Pair Distribution Function for Various Dielectric Functions

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Recently Singwi *et al.* have claimed that the κ^2 dependence of the local-field correction (at large κ) to the Kleinman-Langreth (KL) dielectric function leads to a $1/r$ singularity in the pair distribution function $g(r)$. We have previously emphasized that the self-energy correction must always be included with the local-field correction to the dielectric function. We show that when this is done the $g(0)$ singularity does not occur. We then numerically calculate $g(r)$ using the random-phase approximation (RPA), Hubbard, and KL dielectric constants. Our numerical results for the RPA $g(r)$ agree with Brouers's and are significantly different from Singwi's. The KL $g(0)$ is less negative for large r_s than the RPA or Hubbard $g(0)$.

We have previously derived the following approximation to the dielectric response function containing local-field and self-energy exchange corrections[1]:

$$\epsilon_{\mathrm{KL}}(\kappa,\omega)=1+\tfrac{1}{2}[\chi(\kappa,+\omega)+\chi^*(\kappa,-\omega)]\left\{1-\frac{1}{2}\,\frac{A[\chi^2(\kappa,+\omega)+\chi^{*2}(\kappa,-\omega)]+2B\chi(\kappa,+\omega)\chi^*(\kappa,-\omega)}{\chi(\kappa,+\omega)+\chi^*(\kappa,-\omega)}\right\}^{-1}, \tag{1}$$

where

$$A=\tfrac{1}{2}[\kappa^2/(2\alpha k_F^2+K_S^2)], \tag{2}$$

$$B=\tfrac{1}{2}[\kappa^2/(2\alpha k_F^2+\kappa^2+K_S^2)], \tag{3}$$

and

$$\chi(\kappa,\pm\omega)=\chi_1(\kappa,\pm\omega)-i\chi_2(\kappa,\pm\omega), \tag{4}$$

with

$$\chi_1(\kappa,\pm\omega)=\frac{2}{\pi\kappa^3}\left\{\left[k_F^2-\left(\frac{k^2+\Delta(\kappa)\pm\omega}{2\kappa}\right)^2\right]\ln\left|\frac{\kappa^2+\Delta(\kappa)\pm\omega+2\kappa k_F}{\kappa^2+\Delta(\kappa)\pm\omega-2\kappa k_F}\right|+\frac{k_F}{\kappa}\,[\kappa^2+\Delta(\kappa)\pm\omega]\right\}, \tag{5}$$

$$\chi_2(\kappa,\pm\omega)=\frac{2}{\kappa^3}\left[k_F^3-\left(\frac{\kappa^2+\Delta(\kappa)\pm\omega}{2\kappa}\right)^2\right]\quad\text{if }-(\kappa^2+2\kappa k_F)<(\pm\omega+\Delta)<(2\kappa k_F-\kappa^2)$$
$$=0\quad\text{otherwise}, \tag{6}$$

where the self-energy correction $\Delta(\kappa)$ is given by

$$\Delta(\kappa)=\frac{8}{3\pi}\,\frac{k_F^3}{\kappa^2}(A-B). \tag{7}$$

K_S is an inverse screening length arising from the use of a screened exchange interaction and α is a numerical constant arising from making the following approximation for integrals which appear in $\epsilon(\kappa,\omega)$:

$$\int_0^{k_F}\{f(\vec{k},\vec{k}')/[(\vec{k}-\vec{k}')^2+b^2]\}d^3k\,d^3k' \approx(2\alpha k_F^2+b^2)^{-1}\int_0^{k_F}f(\vec{k},\vec{k}')\,d^3k\,d^3k'. \tag{8}$$

Langreth[2] has derived a variational formula for determining the proper vertex function $\tilde{\Lambda}_{\vec{k}}(\kappa,\omega)$. Assuming $\tilde{\Lambda}$ to be $\vec{k}$ independent, he finds an expression for $\tilde{\Lambda}(\kappa,\omega)$ from his variational formula. Note that this expression [his Eq. (43)] is identical with Eq. (5) in Ref. 1. He then shows that in the limits $\omega=0$, $\kappa\to 0$, and $\kappa\to\infty$, this approximate $\tilde{\Lambda}(\kappa,\omega)$ leads to an exact expression for $\epsilon(\kappa,\omega)$ in terms of $\tilde{I}(\vec{k},\vec{k}')$, the proper spin-symmetric part of the effective particle-hole interaction, assumed to be static. Taking

$$\tilde{I}(\vec{k},\vec{k}')=-8\pi/[(\vec{k}-\vec{k}')^2+K_S^2], \tag{9}$$

the form used both by Kleinman[1] and by Hubbard,[3,4] he compares his dielectric function with an earlier (and slightly incorrect) expression of Kleinman[5] and with Hubbard's[3]

$$\epsilon_H(\kappa,\omega)=1+\overline{\chi}_0(\kappa,\omega)\{1-A\overline{\chi}_0(\kappa,\omega)\}^{-1}. \tag{10}$$

In the $\omega = 0$, $\kappa \to \infty$ limit Eq. (1) as well as the earlier expression[5] for ϵ both become

$$\epsilon_{\mathrm{KL}}(\kappa \to \infty,\ \omega = 0) = 1 + \bar{\chi}(\kappa, 0)\{1 - \tfrac{1}{2}(A+B)\bar{\chi}(\kappa, 0)\}^{-1} \ , \tag{11}$$

where $\bar{\chi}(\kappa, \omega) = \frac{1}{2}[\chi(\kappa, +\omega) + \chi^*(\kappa, -\omega)]$ and $\bar{\chi}_0(\kappa, \omega)$ is obtained from $\bar{\chi}(\kappa, \omega)$ by setting the self-energy correction $\Delta(\kappa)$ equal to zero. Langreth finds in this limit that Eq. (11) gives identical results to his exact ϵ when $\alpha = \frac{1}{2}$ in Eqs. (2) and (3) as long as $K_S^2/(2k_F)^2 > 0.3$. Because $A/\kappa^2 \to 0$, whereas $(A+B)/\kappa^2$ is finite in this limit, Hubbard's approximation is incorrect.

Singwi *et al.*[6] and Shaw[7] have noted that if the ω dependence of ϵ is neglected and ϵ is written in the form

$$\epsilon(\kappa) = 1 + \bar{\chi}_0(\kappa)\{1 - G(\kappa)\bar{\chi}_0(\kappa)\}^{-1} \ , \tag{12}$$

and if $G(\kappa \to \infty)$ is proportional to κ^2, then the pair distribution function $g(r)$ will approach $-\infty$ as $r \to 0$. Because $A + B$ is proportional to κ^2 as $\kappa \to \infty$, they have claimed that our dielectric constant is unphysical. They failed to notice that Eq. (11) contains $\bar{\chi}$ rather than $\bar{\chi}_0$. Note that Eq. (11) can be manipulated to give

$$\begin{aligned}\epsilon_{\mathrm{KL}}(\kappa \to \infty, \omega = 0) &= 1 + \bar{\chi}_0[\bar{\chi}_0/\bar{\chi} - \tfrac{1}{2}(A+B)\bar{\chi}_0]^{-1} \\ &= 1 + \bar{\chi}_0/(1 - G\bar{\chi}_0) \ ,\end{aligned} \tag{13}$$

where

$$G = \tfrac{1}{2}(A+B) + 1/\bar{\chi}_0 - 1/\bar{\chi} \quad . \tag{14}$$

Expanding $\bar{\chi}$ in the $\kappa \to \infty$ limit, we find

$$\bar{\chi} \to (\omega_p^2/\kappa^4)(1 - \Delta_\infty/\kappa^2) \quad , \tag{15}$$

so that

$$\frac{1}{\bar{\chi}_0} - \frac{1}{\bar{\chi}} \to \frac{\kappa^6}{\omega_p^2}\left(\frac{1}{\kappa^2} - \frac{1}{\kappa^2 - \Delta_\infty}\right) \to -\frac{\kappa^2}{\omega_p^2}\,\Delta_\infty \ , \tag{16}$$

where from Eq. (7)

$$\Delta_\infty = (4/3\pi)\,k_F^3/(2\alpha k_F^2 + K_S^2) = \tfrac{1}{4}\,\omega_p^2/(2\alpha k_F^2 + K_S^2) \ . \tag{17}$$

Thus the κ^2 term in $\frac{1}{2}(A+B)$ is exactly canceled by the κ^2 term in the self-energy correction, $1/\bar{\chi}_0 - 1/\bar{\chi}$, and the leading term in $G(\kappa \to \infty)$ is κ independent. Therefore our ϵ does not lead to an infinite $g(0)$. This was independently discovered by Shaw[8] after the publication of his paper.[7]

We have calculated the pair distribution function from the formula[7]

$$g(x) = 1 + \tfrac{3}{2}\int_0^\infty d\eta\,\eta^2 j_0(\eta x)[S(\eta) - 1] \ , \tag{18}$$

where $\eta = k/k_F$, $x = k_F r$, $j_0(\eta x)$ is the zeroth spherical Bessel function, and

$$S(\eta) = -\frac{3}{4}\,\frac{\eta^2}{k_F}\int_0^\infty \mathrm{Im}\frac{1}{\epsilon(\eta, \omega)}\,d\omega . \tag{19}$$

We calculated K_S from

$$K^2\epsilon_{\mathrm{RPA}}(K) = K^2 + K_S^2 \ , \tag{20}$$

where $K^2 = 2\alpha k_F^2$ and $2\alpha k_F^2 + \kappa^2$ in A and B, respectively, and took[9]

$$\alpha = \tfrac{1}{2}(1 + e^{-\kappa/2k_F}) \quad . \tag{21}$$

The choice for α was determined by the fact that for $\kappa \to \infty$ we must have $\alpha = \frac{1}{2}$. Furthermore, for $\kappa = 0$, only electrons on the Fermi surface contribute to the dielectric screening; thus the average value of $\vec{k} - \vec{k}'$ appearing in Eq. (8) is $2k_F$ and $\alpha = 1$. In Fig. 1 we plot $g(r)$ for several electron densities using ϵ_{RPA}, ϵ_H, and ϵ_{KL}. In the RPA case our results differ significantly from Singwi's.[6] For small values of r his $g(r)$ become too large [e.g., for $r_s = 2$, we get $g(0) = -0.65$ and he gets $g(0) = -0.53$].[10] We used $\eta = 100$ for an upper limit in the numerical evaluation of the integral in Eq. (18). We found we were able to reproduce Singwi's RPA results by taking $\eta = 10$ as the upper limit.[11] For large x this is sufficient because of the oscillating Bessel function, but for small x it is not. Our RPA results are identical with Brouers's[12] (as closely as we can read his graphs) even though Brouers used an incorrect formula of Pines[13] for the plasma contribution. In order to check our integration we used the sum rules

$$\int_0^\infty \omega\,\mathrm{Im}\epsilon(\kappa, \omega)\,d\omega = \tfrac{1}{2}\pi\,\omega_p^2 \quad , \tag{22}$$

$$\int_0^\infty \omega\,\mathrm{Im}[1/\epsilon(\kappa, \omega)]d\omega = -\tfrac{1}{2}\pi\omega_p^2 \quad . \tag{23}$$

In the RPA and Hubbard cases they were obeyed to five significant figures. Using ϵ_{KL}, they were obeyed to within 0.1% for $\eta = 0$ and to five significant figures for large η. The reason for this is that the local-field and self-energy terms give canceling added contributions but the approximations [Eq. (8)] made in the local-field and self-energy terms are slightly different, so that the cancellation is not exact.

In Fig. 1 we note that for $r_s \geq 2$, ϵ_{RPA}, ϵ_H, and ϵ_{KL} all yield negative $g(r \to 0)$; this is a probability function and therefore must be positive. We see that the $g(r)$ calculated from ϵ_H are better than those calculated from ϵ_{RPA} and those calculated from ϵ_{KL} are better than those calculated from ϵ_H. We note in passing that considerable improvement in $g(r)$ can be obtained by setting $K_S = 0$ in either ϵ_H or ϵ_{KL} [e.g., for $r_s = 2$, ϵ_{KL} with screening

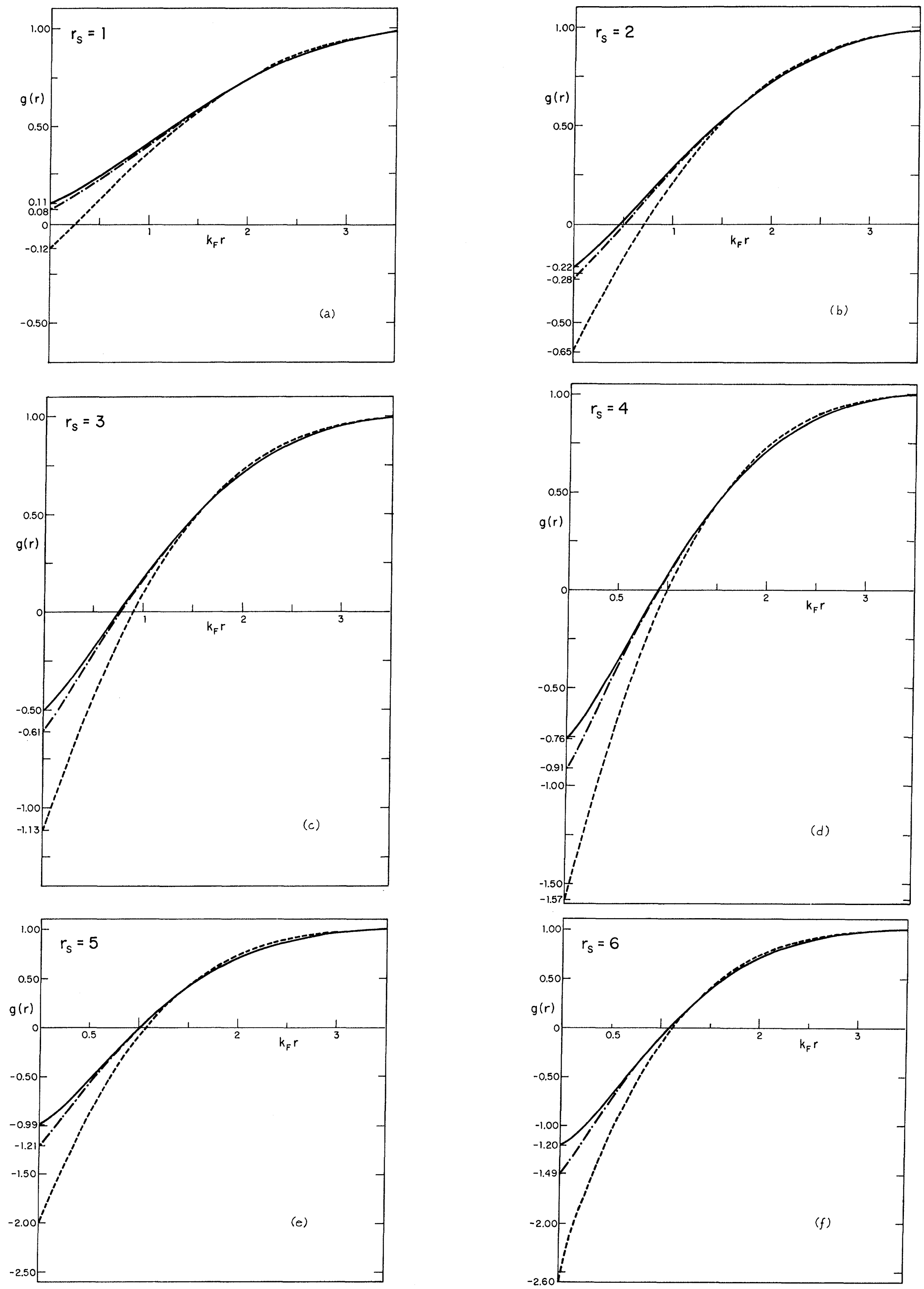

FIG. 1. Pair distribution functions for $r_s = 1$ to $r_s = 6$ calculated using ϵ_{RPA} (dashes), ϵ_H (dots and dashes), and ϵ_{KL} (solid lines).

yields $g(0) = -0.22$ and without screening $g(0) = -0.07$]. This appears to be completely unjustified, however. We further note that Singwi's[14] "self-consistent" dielectric function yields a $g(r)$ much better than ϵ_{KL} [i.e., less negative $g(0)$]. On the other hand, in what Singwi calls the Hartree-Fock limit his ϵ reduces to ϵ_H. Because Langreth[2] has proven ϵ_H is incorrect [see discussion following Eq. (11)], Singwi's ϵ must be incorrect as well. If Singwi's self-consistency procedure could be corrected to yield ϵ_{KL} in the Hartree-Fock limit, it would undoubtedly yield an ϵ far superior to anything yet derived.[15] Finally, we wish to emphasize that just because the Kleinman-Langreth and Hubbard $g(r)$ contain similar corrections to the RPA $g(r)$ does not mean they will give similar corrections to other quantities. In fact, we have found that for a given ionic pseudopotential they yield corrections of opposite sign to the phonon frequencies of magnesium calculated[16] with ϵ_{RPA}.

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[11]We have not recalculated $g(r)$ using the dielectric function ϵ_{STLS} of Singwi *et al.* (Ref. 6), since ϵ_{STLS} is not given in closed form. It is possible that the self-consistent nature of ϵ_{STLS} [i.e., its dependence on $g(r)$] will reduce the error made in $g_{STLS}(r)$ by taking $\eta = 10$ as the upper limit of integration relative to the error in $g_{RPA}(r)$.

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Some Implications of Weak-Scaling Theory*

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The weak-scaling theory developed by the author is extended to facilitate contact with the numerical results of Ferer *et al.* His conclusions are consistent with their results, and certain specific extensions of their numerical work are suggested by the analysis.

In a previous paper,[1] the author outlined the derivation of a set of weak-scaling relations based upon the appearance of two correlation lengths, Λ and ξ. The analysis rested upon an investigation of the form of the density-density correlation function $\hat{F}(\vec{r})$ along the coexistence curve. In order to make contact with the results of Ferer, Moore, and Wortis[2] that hold along the critical isochore, as well as our own techniques[3,4] that involve $\hat{F}(\vec{r})$ along the critical isotherm, we extend here the discussion given in Ref. 1.

We use the notation of Ref. 1, where we introduced the function $\tilde{q}(\vec{r},\kappa)$ by assuming that along the coexistence curve

$$\hat{F}(\vec{r}) - \hat{F}(\vec{r})_c = f(\kappa r)/r^{d-t-\tilde{q}(\vec{r},\kappa)} . \quad (1)$$

Here $\hat{F} = \rho^2 \hat{h}$, where $\hat{h}$ is the correlation function discussed in our earlier work and ρ is the number density. Letting $M = |\rho - \rho_c|$, so that M is proportional (in spin language) to magnetization, we assume that $\kappa = \xi^{-1} \sim M^{\epsilon}$ along the coexistence curve and that $\kappa \sim |T - T_c|^{\nu}$ when $M = 0$ and $T > T_c$. As