Long wavelength behavior of the dynamical spin-resolved local-field factor in a two-dimensional electron liquid

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The high frequency limits of the singular component of the spin-resolved exchange-correlation kernel tensor \( f_{\sigma\sigma'}^{L,T}(q,\omega) = -v(q)G_{\sigma\sigma'}^{L,T}(q,\omega) \) in a two-dimensional isotropic electron liquid with arbitrary spin polarization are studied. Here \( G_{\sigma\sigma'}^{L,T}(q,\omega) \) is the spin-resolved local field factor, \( v(q) \) is the Coulomb interaction in momentum space, and \( \sigma \) denotes spin. Particularly, the real part of \( A(\omega) \) is found to be logarithmically divergent at large \( \omega \). The large wavevector structure of the corresponding spin-resolved static structure factor is also established.

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I. INTRODUCTION

The spin-resolved local field factor \( G_{\sigma\sigma'}^{\prime}(q,\omega) \) has often been used to include exchange-correlation (xc) effects beyond the random phase approximation in many-electron systems. It is also one of the key concepts in the time-dependent (spin) density functional theory (TD(S)DFT) . In TD(S)DFT, however, one frequently uses the equivalent xc kernel, defined as

\[ f_{\sigma\sigma'}^{\prime}(q,\omega) = \frac{\partial^2}{\partial \epsilon^2} \left. G_{\sigma\sigma'}^{\prime}(q,\omega) \right|_{\epsilon=0} \],

instead. Here \( v(q) \) is the Fourier transform of the Coulomb interaction.

Recently it has been found that \( f_{\sigma\sigma'}^{\prime}(q,\omega) \) has quite surprising singular structure at small wavevector \( q \). The singular structure leads to invalidity of a conventional extension of local density approximation of the ground state density functional theory to the TDSDFT. This problem of ultranomalonicity in TDSDFT has been recently solved in a scheme of time dependent spin current density functional theory (TDSCDFT) . In TDSCDFT, in addition to \( f_{\sigma\sigma'}^{\prime}(q,\omega) \) which coincides with the longitudinal component \( f_{\sigma\sigma'}^{L}(q,\omega) \) of the xc kernel tensor \( f_{\sigma\sigma'}^{L}(q,\omega) \), the knowledge of the transverse component \( f_{\sigma\sigma'}^{T}(q,\omega) \) is also required. Note that we are only concerned with an isotropic electron liquid and the directions are relative to the wavevector \( q \). Thus, in general,

\[ f_{\sigma\sigma'}^{L,T}(q,\omega) = -v(q)A_{\sigma\sigma'}^{L,T}(q,\omega). \]

Both \( f_{\sigma\sigma'}^{L}(q,\omega) \) and \( f_{\sigma\sigma'}^{T}(q,\omega) \) have a singular structure at long wavelength and

\[ f_{\sigma\sigma'}^{L,T}(q,\omega) = \frac{\partial^2}{\partial \epsilon^2} G_{\sigma\sigma'}^{L,T}(q,\omega) + O(q^2), \]

where \( n_\sigma \) is the spin-resolved density (\( \sigma = 1 \) for \( \uparrow \)-spin and \( \sigma = -1 \) for \( \downarrow \)-spin), and \( n = n_\uparrow + n_\downarrow \) is the total density. It has been shown \( A(\omega) \) to be well behaved in three dimensions (3-D) and in this note, we point out that the real part of \( A(\omega) \), however, is divergent at high frequency in two dimensions (2-D). In other words the third moment of the spin-density spin-density response function \( \mathcal{F}_3^{\downarrow\downarrow}(0,0) \) is infinity in 2-D. We further show that the imaginary part of \( A(\omega) \) goes as a constant at high frequency, which is consistent with the divergence of \( ReA(\omega) \), in accordance with Kramer-Kröning (KK) relation,

\[ ReA(\omega) = ReA(\infty) + P \int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{ImA(\omega')}{\omega'-\omega}. \]

II. LARGE WAVEVECTOR LIMIT OF THE SPIN-RESOLVED STATIC STRUCTURE FACTOR \( S_{\sigma\sigma'}(k) \)

The third moment of the spin density spin density response function will be shown to be intrinsically related to the spin-resolved static structure factor \( S_{\sigma\sigma'}(k) \). We start with an investigation of the large \( k \) behavior of \( S_{\sigma\sigma'}(k) \). \( S_{\sigma\sigma'}(k) \) can be obtained from the spin-resolved pair-correlation function \( g_{\sigma\sigma'}(r) \) via the following well known relation,

\[ S_{\sigma\sigma'}(k) = \frac{n_\sigma}{n} \delta_{\sigma\sigma'} - \frac{n_\sigma n_\sigma'}{n} \int [g_{\sigma\sigma'}(r) - 1] e^{-ikr} dr. \]

At large \( k \), Eq. \ref{eq:sn} yields

\[ \lim_{k\to\infty} k^3 S_{\sigma\sigma'}(k) = -\frac{4\pi n_{\perp}}{n_\perp} g_{\sigma\sigma'}(0), \]

and

\[ \lim_{k\to\infty} k^5 [S_{\sigma\sigma'}(k) - \frac{n_\sigma}{n}] = \frac{6\pi n_{\perp}^2}{n_\perp} \partial^2 g_{\sigma\sigma'}(r)|_{r=0}. \]

where \( \sigma = -\sigma \). Eq. \ref{eq:sn} was also established before by Rajagopal and Kimball in Ref. \ref{ref:raj}, while Eq. \ref{eq:kn} is new. In obtaining the above results, we have used the following properties of the short range structures of \( g_{\sigma\sigma'}(r) \) \ref{ref:ar}, \ref{ref:ar2}, \ref{ref:ar3},

\[ \frac{\partial}{\partial r} g_{\sigma\sigma'}(r)|_{r=0} = \frac{2}{a_0} g_{\sigma\sigma'}(0), \]
\[
\frac{\partial^3}{\partial r^3} g_{\sigma\sigma}(r)|_{r=0} = \frac{2}{a_0} \frac{\partial^2}{\partial r^2} g_{\sigma\sigma}(r)|_{r=0}, 
\]
where \(a_0\) is the Bohr radius.

Recently an approximate scheme for the spin symmetric and antisymmetric local field factors in 2-D was developed by Atwal et al in Ref. [12], based on the exact limiting results and sum rules. One of the sum rules employed in the scheme is the third moment sum rule. However, the fact of infiniteness of the third moment, as will be demonstrated in the next section, was overlooked in Refs. [12,16]. To be more precise, the quantity \(\lambda_0^\infty\) in the above mentioned scheme, which is defined in Eq. (26) in Ref. [16] (or equivalently \(I_2(q \to 0)\) defined in Eq. (25) in Ref. [16]), is infinite. In fact, Eq. (26) in Ref. [16] can be rewritten as

\[
\lambda_0^\infty\left(r_s\right) = -8 \int_0^\infty dkk^2 S_T(k), \tag{10}
\]

From Eq. (10), one knows that \(S_T\) \(\sim 1/k^3\) at large \(k\). Therefore the rhs of Eq. (10) is divergent. The infiniteness of \(\lambda_0^\infty\) (\(r_s\)) seems not sufficiently realized in Refs. [16,16] and it was evaluated numerically by use of the pair-correlation density \(g(r)\) which is obtained at various \(r_s\) from QMC studies.

III. HIGH FREQUENCY LIMITS OF \(A(\omega)\)

In this section, we will explicitly show the infiniteness of the third moment of the spin-density spin-density response function, or equivalently the first moment of the spin-current spin-current response function \(M_{\sigma\sigma}^{L,T}(q)\). We start from a relation between the latter and \(Re f_{x,\sigma\sigma}^\alpha(q, \omega \to \infty)\),

\[
v^\alpha(q) + Re f_{x,\sigma\sigma}^\alpha(q, \omega \to \infty) = \frac{n^2}{\pi} \frac{M_{\sigma\sigma}^\alpha(q) - M_{\sigma\sigma}^{\alpha(0)}(q)}{q^2}, \tag{11}
\]

where \(\alpha = L, T\), and \(v^L(q) = 2\pi e^2/q\), and \(v^T(q) = 0\). \(M_{\sigma\sigma}^{\alpha(0)}(q)\) is the noninteracting version of \(M_{\sigma\sigma}^\alpha(q)\). As in the case of 3-D [3], \(M_{\sigma\sigma}^\alpha(q)\) has two parts of contributions, one from kinetic energy, and the other from electron interaction,

\[
M_{\sigma\sigma}^\alpha(q) = [M_{\sigma\sigma}^\alpha(q)]_{kin} + [M_{\sigma\sigma}^\alpha(q)]_{int}. \tag{12}
\]

Similar derivations to those in the case of the 3-D lead to

\[
[M_{\sigma\sigma}^\alpha(q)]_{int} = \frac{1}{m^2} q^2 \delta v(q) n_\sigma n_{\sigma'} + \frac{1}{m^2} \left[ \delta_{\sigma\sigma'} \sum_\tau \Gamma^\alpha_{\sigma\tau}(0) - \Gamma^\alpha_{\sigma\sigma'}(q) \right]. \tag{13}
\]

and

\[
[M_{\sigma\sigma}^\alpha(q)]_{kin} = \frac{1}{5m^2} \delta_{\sigma\sigma'}(2q^2 + q^2)(T_{\sigma}), \tag{14}
\]

where

\[
\Gamma_{\sigma\sigma'}^\alpha(q) = -\frac{1}{2} \sum_{k \neq \mathbf{q}} \left( k^2 \delta_{\sigma\sigma'}(q) - \langle \rho_{\sigma}(q-k) \rho_{\sigma'}(q) \rangle \right), \tag{15}
\]

and \((T_{\sigma})\) is the spin-resolved kinetic energy, and \(S\) is the area of the system. At small wavevector, it can be shown that

\[
[M_{\sigma\sigma}^\alpha(q)]_{int} = \frac{1}{m^2} \delta_{\sigma\sigma'}(2q^2 + q^2)(T_{\sigma}), \tag{14}
\]

where \(\beta L = -5/8\) and \(\beta T = 1/8\). Substituting Eqs. (14) and (16) into Eq. (11), one has,

\[
Re A(\omega \to \infty) = -\frac{2}{m} \sum_\mathbf{k} k^2 v(\mathbf{k}) S_T(k), \tag{17}
\]

and

\[
B_{\sigma\sigma'}^{L,T}(\omega \to \infty) = \delta_{\sigma\sigma'} \alpha^{L,T} \frac{\epsilon_{\sigma}}{n_\sigma} + \frac{\beta^{L,T}}{2} \int dr v(r)[1 - g_{\sigma\sigma'}(r)], \tag{18}
\]

where \(\epsilon_{\sigma}\) is spin-resolved correlation kinetic energy for per particle, and \(\alpha = 3, \alpha = 1\). Evidently \(Re A(\omega \to \infty)\) approaches to infinity due to the fact of \(S_T\) \(\sim 1/k^3\) at large \(k\) and subsequently the logarithmic divergence of the summation over \(\mathbf{k}\) on the rhs of Eq. (17).

Next we turn to investigating the high frequency limit of the imaginary part of \(A(\omega)\). Similar calculations to those in the case of 3-D in Ref. [3] lead to the following exact identity,

\[
Im A(\omega) = \frac{2}{S^2 n^2} \sum_{k,k'} v(k)v(k')k \cdot k'
\]

\[
Im \langle \rho_{\sigma} (-\mathbf{k}) \rho_{\sigma}(\mathbf{k}) \rangle = \frac{\beta^{L,T}}{2} \int dr v(r)[1 - g_{\sigma\sigma'}(r)], \tag{19}
\]

where \(\rho_{\sigma}(\mathbf{k})\) is the spin-resolved density operator. At large \(\omega\), the four-point response function coincides with that of a noninteracting electron gas, which is given by

\[
\langle \rho_{\sigma} (-\mathbf{k}) \rho_{\sigma}(\mathbf{k}) \rangle = -\pi \delta(\omega - k^2/m) \delta_{\mathbf{k},\mathbf{k}'} N_1 \tag{20}
\]

Substituting Eq. (20) into Eq. (19), one has

\[
Im A(\omega) \omega \to \infty = \frac{2\pi n_\sigma n_\sigma}{S n^2} \sum_\mathbf{k} \delta(\omega - k^2/m)v^2(\mathbf{k})k^2. \tag{21}
\]
which can be further simplified as

\[ \text{Im} A(\omega) \xrightarrow{\omega \to \infty} -\frac{2\pi^2 n^1 n^1 m e^4}{n^2}. \]  

(22)

Therefore, surprisingly, though reasonably in accordance with the divergent structure of \( \text{Re} A(\omega \to \infty) \), \( \text{Im} A(\omega) \) goes as a constant at large \( \omega \). In fact, with KK relation of Eq. (4), the limiting structure \( \text{Im} A(\omega) \) in Eq. (22) yields

\[ \text{Re} A(\omega) \xrightarrow{\omega \to \infty} 4\pi n^1 n^1 m e^4 \ln \omega. \]  

(23)

In obtaining the above result, we have used the fact of \( \text{Re} A(0) = 0 \), which is proved for 3-D case in Ref. [7, 8], and evidently also holds for 2-D case.

IV. CONCLUSIONS

Several exact results for the spin-resolved static structure factor and the dynamical local field factor of an arbitrary spin-polarized electron liquid in two dimensions have been established in this paper. Particularly, we have found that, at small wavevector, the corresponding third moment of the spin-density spin-density response function is infinite, and the exchange-correlation kernel is divergent logarithmically at high frequency.

Note added in proof: After the paper was finished, it was found that the divergence of the quantity \( \lambda^{\infty}_a(r_s) \) defined in Ref. [15, 16] was also noticed by Dr. P. Gori-Giorgi.

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[1] K. S. Singwi and M. P. Tosi, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1981), Vol. 36, p. 177.
[2] S. Ichimaru, Rev. Mod. Phys. 54, 1017 (1982).
[3] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
[4] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).
[5] E. Runge and E. K. U. Gross, Phys. Rev. Lett. 52, 997 (1984).
[6] E. K. U. Gross, J. F. Dobson, and M. Petersilka, in *Topics in current chemistry*, edited by R. F. Nalewajski (Springer, Berlin, 1996).
[7] Z. Qian, A. Constantinescu, and G. Vignale, Phys. Rev. Lett. 90, 066402 (2003).
[8] Z. Qian and G. Vignale, Phys. Rev. B 68, 195113 (2003).
[9] B. Goodman and A. Sjölander, Phys. Rev. B 8, 200 (1973).
[10] K. L. Liu, Can. J. Phys. 69, 573 (1991).
[11] A. K. Rajagopal and J. C. Kimball, Phys. Rev. B 15, 2819 (1977).
[12] J. C. Kimball, Phys. Rev. A 7, 1648 (1973); J. Phys. A 8, 1513 (1973).
[13] A. K. Rajagopal, J. C. Kimball, and M. Banerjee, Phys. Rev. B 18, 2339 (1978).
[14] A. E. Carlsson and N. W. Ashcroft, Phys. Rev. B 25, 3474 (1982).
[15] G. S. Atwal, I. G. Khalil, and N. W. Ashcroft, Phys. Rev. B 67, 115107 (2003).
[16] G. S. Atwal and N. W. Ashcroft, Phys. Rev. B 67, 233104 (2003).