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Exact limits of the many-body local fields in a two-dimensional electron gas

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We have derived the exact limiting behavior of the many-body local fields $G_{\pm}(\mathbf{q},\omega)$ in a two-dimensional electron gas. At large wave vectors and finite frequencies these functions can be expressed in terms of $g(0)$, the value at the origin of the pair correlation function of the electron gas. We find in particular that in this limit $G_{+}(\infty,\omega)=1-g(0)$, and $G_{-}(\infty,\omega)=g(0)$. Our results provide new insight into the problem of the many-body vertex corrections in this interacting system.

The effect of exchange and correlation can be incorporated into the wave-vector- and frequency-dependent charge and spin susceptibility of an electron gas by introducing many-body local fields.[1] The charge and spin susceptibility of this system can be written as

$$\chi_c(\mathbf{q},\omega)=\frac{\chi_0(\mathbf{q},\omega)}{1-v(q)[1-G_{+}(\mathbf{q},\omega)]\chi_0(\mathbf{q},\omega)}\ , \tag{1}$$

$$\chi_s(\mathbf{q},\omega)=-\mu_B^2\frac{\chi_0(\mathbf{q},\omega)}{1+v(q)G_{-}(\mathbf{q},\omega)\chi_0(\mathbf{q},\omega)}\ , \tag{2}$$

where $\chi_0(\mathbf{q},\omega)$ is the Lindhard response function.[2] $v(q)$ is the Fourier transform of the Coulomb potential and μ_B is the Bohr magneton. Equations (1) and (2) define the many-body local fields $G_{+}(\mathbf{q},\omega)$ and $G_{-}(\mathbf{q},\omega)$. These quantities are the many-body analogues in the electron liquid of the familiar Clausius-Mossotti local fields of electrostatics. Using an alternative but physically equivalent description the $G_{\pm}(\mathbf{q},\omega)$'s can be regarded as vertex corrections.[1,3] The knowledge of the correct form of these functions is necessary in any quantitative calculations of the effects of the electron-electron interaction on many physical properties of interest. The most conspicuous examples are the effective mass and the spin susceptibility. As we shall show this is especially true for a two-dimensional electron gas (2D EG).

In the particular case of a 2D EG these functions are largely unknown and it is therefore useful, and timely, to determine their exact behavior in the limit of large and small wave vectors. This is the purpose of the present paper.

We will discuss first the large wave vector behavior. For the three-dimensional electron gas (3D EG) much work has been done. Some of the earlier studies have attempted to derive expressions for the $G_{\pm}(\mathbf{q},\omega)$'s via approximate solutions of the many-body problem.[4,1] This approach, although useful, has only led to results of uncontrolled validity. More recently however some work has been focused on extracting, via a frontal attack on the many-body problem, the exact properties of the local fields. The present analysis will only deal with the latter and more fundamental viewpoint. Table I provides a summary of the most relevant results.

Kimball[5] has derived the large q behavior of the local fields under the assumption that these functions are independent of frequency. Kimball's assumption however is unjustified since the frequency dependence of the $G_{\pm}(\mathbf{q},\omega)$'s is in fact important. Niklasson[6] has derived an exact expression for the finite frequency and large wave vector limit of $G_{+}(\mathbf{q},\omega)$ in terms of $g(0)$, the value at the origin of the pair distribution function. Following an approach based on the equation-of-motion method he studied the linear response of the system to an external potential and found that $G_{+}(\infty,\omega)=\frac{2}{3}[1-g(0)]$ (see Table I). Zhu and Overhauser[7] carried out a similar analysis for the spin response of the same system and arrived at the complementary result $G_{-}(\infty,\omega)=\frac{1}{3}[4g(0)-1]$ (see Table I). The asymptotic values of $G_{\pm}(\infty,\omega)$ can be then estimated once the value of $g(0)$ is known.[8] In general $g(0)$ will depend on the electronic density and so will the $G_{\pm}(\infty,\omega)$'s.

We turn now to the derivation of the analogous relations for the $G_{\pm}(\mathbf{q},\omega)$ in the 2D EG. Following the method used in Refs. 6 and 7 it can be shown that in any space dimension for finite frequencies and large wave vectors $G_{\pm}(\mathbf{q},\omega)$ can be expressed as

$$G_{\pm}(\mathbf{q},\omega)\approx\frac{1}{2N}\sum_{\mathbf{q}'}\sum_{\sigma,\sigma'}\left[\frac{(\mathbf{q}\cdot\mathbf{q}')^2 v(\mathbf{q}')}{q^4 v(\mathbf{q})}-\eta_{\pm}(\sigma\sigma')\right]\times[S_{\sigma\sigma'}(\mathbf{q}')-\delta_{\sigma\sigma'}], \tag{3}$$

where $\eta_{+}(\sigma\sigma')=1$ and $\eta_{-}(\sigma\sigma')=\mathrm{sgn}(\sigma\sigma')$. In Eq. (3) $S_{\sigma\sigma'}(\mathbf{q})$ is a static structure factor and is defined as

$$S_{\sigma\sigma'}(\mathbf{q})=\frac{2}{N}\langle\Psi_0\,|\,n_\sigma^\dagger(\mathbf{q})n_{\sigma'}(\mathbf{q})\,|\,\Psi_0\rangle-\frac{N}{2}\delta_{\mathbf{q},0}, \tag{4}$$

where $n_\sigma(\mathbf{q})$ is the Fourier transform of the electron density operator for spin projection σ, and the expectation value is taken over $|\Psi_0\rangle$, the ground state of the system. The usual charge and spin static structure factors can be readily related to $S_{\sigma\sigma'}(\mathbf{q})$. A direct inspection of Eq. (3) clearly shows that since in a 2D EG $v(q)=2\pi e^2/q$, in the large q limit the first term can be neglected, and one is left with

$$G_{\pm}(\mathbf{q},\omega)\approx\frac{1}{2}\sum_{\sigma,\sigma'}\eta_{\pm}(\sigma\sigma')[\tfrac{1}{2}-g_{\sigma\sigma'}(0)], \tag{5}$$

TABLE I. Exact asymptotic values ($q \rightarrow \infty$) of the local fields $G_{\pm}(\mathbf{q},\omega)$ for both a 3D EG (first two columns) and a 2D EG (last two columns). On the left the appropriate value of the frequency ω is given. The first row corresponds to a case in which the $G_{\pm}(\mathbf{q},\omega)$'s are assumed to be frequency independent.

	3D		2D	
	G_+	G_-	G_+	G_-
ignoring the ω dependence	$1-g(0)$[a]	$g(0)$[a]	$1-g(0)$[b]	$g(0)$[b]
finite ω	$\frac{2}{3}[1-g(0)]$[c]	$\frac{1}{3}[4g(0)-1]$[d]	$1-g(0)$[b]	$g(0)$[b]
$\omega=\hbar q^2/2m$	$1-g(0)$[b]	$g(0)$[b]	$1-g(0)$[b]	$g(0)$[b]

[a]Kimball, Ref. 5.
[b]Santoro and Giuliani, present work.
[c]Niklasson, Ref. 6.
[d]Zhu and Overhauser, Ref. 7.

where the pair correlation function $g_{\sigma\sigma'}(r)$ has been introduced via the following relation with the structure factor $S_{\sigma\sigma'}(\mathbf{q})$:

$$g_{\sigma\sigma'}(r)=\frac{1}{2}+\frac{1}{N}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}[S_{\sigma\sigma'}(\mathbf{q})-\delta_{\sigma\sigma'}]. \quad (6)$$

The familiar (symmetric) pair correlation function g(r) can be obtained from $g_{\sigma\sigma'}(r)$ by simply summing over the spin indices

$$g(r)=\tfrac{1}{2}\sum_{\sigma,\sigma'} g_{\sigma\sigma'}(r). \quad (7)$$

From Eq. (5) one can then readily obtain the following exact large q (finite ω) asymptotic values: $G_+(\infty,\omega)=1-g(0)$ and $G_-(\infty,\omega)=g(0)$ (see Table I). The following items are worth mentioning: (i) Our results imply that within the Hartree-Fock approximation in which $g^{\mathrm{HF}}(0)=\frac{1}{2}$, for a 2D EG one has $G_{\pm}^{\mathrm{HF}}(\infty,\omega)=\frac{1}{2}$. This can be compared with the corresponding value of $\frac{1}{3}$ in the 3D EG case.[9] (ii) Our result for $G_-(\infty,\omega)$ is by definition a positive number for all electronic densities. This should be contrasted with the corresponding result for the 3D EG of Zhu and Overhauser[7] which for metallic densities seems to predict a perhaps surprising negative value for this quantity. Finally it can be shown that in a 2D EG if the frequency dependence of the local fields is neglected one arrives at the same results, i.e. $G_+(\infty)=1-g(0)$ and $G_-(\infty)=g(0)$ (see Table I).

We next turn our attention to the zero frequency long wavelength limit of the $G_{\pm}(\mathbf{q},\omega)$'s. In this case ω is set to be equal to zero before letting q vanish. The behavior of the local fields in this situation can be simply related to the static response properties of the system. For the case of a 3D EG the reader is referred for instance to the discussion of Refs. 10 and 7.

For a 2D EG the situation is more interesting in that in this limit the $G_{\pm}(\mathbf{q},0)$'s are linearly proportional to $q=|\mathbf{q}|$ as opposed to the q^2 behavior of the corresponding three-dimensional quantities. Making use of the compressibility sum rule and of Eq. (1) one obtains in this case

$$G_+(\mathbf{q},0)\approx(1+\alpha)(q/\pi k_F), \quad q\rightarrow 0, \quad (8)$$

where the constant α depends on the electronic density, and can be determined in terms of $w_c(k_F)$, the correlation energy per particle in a 2D EG. We obtain

$$\alpha=-(3\pi/4e^2)[w_c'(k_F)+\tfrac{1}{3}k_F w_c''(k_F)]. \quad (9)$$

$w_c(k_F)$ can in turn be obtained from the various numerical calculations available in the literature.[11–14]

In an analogous manner the small q limit of $G_-(\mathbf{q},0)$ is related to the many-body enhancement of the spin susceptibility $s=\chi_s(\mathbf{q}\rightarrow 0,0)/\chi_P$, χ_P being the Pauli susceptibility. Making use of Eq. (2) we obtain

$$G_-(\mathbf{q},0)\approx\frac{(s-1)}{s}\frac{q}{q_{\mathrm{TF}}}, \quad q\rightarrow 0, \quad (10)$$

where in a 2D EG the Thomas-Fermi wave vector q_{TF} is given by $2/a_B$, a_B being the effective Bohr radius. Experimental[15] and theoretical[16] values for s are available in the literature and can be used to correctly estimate $G_-(\mathbf{q},0)$ in this limit.

In the previous discussion the frequency variable has been neglected or assumed to acquire finite values. In actual calculations however it is necessary to allow for the frequency dependence of the local fields. In particular for large q it is often relevant to evaluate the behavior of $G_{\pm}(\mathbf{q},\omega)$ when $\omega=\hbar q^2/2m$. This can be accomplished by following a procedure employed by Kimball[5] in his study of the 3D EG. In this case however, at variance with Kimball's original analysis, the frequency dependence of the local fields must be explicitly allowed for. For the sake of brevity we will report here only the calculation related to the case of $G_+(\mathbf{q},\hbar q^2/2m)$ for a 2D EG. One starts with the well known exact relation between the static structure factor $S(\mathbf{q})=\frac{1}{2}\sum_{\sigma,\sigma'}S_{\sigma\sigma'}(\mathbf{q})$, and the response function $\chi_c(\mathbf{q},\omega)$ of Eq. (1):

$$S(\mathbf{q})=-\frac{1}{\pi n}\int_0^{\infty} d\omega\,\mathrm{Im}[\chi_c(\mathbf{q},\omega)]. \quad (11)$$

$S(\mathbf{q})$ is in turn related to $g'(0)$, the value at the origin of the derivative $\partial g(r)/\partial r$, by the following exact relation valid in two dimensions:

$$g'(0)=\lim_{q\to\infty} -\frac{q^3}{2\pi n}[S(\mathbf{q})-1]. \quad (12)$$

Making use of Eqs. (1), (11), and (12) we arrive at the simple result $G_+(\mathbf{q},\hbar q^2/2m)\approx 1-\frac{1}{2}a_B g'(0)=1-g(0)$. In the last step we have made use of the two-dimensional version of the cusp theorem,[17] stating that $g'(0)=2a_B^{-1}g(0)$. The latter is a fundamental formula which is valid for all densities when the two-body potential is Coulombic. A similar analysis can be repeated for $G_-(\mathbf{q},\hbar q^2/2m)$, and for the 3D EG case. The results are summarized in the last row of Table I.

It is important to realize that for a 3D EG particular care must be exercised in selecting the appropriate limiting formulas for the local fields when approximate expressions for the vertex corrections are needed.[18] As we have shown however this problem does not exist for a 2D EG.

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