which sets to zero the mean potential felt by each electron.

The instantaneous correlations between pairs of electrons are described by the distribution functions $g_{\sigma\sigma'}(r)$. We define them according to standard practice for multicomponent fluids by setting equal to $n_{\sigma'}g_{\sigma\sigma'}(r)\ \Omega_D r^{D-1}dr$ the number of electrons with spin σ' contained in a shell of radius r and thickness dr centered on an electron with spin σ ($\Omega_2=2\pi$ and $\Omega_3=4\pi$). Namely, the two-body density-density correlation function is written as $\langle\rho_\sigma(\mathbf{r})\rho_{\sigma'}(\mathbf{r}')\rangle=n_\sigma\delta_{\sigma\sigma'}\delta^{(D)}(\mathbf{r}-\mathbf{r}')+n_\sigma n_{\sigma'}g_{\sigma\sigma'}(|\mathbf{r}-\mathbf{r}'|)$. This definition ensures the symmetry property $g_{\sigma\sigma'}(r)=g_{\sigma'\sigma}(r)$ and the asymptotic value $g_{\sigma\sigma'}(r\to\infty)=1$.

The corresponding partial structure factors are obtained by Fourier transform according to the definiton

$$S_{\sigma\sigma'}(q)=\delta_{\sigma\sigma'}+(n_\sigma n_{\sigma'})^{1/2}\int d\mathbf{r}[g_{\sigma\sigma'}(r)-1]\exp(-i\mathbf{q}\cdot\mathbf{r}). \tag{2}$$

In particular, in $D=2$ we have

$$S_{\sigma\sigma'}(q)=\delta_{\sigma\sigma'}+2\pi(n_\sigma n_{\sigma'})^{1/2}\int_0^\infty dr[g_{\sigma\sigma'}(r)-1]r\,J_0(qr), \tag{3}$$

where $J_0(x)$ is the Bessel function of zero order. Clearly, with these definitions $S_{\sigma\sigma'}(q)=S_{\sigma'\sigma}(q)$.

A. Perturbation Hamiltonian and linear susceptibilities

The EG introduced above is subjected to an external perturbation described by the Hamiltonian

$$\mathcal{H}_1(t)=\sum_\sigma\int d\mathbf{r}[W_\sigma(\mathbf{r},t)\psi^\dagger_\sigma(\mathbf{r})\psi_\sigma(\mathbf{r}) + W_{\sigma\bar\sigma}(\mathbf{r},t)\psi^\dagger_\sigma(\mathbf{r})\psi_{\bar\sigma}(\mathbf{r})]. \tag{4}$$

This notation, which is taken from early work by Caccamo *et al.*,[27] explicitly shows that the external perturbation couples with fluctuations in the spin densities (i.e., in the charge and magnetization densities) through the first term on the right-hand side of Eq. (4) and also induces spin flips through the second term.

Of course, the perturbation Hamiltonian (4) can be rewritten in terms of a weak external electromagnetic field,[26] consisting of an electric potential $\phi(\mathbf{r},t)$ and a magnetic field $\mathbf{b}(\mathbf{r},t)$. We only need to set

$$W_\sigma(\mathbf{r},t)=-e\phi(\mathbf{r},t)-\gamma b_z(\mathbf{r},t)\mathrm{sgn}(\sigma) \tag{5}$$

and

$$W_{\uparrow\downarrow}(\mathbf{r},t)=-\gamma b_+(\mathbf{r},t),\qquad W_{\downarrow\uparrow}(\mathbf{r},t)=-\gamma b_-(\mathbf{r},t) \tag{6}$$

with $b_\pm=b_x\pm ib_y$. In these equations $\gamma=g\mu_B/2$, with g the Landé factor and μ_B the Bohr magneton.

The linear response of the EG is described by a set of longitudinal susceptibilities for the field (5) and by transverse susceptibilities for the spin-flip field (6). Standard linear-response theory yields the changes in density of the two spin populations due to the longitudinal term as

$$\delta n_\sigma(\mathbf{r},t)=\sum_{\sigma'}\int d\mathbf{r}'\int_{-\infty}^{\infty}dt'\,K_{\sigma\sigma'}(|\mathbf{r}-\mathbf{r}'|,t-t')W_{\sigma'}(\mathbf{r}',t') \tag{7}$$

and the density changes due to spin-flip processes as

$$\delta n_{\sigma\bar\sigma}(\mathbf{r},t)=\int d\mathbf{r}'\int_{-\infty}^{\infty}dt'\,\tilde K_{\sigma\bar\sigma}(|\mathbf{r}-\mathbf{r}'|,t-t')W_{\sigma\bar\sigma}(\mathbf{r}',t'). \tag{8}$$

With the notation $\rho_\sigma(\mathbf{r})=\psi^\dagger_\sigma(\mathbf{r})\psi_\sigma(\mathbf{r})$ and $\rho_{\sigma\bar\sigma}(\mathbf{r})=\psi^\dagger_\sigma(\mathbf{r})\psi_{\bar\sigma}(\mathbf{r})$ for the operators entering Eq. (4), the linear susceptibilities are defined by

$$K_{\sigma\sigma'}(|\mathbf{r}-\mathbf{r}'|,t-t')=-i\hbar\,\theta(t-t')\langle[\rho_\sigma(\mathbf{r},t),\rho_{\sigma'}(\mathbf{r}',t')]\rangle \tag{9}$$

and

$$\tilde K_{\sigma\bar\sigma}(|\mathbf{r}-\mathbf{r}'|,t-t')=-i\hbar\,\theta(t-t')\langle[\rho_{\sigma\bar\sigma}(\mathbf{r},t),\rho_{\sigma\bar\sigma}(\mathbf{r}',t')]\rangle. \tag{10}$$

Here $\theta(t)$ is the Heaviside step function, $\langle\cdots\rangle$ denotes an average over the equilibrium ensemble, and all the operators are in the Heisenberg representation.

More explicitly, the linear response of the EG consists of four induced density changes. In Fourier transform these are the charge-density change $\rho(\mathbf{q},\omega)$, the change $m_z(\mathbf{q},\omega)$ in longitudinal magnetization, and the changes $m_\pm(\mathbf{q},\omega)$ in magnetization due to spin flips. The induced density changes are related to the external fields by[26]

$$\begin{pmatrix} \rho \\ m_z \\ m_+ \\ m_- \end{pmatrix} = \begin{pmatrix} \chi_{ee} & \chi_{em} & 0 & 0 \\ \chi_{me} & \chi_{mm} & 0 & 0 \\ 0 & 0 & \chi_m^+ & 0 \\ 0 & 0 & 0 & \chi_m^- \end{pmatrix} \begin{pmatrix} \phi \\ b_z \\ b_+ \\ b_- \end{pmatrix}. \tag{11}$$

In Eq. (11), we have for simplicity suppressed the $(\mathbf{q},\omega)$ variables. The susceptibilities in this equation are linear combinations of the Fourier transforms of those defined in Eqs. (9) and (10) $[\chi_{\sigma\sigma'}(\mathbf{q},\omega)$ and $\tilde{\chi}_{\sigma\bar{\sigma}}(\mathbf{q},\omega)$, say]. These are $\chi_{ee}=e^2\Sigma_{\sigma\sigma'}\chi_{\sigma\sigma'}$, $\chi_{em}=e\gamma\Sigma_{\sigma\sigma'}\chi_{\sigma\sigma'}\mathrm{sgn}(\sigma')$, $\chi_{me}=e\gamma\Sigma_{\sigma\sigma'}\chi_{\sigma\sigma'}\mathrm{sgn}(\sigma)$, $\chi_{mm}=-\gamma^2\Sigma_{\sigma\sigma'}\chi_{\sigma\sigma'}\mathrm{sgn}(\sigma\sigma')$, and $\chi_m^+=-\gamma^2\tilde{\chi}_{\uparrow\downarrow}$, $\chi_m^-=-\gamma^2\tilde{\chi}_{\downarrow\uparrow}$.

B. Local-field factors

The local-field factors $G_\sigma^\pm(\mathbf{q},\omega)$ are introduced by writing an effective one-electron Hamiltonian $H_\sigma(\mathbf{q},\omega)$ in which an electron with spin σ experiences effective fields embodying exchange and correlation with the surrounding EG. The effective fields are the sum of the external fields and of the fields arising from the induced changes $n_\sigma(\mathbf{q},\omega)$ and $n_{\sigma\bar{\sigma}}(\mathbf{q},\omega)$ in the spin densities. This idea underlies the density-functional approach to inhomogeneous electronic systems and, in the linear regime, the functions $G_\sigma^\pm(\mathbf{q},\omega)$ contain the effect of the exchange-correlation hole in determining the effective coupling of the electron with the EG.[12–14]

The expressions of the effective fields are as follows:[26]

$$W_\sigma^{\mathrm{eff}}(\mathbf{q},\omega)=W_\sigma(\mathbf{q},\omega)+v(q)\{[1-G_\sigma^+(\mathbf{q},\omega)]n(\mathbf{q},\omega) - \mathrm{sgn}(\sigma)G_{L,\sigma}^-(\mathbf{q},\omega)m(\mathbf{q},\omega)\} \tag{12}$$

with $n(\mathbf{q},\omega)\equiv\Sigma_\sigma n_\sigma(\mathbf{q},\omega)$ and $m(\mathbf{q},\omega)\equiv\Sigma_\sigma\mathrm{sgn}(\sigma)\times n_\sigma(\mathbf{q},\omega)$,and

$$W_{\sigma\bar{\sigma}}^{\mathrm{eff}}(\mathbf{q},\omega)=W_{\sigma\bar{\sigma}}(\mathbf{q},\omega)-v(q)G_{T,\bar{\sigma}}^-(\mathbf{q},\omega)n_{\sigma\bar{\sigma}}(\mathbf{q},\omega). \tag{13}$$

The fields W_σ^{eff} induce changes in the electron density and in the density of electrons with spin along the quantization direction, while the fields $W_{\sigma\bar{\sigma}}^{\mathrm{eff}}$ govern spin flips, hence the anisotropy in $G_\sigma^-(\mathbf{q},\omega)$, which gives origin to a longitudinal (L) and a transverse (T) local field. We also note the symmetry property $G_\uparrow^\pm(\mathbf{q},\omega;\zeta)=G_\downarrow^\pm(\mathbf{q},\omega;-\zeta)$.

The response of the EG to the effective fields (12) and (13) is given by the single-particle susceptibilities $\Pi_{\sigma\sigma'}(\mathbf{q},\omega)$. Considering first the longitudinal response, the induced changes in the spin densities are written in the two alternative forms

$$n_\sigma(\mathbf{q},\omega)=\sum_{\sigma'}\chi_{\sigma\sigma'}(\mathbf{q},\omega)W_{\sigma'}(\mathbf{q},\omega) =\sum_{\sigma'}\Pi_{\sigma\sigma'}(\mathbf{q},\omega)W_{\sigma'}^{\mathrm{eff}}(\mathbf{q},\omega). \tag{14}$$

It is then easy to see that the local-field factors are given by

$$G_\uparrow^+=1+\frac{1}{2v(q)}\left(\frac{\chi_{\downarrow\downarrow}-\chi_{\uparrow\downarrow}}{\chi_{\uparrow\uparrow}\chi_{\downarrow\downarrow}-\chi_{\uparrow\downarrow}\chi_{\downarrow\uparrow}}-\frac{1}{\Pi_{\uparrow\uparrow}}\right) \tag{15}$$

and

$$G_{L,\uparrow}^-=\frac{1}{2v(q)}\left(\frac{\chi_{\downarrow\downarrow}+\chi_{\uparrow\downarrow}}{\chi_{\uparrow\uparrow}\chi_{\downarrow\downarrow}-\chi_{\uparrow\downarrow}\chi_{\downarrow\uparrow}}-\frac{1}{\Pi_{\uparrow\uparrow}}\right). \tag{16}$$

Similarly, for the transverse response we have

$$G_{T,\uparrow}^-=\frac{1}{v(q)}\left(\frac{1}{\tilde{\chi}_{\downarrow\uparrow}}-\frac{1}{\Pi_{\downarrow\uparrow}}\right). \tag{17}$$

In these equations we have again suppressed the $(\mathbf{q},\omega)$ variables. The expressions for $G_\downarrow^\pm(\mathbf{q},\omega)$ follow by inverting all spin arrows.

The single-particle response functions are given by

$$\Pi_{\sigma\sigma'}(\mathbf{q},\omega)=\sum_{\mathbf{k}}\frac{n_{\mathbf{k}-\mathbf{q}/2,\sigma}-n_{\mathbf{k}+\mathbf{q}/2,\sigma'}}{\hbar\omega-(\varepsilon_{\mathbf{k}+\mathbf{q}/2,\sigma'}-\varepsilon_{\mathbf{k}-\mathbf{q}/2,\sigma})+i0^+}. \tag{18}$$

In this expression, $\varepsilon_{\mathbf{k},\sigma}$ are the single-particle energies $[\varepsilon_{\mathbf{k},\sigma}=\hbar^2q^2/2m-\gamma\,\mathrm{sgn}(\sigma)B_z$ in the presence of a static magnetic field $B_z]$ and $n_{\mathbf{k},\sigma}$ are the momentum distributions for the two spin populations. In the EG literature, the distribution $n_{\mathbf{k},\sigma}$ in Eq. (18) has been alternatively chosen as the ideal Fermi distribution[28] or as the true momentum distribution of the interacting EG.[23] These alternative choices imply different expressions for the local-field factors.[29]

We conclude this section by remarking that the explicit expression for the matrix of susceptibilities in Eq. (11), written in terms of the single-particle susceptibilities $\Pi_{\sigma\sigma'}$ and of the local-field factors $G_\sigma^\pm$, can be found in the paper of Marinescu and Quinn.[26]

III. THE LIMIT OF LARGE WAVE NUMBER

In this section, we use the method developed by Niklasson[23] and by Zhu and Overhauser[24] to calculate the asymptotic values of the local-field factors at large wave number in the case in which $n_{\mathbf{k},\sigma}$ in Eq. (18) is the true momentum distribution function. In this method, one evaluates the equation of motion for the one-particle Wigner distribution function (see also Ref. 26) and uses an exact relationship between the two-particle Wigner distribution function at equilibrium $[f^{(2)}_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}(\mathbf{q})$, say] and the partial structure factors $S_{\sigma\sigma'}(q)$ defined in Eq. (2). This relation is

$$\sum_{\mathbf{k},\mathbf{k}'}f^{(2)}_{\mathbf{k},\sigma;\mathbf{k}',\sigma'}(\mathbf{q})=(n_\sigma n_{\sigma'})^{1/2}[S_{\sigma\sigma'}(q)-\delta_{\sigma\sigma'}]. \tag{19}$$

One can then show that in any space dimension the functions $G^{\pm}_{\uparrow}(\mathbf{q},\omega)$ for finite frequency and large wave number take the following expressions:

$$G^{+}_{\uparrow}(\mathbf{q},\omega)\to\frac{(1-\zeta)}{(1-\zeta^2)^2}\sum_{\mathbf{q}'}\sum_{\sigma,\sigma'}\frac{(n_\sigma n_{\sigma'})^{1/2}}{n^2}[1+\mathrm{sgn}(\sigma)]\times\{[1-\zeta\,\mathrm{sgn}(\sigma)]f_1(\mathbf{q},\mathbf{q}')-[1-\zeta\,\mathrm{sgn}(\sigma')]f_2(\mathbf{q},\mathbf{q}')\}[S_{\sigma\sigma'}(q')-\delta_{\sigma\sigma'}], \tag{20}$$

$$G^{-}_{L,\uparrow}(\mathbf{q},\omega)\to\frac{(1-\zeta)}{(1-\zeta^2)^2}\sum_{\mathbf{q}'}\sum_{\sigma,\sigma'}\frac{(n_\sigma n_{\sigma'})^{1/2}}{n^2}[1+\mathrm{sgn}(\sigma)]\times\{[\mathrm{sgn}(\sigma)-\zeta]f_1(\mathbf{q},\mathbf{q}')-[\mathrm{sgn}(\sigma')-\zeta]f_2(\mathbf{q},\mathbf{q}')\}[S_{\sigma\sigma'}(q')-\delta_{\sigma\sigma'}], \tag{21}$$

and

$$G^{-}_{T,\uparrow}(\mathbf{q},\omega)\to\sum_{\mathbf{q}'}\sum_{\sigma,\sigma'}\frac{(n_\sigma n_{\sigma'})^{1/2}}{n^2}[f_1(\mathbf{q},\mathbf{q}')-\mathrm{sgn}(\sigma\sigma')f_2(\mathbf{q},\mathbf{q}')][S_{\sigma\sigma'}(q')-\delta_{\sigma\sigma'}]. \tag{22}$$

In Eqs. (20)–(22), we have defined $f_1(\mathbf{q},\mathbf{q}')=[(\mathbf{q}\cdot\mathbf{q}')^2v(q')]/[q^4v(q)]$ and $f_2(\mathbf{q},\mathbf{q}')=\{[\mathbf{q}\cdot(\mathbf{q}+\mathbf{q}')]^2v(|\mathbf{q}+\mathbf{q}'|)\}/[q^4v(q)]$.

In dimensionality $D=2$, we have $v(q)=2\pi e^2/q$ and hence $f_1(\mathbf{q},\mathbf{q}')\to0$ and $f_2(\mathbf{q},\mathbf{q}')\to1$ in the limit $q\to\infty$. Furthermore, from Eq. (2) we have

$$\sum_{\mathbf{q}'}[S_{\sigma\sigma'}(q')-\delta_{\sigma\sigma'}]=(n_\sigma n_{\sigma'})^{1/2}[g_{\sigma\sigma'}(0)-1]. \tag{23}$$

Hence,

$$G^{+}_{\uparrow}(\mathbf{q},\omega)\to-\frac{(1-\zeta)}{(1-\zeta^2)^2}\sum_{\sigma,\sigma'}\frac{n_\sigma n_{\sigma'}}{n^2}[1+\mathrm{sgn}(\sigma)]\times[1-\zeta\,\mathrm{sgn}(\sigma')][g_{\sigma\sigma'}(0)-1], \tag{24}$$

$$G^{-}_{L,\uparrow}(\mathbf{q},\omega)\to\frac{(1-\zeta)}{(1-\zeta^2)^2}\sum_{\sigma,\sigma'}\frac{n_\sigma n_{\sigma'}}{n^2}[1+\mathrm{sgn}(\sigma)]\times[\zeta-\mathrm{sgn}(\sigma')][g_{\sigma\sigma'}(0)-1], \tag{25}$$

and

$$G^{-}_{T,\uparrow}(\mathbf{q},\omega)\to-\sum_{\sigma,\sigma'}\frac{n_\sigma n_{\sigma'}}{n^2}\mathrm{sgn}(\sigma\sigma')[g_{\sigma\sigma'}(0)-1]. \tag{26}$$

To complete the calculation, we only need to use the values $g_{\uparrow\uparrow}(0)=g_{\downarrow\downarrow}(0)=0$ from the Pauli principle and the symmetry property $g_{\uparrow\downarrow}(0)=g_{\downarrow\uparrow}(0)$. The results are collected in Table I together with those obtained in $D=3$ by Marinescu and Quinn.[26] Notice that their definition of $g_{\sigma\sigma'}(r)$ differs from that given in Sec. II: Table I consistently uses our definition. These values can be rewritten in terms of $g(0)$ through the relation $g(0)=(1-\zeta^2)g_{\uparrow\downarrow}(0)/2$.

TABLE I. Exact limiting values of the local-field factors $G^{\pm}_{\sigma}(\mathbf{q}\to\infty,\omega)$ for a spin-polarized EG in dimensionality $D=2$ (first column) and $D=3$ (second column).

	2D	3D[a]
$G^{+}_{\uparrow}$	$1-\frac{1}{2}g_{\uparrow\downarrow}(0)$	$\frac{1}{3(1+\zeta)}[2+3\zeta-(1+2\zeta)g_{\uparrow\downarrow}(0)]$
$G^{-}_{L,\uparrow}$	$\frac{1}{2}g_{\uparrow\downarrow}(0)$	$\frac{1}{3(1+\zeta)}[-1+(2+\zeta)g_{\uparrow\downarrow}(0)]$
$G^{-}_{T,\uparrow}$	$\zeta^2+\frac{1}{2}(1-\zeta^2)g_{\uparrow\downarrow}(0)$	$\frac{1}{3}[-1+3\zeta^2+2(1-\zeta^2)g_{\uparrow\downarrow}(0)]$

[a]From Marinescu and Quinn (Ref. 26).

Two further comments are needed on our results for $D=2$ in Table I. First, in the case $\zeta=0$ we recover the results of Santoro and Giuliani[25] for the paramagnetic state, i.e., $G^{+}\to1-g(0)$ and $G^{-}_{L}=G^{-}_{T}\to g(0)$. Second, the value of $g_{\uparrow\downarrow}(0)$ is mainly determined by two-body collisions[30,31] and (with our definitions) may be expected to show little sensitivity to the degree of spin polarization at any given value of the coupling strength. Calculations of $g_{\uparrow\downarrow}(0)$ as a function of the coupling strength in the 2D EG are already available in the literature.[32,33]

The asymptotic expressions for the local-field factors in the case when $n_{\mathbf{k},\sigma}$ in Eq. (18) is replaced by the ideal Fermi distribution are derived in Appendix A. We proceed instead in the next section to evaluate the quantities $G^{\pm}_{\sigma}(\mathbf{q},0)$ in the limit $q\to0$.

IV. THE THERMODYNAMIC LIMIT

We have recalled in Sec. II that the values of $G^{\pm}(q\to0,0)$ for the EG in the paramagnetic state are related to its thermodynamic compressibility K and magnetic susceptibility χ. In 2D these relations are[25]

$$G^{+}(q\to0,0)=\frac{q}{2\pi n^2e^2}\left(\frac{1}{K_0}-\frac{1}{K}\right) \tag{27}$$

and

$$G^{-}(q\to0,0)=\frac{\hbar^2q}{2me^2}\left(1-\frac{\chi_0}{\chi}\right), \tag{28}$$

where K_0 and χ_0 refer to the ideal Fermi gas. In this context, the local-field factors are defined with reference to the noninteracting EG, i.e., by using the ideal Fermi distribution in place of the true momentum distribution $n_{\mathbf{k},\sigma}$ in Eq. (18).

Let us first consider the longitudinal response matrix and the corresponding local fields in the spin-polarized fluid. These take the forms given in Eqs. (15) and (16) except for the replacement of $\Pi_{\sigma\sigma'}(\mathbf{q},\omega)$ by the susceptibilities of the ideal Fermi gas. We may now refer to the work of Caccamo *et al.*,[27] in which the structure of the susceptibilities $\chi_{\sigma\sigma'}(\mathbf{q},\omega)$ for the spin-polarized 3D EG was derived from the equation of motion of $n_\sigma(\mathbf{q},\omega)$ by means of a functional differentiation technique. This approach is especially useful at long wavelengths and low frequencies, where the functional derivatives reduce to local derivatives. In fact, Caccamo *et al.*[27] obtained explicit expressions for the susceptibilities not only for the static (thermodynamic) susceptibilities, but also for the leading (hydrodynamic) terms in a low-frequency expansion.

Using this method, therefore, it is easy to show that in space dimension D the thermodynamic values of the longitudinal local-field factors are given by

$$G_{\uparrow}^{+}(q\to 0,0)\to -\frac{1}{n_{\uparrow}Dv(q)}\frac{\partial}{\partial n}(2t_{\uparrow}+u_{\uparrow}-2t_{\uparrow}^{(0)}) \quad (29)$$

and

$$G_{L,\uparrow}^{-}(q\to 0,0)\to -\frac{1}{n\, n_{\uparrow}Dv(q)}\frac{\partial}{\partial \zeta}(2t_{\uparrow}+u_{\uparrow}-2t_{\uparrow}^{(0)}). \quad (30)$$

The values of $G_{\downarrow}^{+}(q\to 0,0)$ and $G_{L,\downarrow}^{-}(q\to 0,0)$ are obtained by inverting all spin arrows. In Eqs. (29) and (30), we have introduced the equilibrium quantities

$$t_{\sigma}=\sum_{\mathbf{k}} n_{\mathbf{k},\sigma}\frac{\hbar^2k^2}{2m} \quad (31)$$

and

$$u_{\sigma}=\tfrac{1}{2}\int d\mathbf{r}\, v(r)[\langle \rho_{\sigma}(\mathbf{R})\rho(\mathbf{R}+\mathbf{r})\rangle - n_{\sigma}n]. \quad (32)$$

These are the kinetic- and potential-energy densities for electrons of spin σ. The quantity $t_{\sigma}^{(0)}$ is given by Eq. (31) as calculated on the ideal Fermi gas.

It is immediately evident from Eqs. (29) and (30) that the local-field factors in the thermodynamic limit are proportional to q^2 in 3D and to q in 2D. Furthermore, the appropriate generalizations of Eqs. (27) and (28) are

$$n_{\uparrow}G_{\uparrow}^{+}(q\to 0,0)+n_{\downarrow}G_{\downarrow}^{+}(q\to 0,0) \to -\frac{1}{Dv(q)}\frac{\partial}{\partial n}(2t+u-2t^{(0)}) \quad (33)$$

and

$$n_{\uparrow}G_{L,\uparrow}^{-}(q\to 0,0)+n_{\downarrow}G_{L,\downarrow}^{-}(q\to 0,0) \to -\frac{1}{D\, n\, v(q)}\frac{\partial}{\partial \zeta}\left[\sum_{\sigma} \mathrm{sgn}(\sigma)(2t_{\sigma}+u_{\sigma}-2t_{\sigma}^{(0)})\right]. \quad (34)$$

For Eq. (33), the virial theorem in the usual form $2t+u=DP$, P being the pressure, yields

$$n_{\uparrow}G_{\uparrow}^{+}(q\to 0,0)+n_{\downarrow}G_{\downarrow}^{+}(q\to 0,0)\to \frac{1}{n\, v(q)}\left(\frac{1}{K_0}-\frac{1}{K}\right). \quad (35)$$

Similarly, Eq. (34) can be handled by means of a magnetic virial theorem, first reported for the paramagnetic EG by Caccamo *et al.*[34] A general proof is given in Appendix B. We have

$$2(t_{\uparrow}-t_{\downarrow})+(u_{\uparrow}-u_{\downarrow})=Dn\gamma b_z \quad (36)$$

and hence

$$\gamma[n_{\uparrow}G_{L,\uparrow}^{-}(q\to 0,0)+n_{\downarrow}G_{L,\downarrow}^{-}(q\to 0,0)]\to \frac{n\gamma^2}{v(q)}\left(\frac{1}{\chi_0}-\frac{1}{\chi}\right), \quad (37)$$

having defined $\chi^{-1}=n^{-1}\partial b_z/\partial \zeta$. Evidently, the sum rules on compressibility and on longitudinal susceptibility are valid for arbitrary spin polarization and EG dimensionality.

Turning to the spin-flip response, the method of Caccamo *et al.*[27] is easily applied to find the result

$$G_{T,\uparrow}^{-}(q\to 0,0)\to -\frac{2}{Dnv(q)}\frac{\partial}{\partial n_{\downarrow\uparrow}}(2t_{\downarrow\uparrow}+u_{\downarrow\uparrow}-2t_{\downarrow\uparrow}^{(0)}) \quad (38)$$

with the further definitions

$$t_{\sigma\bar{\sigma}}=\sum_{\mathbf{k}} n_{\mathbf{k},\sigma\bar{\sigma}}\frac{\hbar^2k^2}{2m}, \quad (39)$$

$$u_{\sigma\bar{\sigma}}=\tfrac{1}{2}\int d\mathbf{r}\, v(r)\langle \rho_{\sigma\bar{\sigma}}(\mathbf{R})\rho(\mathbf{R}+\mathbf{r})\rangle, \quad (40)$$

and

$$n_{\mathbf{k},\sigma\bar{\sigma}}=\int d\mathbf{r}\langle \psi_{\sigma}^{\dagger}(\mathbf{R}+\tfrac{1}{2}\mathbf{r})\psi_{\bar{\sigma}}(\mathbf{R}-\tfrac{1}{2}\mathbf{r})\rangle \exp(i\mathbf{k}\cdot\mathbf{r}). \quad (41)$$

Again, the value of $G_{T,\downarrow}^{-}(q\to 0,0)$ is obtained from Eq. (38) by inverting all spin arrows.

Another form of the virial theorem concerning the transverse spin-flip susceptibility suggests itself from Eq. (38). This theorem is also proved in Appendix B and reads

$$\begin{aligned} 2t_{\uparrow\downarrow}+u_{\uparrow\downarrow}&=D\gamma n_{\uparrow}b_{+},\\ 2t_{\downarrow\uparrow}+u_{\downarrow\uparrow}&=D\gamma n_{\downarrow}b_{-}. \end{aligned} \quad (42)$$

We accordingly find from Eq. (38)

$$G_{T,\uparrow}^{-}(q\to 0,0)\to -\frac{2n_{\downarrow}}{nv(q)}\left(\frac{1}{\tilde{\chi}_{\downarrow\uparrow}^{(0)}}-\frac{1}{\tilde{\chi}_{\downarrow\uparrow}}\right). \quad (43)$$

This relation, with its analog for $G_{T,\downarrow}^{-}(q\to 0,0)$, is a thermodynamic sum rule applying to the transverse susceptibility in a spin-polarized EG.

V. CONCLUSIONS

The local-field factors incorporate the effects of exchange and correlation in the linear-response functions of the EG. Knowledge of them is essential for the evaluation of the many-body contributions to a number of physical properties for systems of electronic carriers in semiconductors and metals. They also give the basic information for density-functional calculations on weakly inhomogeneous electronic systems.

In a strong-coupling regime, the Coulomb interaction between electrons may induce a finite spin polarization in the EG. Recent quantal simulations[5,8] have reported different behaviors of the ground state as a function of coupling strength and spin polarization in different space dimensions. At any rate, in a two-dimensional EG the application of an in-plane magnetic field can be used to induce such spin polarization and to explore the role of this system parameter over a wide range of values in the absence of diamagnetic effects.

With the above facts in mind, we have studied the exact limiting behaviors of the local-field factors in a spin-polarized EG. In the regime of large wave number, we have recovered the results of Marinescu and Quinn[26] in space dimension $D=3$ and derived the corresponding results in $D=2$. We have also examined an alternative definition of the local-field factors for both dimensionalities in this regime. Finally, we have extended to a spin-polarized EG the sum rules on the thermodynamic compressibility and on the longitudinal magnetic susceptibility, and we derived a rule regarding the transverse magnetic susceptibility.

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APPENDIX A: ASYMPTOTIC EXPRESSIONS OF THE LOCAL-FIELD FACTORS WITH REFERENCE TO THE IDEAL FERMI GAS

As noted in Sec. III, an alternative definition of the local-field factors $[G_\sigma^{\pm(0)}(\mathbf{q},\omega)$, say$]$ is obtained form Eqs. (15)–(17) when the single-particle susceptibility is calculated from Eq. (18) by using the ideal Fermi distribution $n_{\mathbf{k},\sigma}^{(0)}$ in place of the true momentum distribution $n_{\mathbf{k},\sigma}$. This behavior is relevant to the evaluation of static local-field factors by quantal simulation techniques (see, e.g., Ref. 7). We follow the approach of Holas[29] to obtain the expressions of $\Delta G_\sigma^{\pm} \equiv G_\sigma^{\pm(0)} - G_\sigma^{\pm}$ at large wave number and finite frequency.

The calculation hinges on the large-q expansion of $\Pi_{\sigma\sigma'}(\mathbf{q},\omega)$, which reads

$$\Pi_{\sigma\sigma'}(\mathbf{q},\omega)\to -\frac{2m}{\hbar^2 q^2}\left\{ n_\sigma + n_{\sigma'} + \frac{4}{q^2}[\langle(\hat{\mathbf{q}}\cdot\mathbf{k})^2\rangle_\sigma + \langle(\hat{\mathbf{q}}\cdot\mathbf{k})^2\rangle_{\sigma'}]\right\}, \tag{A1}$$

where we have defined $\langle(\hat{\mathbf{q}}\cdot\mathbf{k})^2\rangle_\sigma = \Sigma_{\mathbf{k}} n_{\mathbf{k},\sigma}(\hat{\mathbf{q}}\cdot\mathbf{k})^2$. A straightforward calculation yields

$$\Delta G_\uparrow^+(\mathbf{q},\omega)\to\Delta G_{L,\uparrow}^-(\mathbf{q},\omega)\to\frac{n\hbar^2 q^2\Delta_\uparrow}{2n_\uparrow^2 m^2\omega_p^2(q)} \tag{A2}$$

and

$$\Delta G_{T,\uparrow}^-(\mathbf{q},\omega)\to\frac{2\hbar^2 q^2\Delta}{nm^2\omega_p^2(q)} \tag{A3}$$

for the 2D EG, with the value of the plasma frequency given by $\omega_p^2(q)=2\pi n e^2 q/m$. The quantities Δ_σ and Δ in these equations are given by

$$\Delta_\sigma = \sum_{\mathbf{k}} (n_{\mathbf{k},\sigma} - n_{\mathbf{k},\sigma}^{(0)})(\hat{\mathbf{q}}\cdot\mathbf{k})^2 \tag{A4}$$

and $\Delta = \Sigma_\sigma \Delta_\sigma$. These quantities are proportional to the shifts in kinetic energy associated with the difference between the two types of momentum distribution. Clearly, the shifts $\Delta G_\sigma^{\pm}$ grow linearly with q in 2D.

Equations (A2)–(A4) also give the leading terms of $\Delta G_\sigma^{\pm}$ in $D=3$, provided that the plasma frequency is replaced by $\omega_p^2 = 4\pi n e^2/m$. Thus the shift in local-field factors grows as q^2 to leading order in 3D.[29] However, in this space dimension one also finds a constant contribution to $\Delta G_\sigma^{\pm}$, which is determined by the shift in the mean-square kinetic energy. The results are

$$\Delta G_\uparrow^+(\mathbf{q},\omega)\to\Delta G_{L,\uparrow}^-(\mathbf{q},\omega)\to\frac{n\hbar^2}{2n_\uparrow^2 m^2\omega_p^2}\left(\Delta_\uparrow q^2 - 4\frac{\Delta_\uparrow'}{n_\uparrow}\right) \tag{A5}$$

and

$$\Delta G_{T,\uparrow}^-(\mathbf{q},\omega)\to\frac{2\hbar^2}{nm^2\omega_p^2}\left(\Delta\, q^2 - 4\frac{\Delta'}{n}\right), \tag{A6}$$

where we have defined

$$\Delta_\uparrow' = \left[\sum_{\mathbf{k}} n_{\mathbf{k},\uparrow}(\hat{\mathbf{q}}\cdot\mathbf{k})^2\right]^2 - \left[\sum_{\mathbf{k}} n_{\mathbf{k},\uparrow}^{(0)}(\hat{\mathbf{q}}\cdot\mathbf{k})^2\right]^2 \tag{A7}$$

and

$$\Delta' = \left[\sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma}(\hat{\mathbf{q}}\cdot\mathbf{k})^2\right]^2 - \left[\sum_{\mathbf{k},\sigma} n_{\mathbf{k},\sigma}^{(0)}(\hat{\mathbf{q}}\cdot\mathbf{k})^2\right]^2. \tag{A8}$$

APPENDIX B: MAGNETIC VIRIAL THEOREMS

We introduce the operator

$$A_\sigma = -\tfrac{1}{2} i\hbar\,\mathrm{sgn}(\sigma)\int d^D\mathbf{r}\,\psi_\sigma^\dagger(\mathbf{r})\mathbf{r}\cdot\frac{\partial}{\partial\mathbf{r}}\psi_\sigma(\mathbf{r}) \tag{B1}$$

and evaluate its commutator with the Hamiltonian $\mathcal{H}=\mathcal{H}_0+\mathcal{H}_z$, where $\mathcal{H}_0$ is given by Eq. (1) and $\mathcal{H}_z$ is the Zeeman Hamiltonian,

$$\mathcal{H}_z = -\gamma\int d^D\mathbf{r}\,b_z(\mathbf{r})\sum_\sigma \mathrm{sgn}(\sigma)\psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r}). \tag{B2}$$

The magnetic field is being taken as position-dependent in order to correctly treat boundary terms, but will ultimately be allowed to attain a constant value.

The commutator of A_σ with $\mathcal{H}_0$ is easily calculated using the canonical anticommutator relations, with the result

$$\langle[A_\sigma,\mathcal{H}_0]\rangle=-\tfrac{1}{2}i\hbar\,\mathrm{sgn}(\sigma)(2t_\sigma+u_\sigma) \tag{B3}$$

for its ground-state expectation value. The definitions in Eqs. (31) and (32) have been used. On the other hand, the commutator with the Zeeman term is

$$[A_\sigma,\mathcal{H}_z]=\frac{1}{2}i\hbar\gamma\int d^D\mathbf{r}[\mathbf{r}\cdot\boldsymbol{\nabla}b_z(\mathbf{r})]\psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r}). \tag{B4}$$

After an integration by parts and use of the divergence theorem, the limit of a constant magnetic field can be taken and Eq. (B4) becomes

$$[A_\sigma,\mathcal{H}_z]=-\tfrac{1}{2}i\hbar\gamma b_z\int_{\mathrm{surface}}\mathbf{r}\cdot d\mathbf{s}\,\psi_\sigma^\dagger(\mathbf{r})\psi_\sigma(\mathbf{r}). \tag{B5}$$

This yields

$$\langle[A_\sigma,\mathcal{H}_z]\rangle=-\tfrac{1}{2}i\hbar D\,\gamma n_\sigma b_z. \tag{B6}$$

Finally, by imposing that the expectation value of $\Sigma_\sigma A_\sigma$ should be constant in time, we find from Eqs. (B3) and (B6) the result given in Eq. (36) of the main text.

A similar theorem holds for the transverse susceptibility. We consider the operator

$$A_+=-i\hbar\int d^D\mathbf{r}\,\psi_\uparrow^\dagger(\mathbf{r})\mathbf{r}\cdot\frac{\partial}{\partial\mathbf{r}}\psi_\downarrow(\mathbf{r}) \tag{B7}$$

and its commutator with $\mathcal{H}_0+\mathcal{H}_+$, where

$$\mathcal{H}_+=-\gamma\int d^D\mathbf{r}\,b_+(\mathbf{r})\psi_\downarrow^\dagger(\mathbf{r})\psi_\uparrow(\mathbf{r}). \tag{B8}$$

The same steps as given above to obtain Eqs. (B3) and (B6) lead to the first of Eqs. (42) in the main text. A similar calculation for the field $b_-(\mathbf{r},t)$ completes the derivation of Eqs. (42).

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