Correlation effects on the third-frequency-moment sum rule of electron liquids

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The exact form of the third-frequency-moment sum rule is used to obtain the long-wavelength limit of the dynamic local-field correction of electron liquids within the formalism of Gross and Kohn. The effects of correlation modify the high-frequency behavior of the local-field correction typically by a factor 2—3 at metallic densities.

Recently, Gross and Kohn[1] extended the density-functional formalism to treat the dynamic response of electron liquids within the local-density approximation. They constructed a linear density-density response function in such a way that it satisfied some exact conditions, which include the compressibility sum rule and the third-frequency-moment ($\langle \omega^3 \rangle$) sum rule. In the application of the latter sum rule, however, they used an approximate form in which correlation effects were partially neglected.[2] The purpose of the present Brief Report is to obtain the frequency-dependent local-field correction in the long-wavelength limit by using the exact form of the $\langle \omega^3 \rangle$ sum rule.[3]

The $\langle \omega^3 \rangle$ sum rule[4] gives a constraint on the asymptotic form of the local-field correction $G(q,\omega)$ in the long-wavelength limit,[5]

$$\lim_{q\to 0} G(q,\infty) = -\frac{q^2}{2\pi n e^2}\left(\tfrac{2}{15}\langle V \rangle + \langle E_{\rm kin} \rangle - \langle E_{\rm kin} \rangle_0\right), \tag{1}$$

where $\langle V \rangle$ and $\langle E_{\rm kin} \rangle$ are the average potential and kinetic energies per particle, respectively, and $\langle E_{\rm kin} \rangle_0$ is the noninteracting Fermi-gas value of the latter. Using the virial forms for $\langle V \rangle$ and $\langle E_{\rm kin} \rangle$ one obtains

$$\lim_{q\to 0} f^h_{\rm xc}(q,\infty) = -\tfrac{4}{5} n^{2/3} \frac{d}{dn}\left[\frac{\varepsilon_{\rm xc}}{n^{2/3}}\right] + 6 n^{1/3} \frac{d}{dn}\left[\frac{\varepsilon_{\rm xc}}{n^{1/3}}\right], \tag{2}$$

where $f^h_{\rm xc}(q,\omega) = -(4\pi/q^2) G(q,\omega)$, and $\varepsilon_{\rm xc}$ is the exchange-correlation energy per particle. Neglecting the second term on the right-hand side of Eq. (2), which corresponds to neglecting the difference between $\langle E_{\rm kin} \rangle$ and $\langle E_{\rm kin} \rangle_0$ in Eq. (1), one recovers the expression $f_\infty(n)$ of Ref. 1. It should be noted that the second term of Eq. (2) is entirely due to correlation; the exchange part, $\varepsilon_x = -\frac{3}{4}(3/\pi)^{1/3} n^{1/3}$, does not contribute. If the second term of Eq. (2) is included in the parametrization (14) of Ref. 1, the coefficients $a(n)$ and $b(n)$ are considerably changed. In place of Figs. 1 and 2 of Ref. 1, one now obtains Figs. 1 and 2 below. At $\omega=0$, there is no difference. On the other hand, the high-frequency limits of Re $f^h_{\rm xc}$ are reduced by factors of 2.6 and 3.2 for $r_s=2$ and 4, respectively, leading to a much stronger frequency dependence of $f^h_{\rm xc}$ than in the approximation of Ref. 1. The

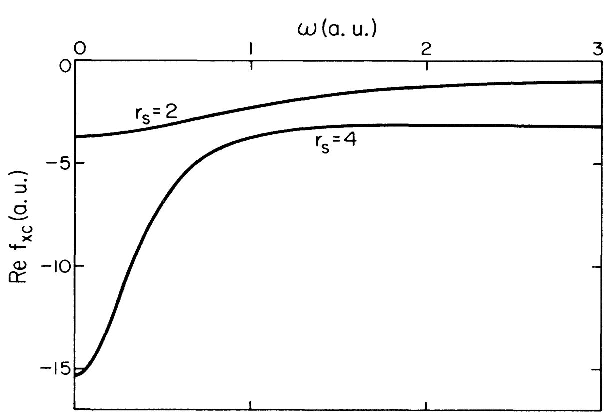

FIG. 1. Real part of the parametrization for $f^h_{\rm xc}(q=0,\omega)$.

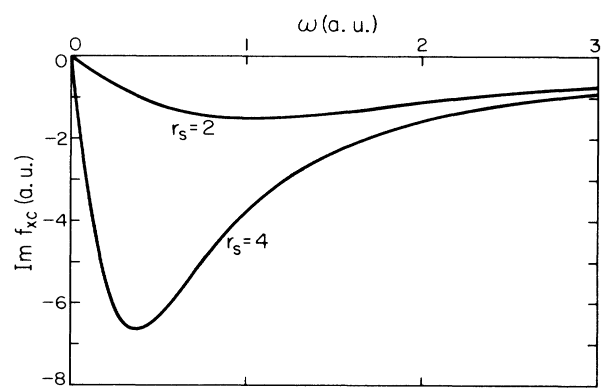

FIG. 2. Imaginary part of the parametrization for $f^h_{\rm xc}(q=0,\omega)$.

difference between $f_{xc}(r,\omega=0)$, as used in the original paper by Zangwill and Soven,[6] and $f_{xc}(r,\bar{\omega})$ at an appropriate frequency $\bar{\omega}$, is now estimated to be about 2% to 6%.

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