Static local-field correction from Monte Carlo studies of the homogeneous electron gas

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From the fixed-node diffusion Monte Carlo (DMC) results obtained by Ortiz and Ballone [Phys. Rev. B **50**, 1391 (1994)], we develop semianalytic expressions of the static local-field correction (LFC) for the dielectric function describing exchange and correlation effects in a homogeneous electron gas. These expressions, correcting some errors of earlier papers, are derived following the Vashista-Singwi [Phys. Rev. B **6**, 875 (1972)] and Utsumi-Ichimaru [Phys. Rev. B **22**, 5203 (1980)] schemes. Both satisfy physical requirements as the ''compressibility sum rule'' for an interacting fermion system. The behavior of these LFC functions is discussed and compared with the well-known LFC's given in the literature. More tractable density-dependent expressions are given in order to allow easy calculations of physical properties without losing accuracy relative to DMC numerical results.

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I. INTRODUCTION

The local-field correction (LFC) function describes exchange and correlation effects in an electron gas. Its determination is one of the fundamental problems of physics and stays always of topicality.[1–13] Several theories based on the so-called ''equation of motion'' [14–25] or on diagrammatic techniques[26–29] lead to various forms $G(q)$ of this important quantity. The quantum Monte Carlo simulation[6,10] is an interesting tool of investigation of the electron system. Ortiz and Ballone[6] (OB) performed such calculations by using the variational Monte Carlo (VMC) method and the fixed-node diffusion Monte Carlo (DMC) method. These authors gave a parametrized expression of the spin-dependent electron-pair correlation function $g^{\sigma,\sigma'}(r)$ from which one can deduce in a straightforward manner the total (number-number) pair-correlation function $g(r)$ and the static electron structure factor $S(q)$. Within the ''equation of motion'' formalism, Singwi *et al.*[24] (STLS) gave $G(q)$ as a functional of $S(q)$. Bretonnet and Boulahbak[9] using this functional and OB Monte Carlo results, obtained a semianalytical expression for $G(q)$. In their original paper[9] and in the applications to liquid metals which followed,[8] they used a mathematical approximation and omitted the spin-parallel contribution to $G(q)$. Furthermore and beyond this remark, it is well known[20,23] that the STLS approach leads to a lack of consistency and a failure to satisfy the ''compressibility sum rule'' which is very important for the study of metal properties. So, in the present work, we take into account the improvements to the original formalism proposed by Vashista-Singwi[20] (VS) and Utsumi-Ichimaru[17] (UI) to get numerically the local-field correction $G(q)$ and parametrize it with an ''*ad hoc*'' expression.

This paper is organized as follows: in Sec. II, we introduce briefly some of the main ingredients of the dielectric function within the semiclassical formalism since a very thorough description is given by many authors. We show how the self-consistent calculation of the local-field correction may be replaced by a direct calculation following three approaches referenced by OB-STLS, OB-VS, and OB-UI and described shortly, respectively, in Secs. II A, II B, and II C. In Sec. II D, we give simple and useful expressions very close to the numerical calculations carried out, respectively, in OB-VS and OB-UI schemes. The behavior of our Monte Carlo–derived LFC functions are discussed and compared to the corresponding self-consistent calculations and to other well-known LFC functions in Sec. III. Finally, in Sec. IV we present our conclusion. Later in the paper we use atomic units throughout: $\hbar = m = e = 1$.

II. THEORETICAL BACKGROUND

The dynamical local-field correction $G(q,\omega)$ and the dielectric function $\varepsilon(q,\omega)$ are related through the most general equation[22,25]

$$\varepsilon(q,\omega) = 1 - \frac{v(q)\chi_0(q,\omega)}{1 + v(q)G(q,\omega)\chi_0(q,\omega)}, \tag{1}$$

where $\chi_0(q,\omega)$ is the usual dynamical polarizability of a free-electron gas and $v(q) = 4\pi/q^2$ is the Fourier transform of the Coulomb potential. One notes that the random-phase approximation (RPA) corresponds to $G(q,\omega) = 0$ and that the Hartree-Fock approximation corresponds to $G(q,\omega) = 1$. Equation (1) serves in a sense as the usual definition of the dynamical LFC. The latter depends on the wave vector $\vec{q}$ and the frequency ω although in the literature $G(q,\omega)$ is thought to be weakly dependent on ω. So, in the static approximation, Eq. (1) is mostly written with only the static local-field correction $G(q)$ in place of the dynamical one. In the classical formalism, the fluctuation-dissipation theorem[14,15] takes an important place and leads to the fundamental expression in which the static electron structure factor is given as a functional of the imaginary part of the dielectric function:[26]

$$S(q) = -\frac{1}{4\pi^2 n_0} q^2 \int_0^\infty d\omega I_m\left[\frac{1}{\varepsilon(q,\omega)}\right], \tag{2}$$

where n_0 is the number density.

So, a semiclassical and self-consistent calculation of the LFC and other quantities defined above combines previous equations and a closure relation to be found. This relation supposes a detailed knowledge of the electron system. Such a relation may be obtained if we solve the Born-Green ''equation of motion'' [14] relating the three-body distribution function to the two-body distribution function. With the aim of solving the Born-Green equation, different approaches or schemes with more or less justified assumptions and approximations were proposed in the past. Each of them leads to a specific form of the closure relation. Another possibility offers interesting perspectives, the one that uses the results of Monte Carlo simulation. We choose this solution because these results like those of Ortiz and Ballone[6] and Ceperley *et al.*[10] are more and more refined. In our work, in place of a self-consistent calculation, we used the parametrized expression for the spin-dependent electron-pair-correlation function $g^{\sigma,\sigma'}(r)$ published by Ortiz and Ballone,[6] and performed a straightforwardly $G(q)$ calculation by successively considering three different closure relations that we call also schemes or approaches. The interest of the method that we used lies in the fact that physical requirements ''sum rules'' (Refs. 3, 15, and 19) impose drastic conditions on $g^{\sigma,\sigma'}(r)$ which are verified in the accurate OB-Monte Carlo calculation.

A. STLS scheme

In the past, Singwi *et al.*[24] (STLS) derived a famous relation within the so-called ''equation of the motion.'' This relation connects the local-field correction $G(q)$ and the electron static structure factor $S(q)$ through the functional

$$G(q) = -\frac{1}{n_0}\int \frac{\vec{q}\cdot\vec{q}'}{q'^2}[S(\vec{q}-\vec{q}')]\frac{d\vec{q}'}{(2\pi)^3}. \tag{3}$$

Shaw,[22] using the well-known reciprocal equation between $S(q)$ and the total (number-number) pair-correlation function $g(r)$, transformed Eq. (3) into the more tractable form that we used,

$$G(\eta) = 1 - g(0) - \int_0^\infty dx \frac{dg(x)}{dx}\frac{\sin(\eta x)}{\eta x}, \tag{4}$$

where $\eta = q/k_F$, k_F is the Fermi wave vector, and $x = k_F r$. The behavior of $G(q)$ in the long- and short-range wavelength limits are, respectively,

$$\lim_{\eta\to 0} G(\eta) = \gamma\eta^2, \tag{5}$$

and,

$$\lim_{\eta\to\infty} G(\eta) = 1 - g(0). \tag{6}$$

The latter equation [Eq. (6)] is precisely the self-consistency condition for the dielectric function $\varepsilon(q,\omega)$ according to Kimball's analysis[19] of the fluctuation-dissipation theorem [Eq. (2)]. Later in this paper, the coefficient γ in Eq. (5) is evaluated and interpreted in connection with the ''compressibility sum rule.'' The total (number-number) pair-correlation function is given in terms of the partial spin-dependent electron-pair-correlation functions[3] $g^{\sigma,\sigma'}(r)$, where the indexes σ,σ' denote spin up ($\uparrow$) or spin down ($\downarrow$). In the case of an unpolarized electron gas, we have[3,6]

$$g(r) = \frac{1}{2}[g^{\uparrow\downarrow}(r) + g^{\uparrow\uparrow}(r)]. \tag{7}$$

The linearity of Eq. (4) shows that similar expressions can be written for each spin-parallel or spin-anti-parallel contribution $G^{\uparrow\uparrow}(q)$ and $G^{\uparrow\downarrow}(q)$. So, we must write the static local-field correction as

$$G(q) = \frac{1}{2}[G^{\uparrow\downarrow}(q) + G^{\uparrow\uparrow}(q)]. \tag{8}$$

Using in Eq. (4) the fitted form of $g^{\sigma\sigma'}(r)$ given by Ortiz and Ballone,[6] Bretonnet and Boulahbak[9] derived the analytic expression

$$G(\eta) = 1 - g(0) - e^{-z}\sum_{\mu=0}^{6} C_\mu \times {}_1F_1\left(1 - \frac{\mu}{2}; \frac{3}{2}; z\right), \tag{9}$$

where ${}_1F_1(\alpha;\gamma;z)$ is the degenerate hypergeometric function and $z = (1/4)(9\pi/4)^{2/3}\eta^2/a$. The coefficients C_μ are related to the Monte Carlo fit parameters of the spin-dependent electron-pair-correlation function $g^{\sigma\sigma'}(r)$ [see Eq. (17) in Ref. 9] and a is one of those.

So, Eq. (9) gives the partial spin-spin-dependent contributions $G^{\sigma,\sigma'}(q)$, namely, $G^{\uparrow\downarrow}(q)$ or $G^{\uparrow\uparrow}(q)$. It should be normally indexed as shown below, Eq. (10)–Eq. (13). However, to simplify the notation, the indices σ and σ', denoting spin up ($\uparrow$) or spin down ($\downarrow$), are conveniently omitted in Eqs. (10)–(13).

In their calculations, the same authors[8,9] employed the spin-anti-parallel contribution $G^{\uparrow\downarrow}(q)$ instead of the total LFC given by Eq. (8). They also used the eighth-order development in Taylor's series of the degenerate hypergeometric function which appears in Eq. (9). So, we have derived an equivalent expression which is a useful improvement for an exact computation. Indeed, owing to properties of ${}_1F_1(\alpha;\gamma;z)$, we rewrite Eq. (9) in terms of well-known functions,

$$G(\eta) = P_1(z) - P_2(z)\exp(-z^2) - P_3(z)\frac{\mathrm{erf}(z)}{z} - P_4(z)\frac{\boldsymbol{D}(z)}{z}. \tag{10}$$

The expressions for the polynomials $P_k(z)$ are

$$P_1(z)=1-g(0)-\frac{C_3}{2}-\frac{C_5}{8}(5-2z^2),\quad P_3(z)=\frac{\sqrt{\pi}}{2}C_0,\tag{11}$$

$$P_2(z)=C_2+C_4\left(1-\frac{2}{3}z^2\right)+C_6\left(1-\frac{4}{3}z^2+\frac{4}{15}z^4\right),$$

$$P_4(z)=C_1+\frac{C_3}{2}(1-2z^2)+\frac{C_5}{2}\left(\frac{3}{4}-3z^2+z^4\right),$$

whereas erf(z) is the well-known error function and $\boldsymbol{D}(z)$ is Dawson's[22] integral defined by

$$\boldsymbol{D}(z)=\exp(-z^2)\int_0^z \exp(\xi^2)d\xi.\tag{12}$$

From Eq. (5) and Eq. (10), we easily deduce the relationship

$$\gamma=\frac{1}{12a\alpha^2}\sum_{\mu=0}^{6}(\mu+1)C_\mu,\tag{13}$$

where $\alpha=(4/9\pi)^{1/3}$ and the spin-dependent coefficients C_μ are calculated for ($\uparrow\downarrow$) and ($\uparrow\uparrow$). It is very important to remember that any implemented calculation of Eq. (9) or equivalently Eq. (10) with a set of optimal fit parameters corresponding to the relative polarization of two spins (parallel $\uparrow\uparrow$ or antiparallel $\uparrow\downarrow$) gives only the partial contributions, respectively, $G^{\uparrow\uparrow}(q)$ and $G^{\uparrow\downarrow}(q)$. The behavior at the long-wavelength limit ($q\to 0$) of the total local-field correction [Eq. (8)] is parabolic and the coefficient γ [Eq. (5)] is expressed in terms of the quantities $\gamma^{\uparrow\downarrow}$ and $\gamma^{\uparrow\uparrow}$ evaluated according to Eq. (13), i.e.,

$$\gamma=\frac{1}{2}(\gamma^{\uparrow\downarrow}+\gamma^{\uparrow\uparrow}).\tag{14}$$

At this stage, the main defect that STLS formalism presents lies on the ''compressibility sum rule'' which is not fulfilled.[20,23] Indeed, the compressibility Ξ of the interacting electron gas can be evaluated by two manners. It can first be deduced from the correlation energy $E_c(r_s)$ through the equation.[17]

$$\frac{\Xi_0}{\Xi}=1-\frac{\alpha r_s}{\pi}+\frac{\alpha^2}{6}r_s^6\frac{d}{dr_s}\left[\frac{1}{r_s^2}\frac{dE_c(r_s)}{dr_s}\right],\tag{15}$$

or it can be evaluated via the following ''sum rule,'' [26] which connects γ and Ξ:

$$\frac{\Xi_0}{\Xi}=1-\frac{4\alpha r_s}{\pi}\gamma,\tag{16}$$

where $\Xi_0=(3/2)E_F n_0$ is the free-electron compressibility, E_F is the Fermi level, and α has the same value as in Eq. (13) whereas the electron-sphere radius r_s is related to the electron density n_0 as $r_s=(3/4\pi n_0)^{1/3}$. With both Eq. (15) and Eq. (16) having to be equal, the STLS formalism did not fulfill this condition.[20,23] Thus the STLS scheme is inconsistent.

B. Vashista-Singwi scheme

Vashista and Singwi[20] (VS), following upon the preceding work of Singwi *et al.*,[23] improve the inconsistent STLS scheme by assuming the ''*ansatz*'' [Eq. (29) in Ref. 20] that, in the present context, we can rewrite with our notation

$$G_{\text{OB-VS}}(q)=G_{\text{OB-STLS}}(q)+a_{\text{OB-VS}}\left(-\frac{q}{3}\frac{\partial}{\partial q}-\frac{r_s}{3}\frac{\partial}{\partial r_s}\right)G_{\text{OB-STLS}}(q).\tag{17}$$

In the precedent equation and hereafter, the abbreviation OB-VS means that the static local-field correction is deduced in the VS scheme from OB Monte Carlo data, and the OB-STLS and OB-UI are defined in a similar manner. Those corresponding to self-consistent calculations are simply notated as STLS, VS, or UI. Likewise for Eq. (5), at the long-wavelength limit, we may write

$$\lim_{q\to 0}G_{\text{OB-VS}}(q)=\gamma_{\text{OB-VS}}\left(\frac{q}{k_F}\right)^2.\tag{18}$$

We select the parameter $a_{\text{OB-VS}}$ in Eq. (17) and consequently the coefficient $\gamma_{\text{OB-VS}}$ in Eq. (18) such that the ''compressibility sum rule'' [Eq. (16)] is exactly verified. So, we get

$$a_{\text{OB-VS}}=\frac{3(\gamma_{\text{OB-STLS}}-\gamma_{\text{OB-VS}})}{2\gamma_{\text{OB-STLS}}+r_s\dfrac{\partial\gamma_{\text{OB-STLS}}}{\partial r_s}}.\tag{19}$$

The coefficient $\gamma_{\text{OB-STLS}}$ is evaluated according to Eq. (14) and $\gamma_{\text{OB-VS}}$ is deduced from Eq. (15) where the correlation energy $E_c(r_s)$ is the one computed and interpolated by Ortiz and Ballone[6] in Perdew-Zunger[16] form. In the metallic-density range, the fitted parameter $a_{\text{OB-VS}}$ is found to be a very slowly varying function of r_s and is close to the value given in Ref. 20, $a_{\text{VS}}=2/3$. We found

$$a_{\text{OB-VS}}=0.610\,33+0.020\,33r_s-0.001\,49r_s^2+1.606\,92\times 10^{-5}r_s^3.\tag{20}$$

Combining Eq. (6) and Eq. (17), it follows the expression of the asymptotic value,

$$\lim_{q\to\infty}G_{\text{OB-VS}}(q)=1-g(0)-\frac{a_{\text{OB-VS}}}{3}r_s\frac{\partial[1-g(0)]}{\partial r_s}.\tag{21}$$

From Table I, we verify the inequality

$$\lim_{q\to\infty}G_{\text{OB-VS}}(q)\leqslant\lim_{q\to\infty}G_{\text{OB-STLS}}(q).\tag{22}$$

Likewise, Shaw[22] inequalities are verified as

$$\frac{1}{2}\leqslant\lim_{q\to\infty}G_{\text{OB-STLS}}(q)\leqslant 1,\quad\frac{1}{2}\leqslant\lim_{q\to\infty}G_{\text{OB-VS}}(q)\leqslant 1.\tag{23}$$

TABLE I. Numerical values of γ defined in Eq. (5), and of the limit $q\to\infty$ of LFC functions versus r_s.

	r_s	1	3	5	10
γ	OB-STLS [this work: Eqs. (8) and (10)]	0.4547	0.5114	0.5454	0.5814
	STLS (Ref. 24)	0.4561	0.5107	0.5378	0.5715
	OB-VS [this work: Eq. (17)]	0.2567	0.2722	0.2850	0.3079
	VS (Ref. 20)	0.24284	0.27433	0.29184	
	OB-UI [this work: Eq. (27)]	0.2584	0.2664	0.2708	0.2751
	UI (Ref. 17)	0.29	0.32	0.33	
	TW (Ref. 25)	0.25	0.25	0.25	0.25
$\lim_{q\to\infty} G(q)$	OB-STLS [this work: Eqs. (8) and (10)]	0.7276	0.9078	0.9768	0.9976
	OB-VS [this work: Eq. (17)]	0.6941	0.8781	0.9594	0.9940
	VS (Ref. 20)	0.7619	0.9958	1.0644	1.0724
	OB-UI [this work: Eq. (27)]	0.7095	0.8893	0.9689	0.9964
	UI (Ref. 17)	0.724	0.893	0.953	
	TW (Ref. 25)	0.762	0.762	0.762	0.762

Undoubtedly Eq. (21) shows that the LFC deduced according to the Vashista-Singwi scheme is not in agreement with Kimball's self-consistent condition [Eq. (6)], whereas this condition is exactly verified in the STLS scheme. Nevertheless, this ascertainment must be relativized since it is known that the Kimball analysis is based on the static approximation for the dielectric function, i.e., with static LFC function $G(q)$ in place of the dynamical one $G(q,\omega)$ in Eq. (1). Precisely, Niklasson,[18] considering the frequency-dependent theory of the LFC, obtained the self-consistency condition given by Eq. (24),

$$\lim_{q\to\infty} G(q,\omega)=\frac{2}{3}[1-g(0)]. \tag{24}$$

However, Holas[13] inquired further into the matter and, taking account of the so-called ''kinetic-energy correlation'' [12] neglected previously, has shown that the large q behavior is actually a parabolic type. Such a correlation corresponds to the difference between the kinetic energy of a noninteracting electron system and the exact kinetic energy of an interacting electron system.[12] Nevertheless, in the theoretical schemes that we used and for which the kinetic energy is that of a noninteracting electron system (see, for instance, Ref. 23 and the Appendix of Ref. 24), this ''kinetic-energy'' part of LFC is neglected. Therefore, the studied LFC's converge to a constant at large enough q values. This constant is in keeping with the approximate relation connecting the local-field correction and the pair-correlation function [Eq. (4) in the STLS case or, with Vashista-Singwi improvements, Eq. (17)]. In comparison, one will now consider a LFC, which is compatible with the Holas result. This one is obtained by extensive diffusion Monte Carlo simulations performed by Moroni *et al.*[10]

It is also interesting to note that $g(0)$, calculated from OB Monte Carlo data,[6] verifies the analytical form of Yasuhara:[21]

$$g(0)=\frac{\zeta}{8}\left[\frac{x}{I_1(x)}\right]^2, \tag{25}$$

where $x=4(4/9\pi)^{1/6}(r_s/\pi)^{1/2}$ and $I_\nu(x)$ is the modified Bessel's function of the first kind. We have found that ζ is very close to 1.0, as in Yasuhara's paper:

$$\zeta=0.984\,92+0.004\,72\times r_s. \tag{26}$$

C. Utsumi-Ichimaru scheme

The method that Utsumi and Ichimaru[17] used consists of splitting the LFC function into two parts corresponding, respectively, to the exchange contribution $G_x(q)$ and the correlation effect $G_c(q)$, so that

$$G(q)=G_x(q)+G_c(q). \tag{27}$$

These authors adopt the following expression for the exchange term:

$$G_x(q)=\frac{\eta^2}{128}\left[11+\frac{15\eta^2}{4}+\frac{3(4-\eta^2)(28+5\eta^2)}{16\eta}\ln\left|\frac{2+\eta}{2-\eta}\right|\right] \quad \text{with} \quad \eta=\frac{q}{k_F}, \tag{28a}$$

and from the Heisenberg ''equation of motion,'' they approximate $G_c(q)$ as

$$G_c(q)=-\frac{1}{n_0}\int\frac{d^3\vec{k}}{(2\pi)^3}K(\vec{q},\vec{k})S_{\rm WS}(k)[S(|\vec{q}-\vec{k}|)-S_{\rm HF}(|\vec{q}-\vec{k}|)], \tag{28b}$$

where the kernel $K(\vec{q},\vec{k})$ has the form

$$K(\vec{q},\vec{k})=\frac{\vec{q}\cdot\vec{k}}{k^2}+\frac{\vec{q}\cdot(\vec{q}-\vec{k})}{|\vec{q}-\vec{k}|^2}. \tag{29}$$

$S_{\rm HF}(q)$ and $S_{\rm WS}(q)$ are, respectively, the Hartree-Fock structure factor and the Wigner-Seitz screening factor whose expressions are given by

TABLE II. Expression of $D_n(r_s)$, $n \in [0,5]$ [Eq. (32)] in OB-VS expansion, accurate in the ranges $1 \leqslant r_s \leqslant 3$ and $3 \leqslant r_s \leqslant 5$.

$$1 \leqslant r_s \leqslant 3$$
$$D_0(r_s) = 0.59334 + 0.10489 r_s - 0.00491 r_s^2 + 1.74007 \times 10^{-4} r_s^3 - 8.95027 \times 10^{-5} r_s^4$$
$$D_1(r_s) = -0.32951 - 0.21230 r_s + 0.00965 r_s^2 + 130.44007 \times 10^{-4} r_s^3 - 145.95027 \times 10^{-5} r_s^4$$
$$D_2(r_s) = 5.30593 + 1.31679 r_s + 0.21208 r_s^2 - 1684.25993 \times 10^{-4} r_s^3 + 1560.04973 \times 10^{-5} r_s^4$$
$$D_3(r_s) = -15.07056 - 3.26070 r_s - 1.37773 r_s^2 + 7830.94007 \times 10^{-4} r_s^3 - 7529.95027 \times 10^{-5} r_s^4$$
$$D_4(r_s) = 22.02554 + 4.48947 r_s + 2.61918 r_s^2 - 13727.75993 \times 10^{-4} r_s^3 + 13490.04973 \times 10^{-5} r_s^4$$
$$D_5(r_s) = -9.81589 - 2.40712 r_s - 1.47717 r_s^2 + 7868.54007 \times 10^{-4} r_s^3 - 8063.95027 \times 10^{-5} r_s^4$$
$$3 \leqslant r_s \leqslant 5$$
$$D_0(r_s) = 0.64995 + 0.09479 r_s - 0.01191 r_s^2 + 16.30000 \times 10^{-4} r_s^3 - 0.12052 \times 10^{-3} r_s^4$$
$$D_1(r_s) = 3.29115 - 2.55653 r_s + 0.43412 r_s^2 + 6.94645 \times 10^{-4} r_s^3 - 2.39052 \times 10^{-3} r_s^4$$
$$D_2(r_s) = -24.77987 + 21.24814 r_s - 3.78282 r_s^2 + 747.24645 \times 10^{-4} r_s^3 + 11.70948 \times 10^{-3} r_s^4$$
$$D_3(r_s) = 116.18740 - 88.97349 r_s + 15.72466 r_s^2 - 3562.35355 \times 10^{-4} r_s^3 - 41.95052 \times 10^{-3} r_s^4$$
$$D_4(r_s) = -211.65547 + 156.15424 r_s - 27.61189 r_s^2 + 7240.34645 \times 10^{-4} r_s^3 + 63.13948 \times 10^{-3} r_s^4$$
$$D_5(r_s) = 136.96029 - 97.22916 r_s + 17.26022 r_s^2 - 4878.05355 \times 10^{-4} r_s^3 - 38.08052 \times 10^{-3} r_s^4$$

$$S_{\mathrm{HF}}(q) = \begin{cases} \frac{3}{4}\frac{q}{k_F} - \frac{1}{16}\left|\frac{q}{k_F}\right|^3 & q \leqslant k_F, \\ 1 & q > k_F, \end{cases} \tag{30}$$

and

$$S_{\mathrm{WS}}(q) = \frac{q^2}{q^2 + q_{\mathrm{WS}}^2}, \tag{31}$$

where q_{WS} is a characteristic wave number (see Ref. 15).

D. New expression of parametrized local-field correction

The expressions of OB-STLS local-field corrections [Eq. (9) or Eq. (10)] are very complex and those in OB-VS [Eq. (17)] or OB-UI [Eq. (27)] schemes are obtained numerically. So, we give here a very simple analytical expression which accurately reproduces these numerical values in the whole q-range variation and for metallic densities. We assume the following expansion of $G(\eta)$ in terms of the usual Lindhard function $Z(\eta)$,

$$G(\eta) = [1 - Z(\eta)] \times \sum_n D_n(r_s) Z(\eta)^n, \tag{32}$$

with

$$Z(\eta) = \frac{1}{2} + \frac{4 - \eta^2}{8\eta} \ln\left|\frac{2+\eta}{2-\eta}\right|, \quad \eta = \frac{q}{k_F}, \tag{33}$$

where $D_n(r_s)$ are density-dependent coefficients of the expansion and the prefactor $[1 - Z(\eta)]$, in the right-hand side of Eq. (32), ensures the requirement $G(0) = 0$. There is no reason for supposing that the exponent n in Eq. (32) is positive if one does not want to restrict the generality. In fact, if we consider the class of local-field corrections which have the Holas parabolic behavior at the short-wavelength limit (Refs. 10–13), the development must be considered as a Laurent series whose first term is $[D_{-1}(r_s)]/Z(\eta)$. In this case, the Lindhard function appears as a singularity of the LFC ($Z = 0$). Indeed at a short-wavelength limit, we have

$$\lim_{\eta \to \infty} G(\eta) = D_0 - D_{-1} + \frac{3 D_{-1}}{4} \eta^2 + O\left(\frac{1}{\eta^2}\right). \tag{34}$$

On the other hand, the term with the coefficient D_{-1} does not appear if the local-field correction is limited, as it is in the case of the present work. The coefficients $D_n(r_s)$ which contain the physical information on the exchange and correlation effects are really unknown. They may be obtained by a fitting as in this work. From the properties of the Lindhard function, one can write three criteria that these coefficients should verify,

$$D_{-1}(r_s) = 0,$$

$$D_0(r_s) = \lim_{\eta \to \infty} G(\eta) \quad \text{(if the LFC is limited)}, \tag{35}$$

$$\sum_n D_n(r_s) = 0, \tag{36}$$

and for γ already defined in Eq. (5),

$$\gamma = -\frac{1}{12} \sum_n n [D_n(r_s) - D_{n-1}(r_s)]. \tag{37}$$

III. RESULTS AND DISCUSSION

We carried out the local-field correction $G(q)$ following the three theoretical approaches described in the previous sections. For every considered case, we used the spin-dependent electron-pair-correlation function $g^{\sigma,\sigma'}(r)$ and the correlation energy $E_c(r_s)$, both parametrized by Ortiz and Ballone.[6] Our numerical results are displayed from Table I to Table III and in Fig. 1 to Fig. 5.

In Table I, the limit behavior in the long and short wavelengths of calculated LFC's are reported for different values of r_s. The accurate fitting parameters $D_n(r_s)$ defined in Eq. (32) are reported in Table II (OB-VS case) and in Table III (OB-IU case).

We plot in Fig. 1 the shape of the spin-anti-parallel con-

TABLE III. Expression of $D_n(r_s)$, $n \in [0,6]$ [Eq. (32)] in OB-UI expansion, accurate in the range $1 \leqslant r_s \leqslant 5$.

$$1 \leqslant r_s \leqslant 5$$
$$D_0(r_s) = 0.57353 + 0.15100 r_s - 0.01472 r_s^2 - 0.510009 \times 10^{-3} r_s^3 + 1.17066 \times 10^{-4} r_s^4$$
$$D_1(r_s) = -0.28578 - 0.78691 r_s - 0.12015 r_s^2 + 71.52999 \times 10^{-3} r_s^3 - 69.12934 \times 10^{-4} r_s^4$$
$$D_2(r_s) = 12.50176 + 3.83749 r_s + 1.11258 r_s^2 - 554.48001 \times 10^{-3} r_s^3 + 531.37066 \times 10^{-4} r_s^4$$
$$D_3(r_s) = -61.25749 - 11.63239 r_s - 4.21829 r_s^2 + 2035.03999 \times 10^{-3} r_s^3 - 1952.62934 \times 10^{-4} r_s^4$$
$$D_4(r_s) = 167.31876 + 20.85378 r_s + 7.66303 r_s^2 - 3744.64001 \times 10^{-3} r_s^3 + 3608.57066 \times 10^{-4} r_s^4$$
$$D_5(r_s) = -186.10675 - 18.83851 r_s - 6.79233 r_s^2 + 3367.47999 \times 10^{-3} r_s^3 - 3256.52934 \times 10^{-4} r_s^4$$
$$D_6(r_s) = 70.45671 + 6.56586 r_s + 2.34771 r_s^2 - 1173.68001 \times 10^{-3} r_s^3 + 1137.67066 \times 10^{-4} r_s^4$$

tribution $G^{\uparrow\downarrow}(q)$ in the STLS scheme [the curve called "exact OB-STLS ($\uparrow\downarrow$)"] calculated exactly according to Eq. (10) and under the control of Eq. (4) which also may be carried out numerically. We reproduce in the same figure $G^{\uparrow\downarrow}(q)$ calculated following Bretonnet-Boulahbak[9] and Boulahbak *et al.*[8] according to Eq. (9) and using as these authors the eighth-order expansion of the degenerate hypergeometric function [the curve called "approximate OB-STLS ($\uparrow\downarrow$)"]. As may be seen, the mathematical approximation assumed by these authors is only found in the range $q \lesssim 1.2 k_F$. The correct total STLS $G(q)$ [the curve called "exact total OB-STLS" including ($\uparrow\downarrow$) and ($\uparrow\uparrow$) contributions] calculated according to Eq. (8) and Eq. (10) is also reproduced.

We compare, in Fig. 2, the LFC determined numerically within a Monte Carlo OB-VS scheme [Eq. (17)] to the LFC according to the initially self-consistent screening theory of Vashista and Singwi (the numerical values are from Table IV in Ref. 20). We should notice here that both curves are remarkably identical for $q \lesssim 2 k_F$. The differences for higher q values which one observes between OB-VS and VS (self-consistent) are, from a theoretical point of view, significant. They show the limit of the theoretical model in the short-range correlation. We explain the differences for large q values by the fact that, in real space and for small distances, the VS radial distribution function $g(r)$ has an unsatisfactory behavior. It takes even unphysical negative values for $r \lesssim 1/2 k_F$ (Fig. 2 in Ref. 20). On the other hand, as input in the OB-VS calculation (present work), the function $g(r)$ is positive in the whole range of distance r and satisfies main physicals requirements ("sum rules").[6] Both LFC curves of OB-VS obtained numerically according to Eq. (17) or by our fitting expression [Eq. (32)] can practically not be distin-

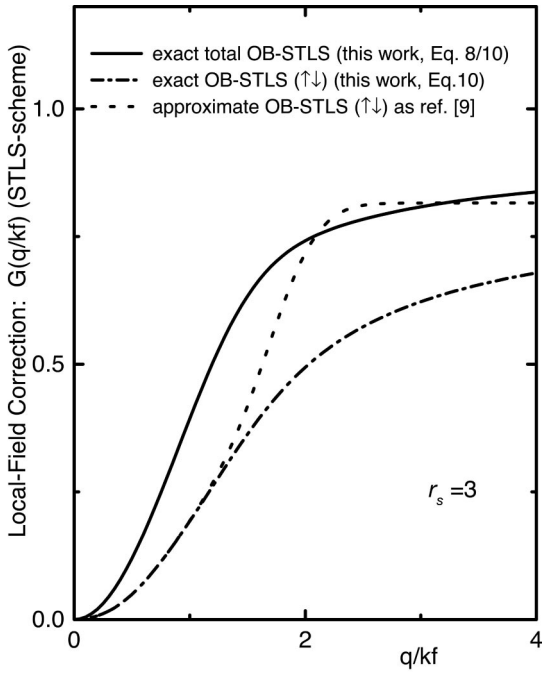

FIG. 1. Static local-field correction in the STLS scheme for $r_s = 3$. Our exact calculation [Eq. (10)] of the anti-parallel-spin part OB-STLS ($\uparrow\downarrow$) (short-dash-dotted line) is compared with the other one based on Eq. (9) with the hypergeometric function expanded up to eighth order (dotted line) as in Ref. 9. The exact total local-field correction OB-STLS [Eq. (8) and Eq. (10)] including ($\uparrow\downarrow$) and ($\uparrow\uparrow$) contributions, is also shown (continuous line).

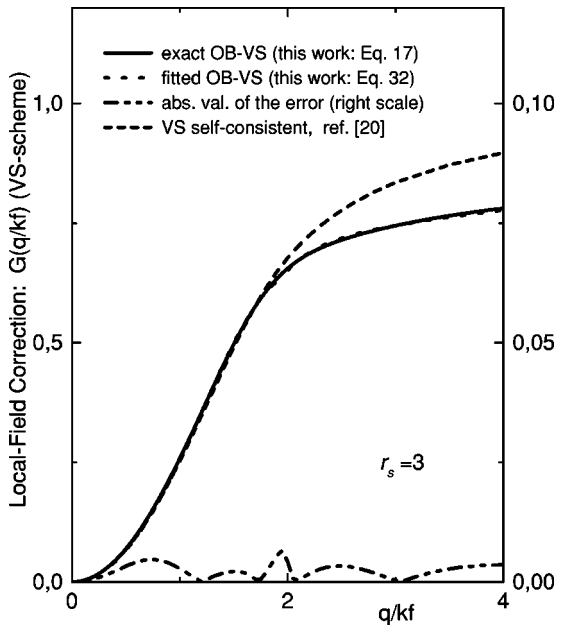

FIG. 2. Static local-field correction in the VS scheme for $r_s = 3$. The VS self-consistent calculation (Ref. 20) (short-dashed line) is compared with our results: the exact OB-VS [Eq. (17)] (continuous line) and the accurate fitting of OB-VS [Eq. (32)] (dotted line) can practically not be distinguished in the whole q range. The absolute value of their difference (error) is scaled by a factor of 10 (dash-dot-dotted line, right scale).

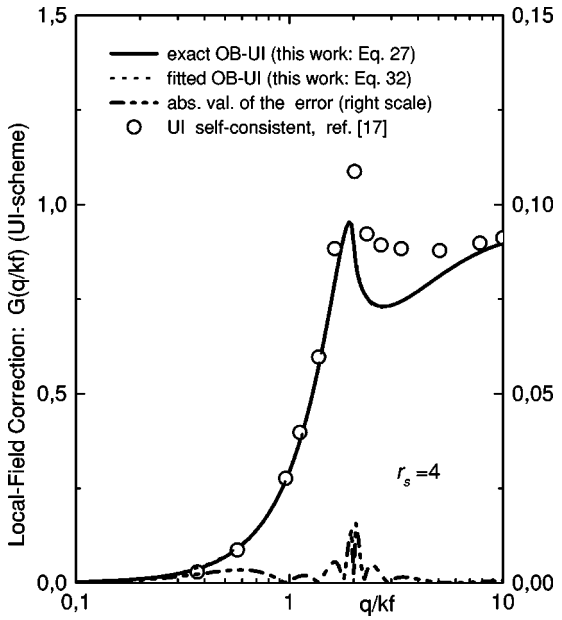

FIG. 3. Static local-field correction in the UI scheme for $r_s=4$. The few points of UI's LFC picked up from Ref. 17 (open circles) are compared with our corresponding LFC's: the exact OB-UI [Eq. (27)] curve (continuous line) practically masks the accurate fitting [Eq. (32)] of the OB-UI curve (dotted line). The absolute value of their difference (error) is scaled by a factor of 10 (dash-dot-dotted line, right scale).

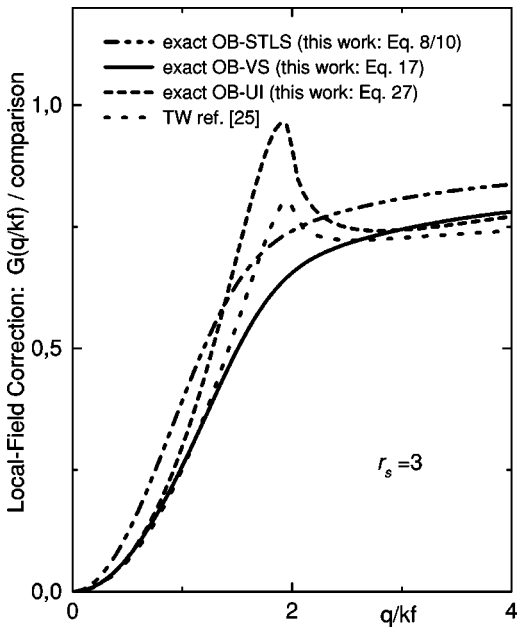

FIG. 4. Our exact Monte Carlo–derived results are grouped together to be compared: OB-STLS (dash-dot-dotted line), OB-VS (continuous line), and OB-UI (short-dashed line). The LFC of Toigo-Woodruff (Ref. 25) (TW) is also presented (dotted line).

guished in the whole q range. They are in agreement to within 1%. Their difference (''absolute value of the error'') is also shown in the same figure with another scale and can be neglected.

Our results performed in the OB-UI scheme are displayed in Fig. 3. For the sake of comparison with the corresponding self-consistent LFC curve shown in Refs. 15 and 17, some points are picked up from the latter and are reported in the same figure. The calculations are carried out with $r_s=4$ and we used a logarithmic scale for the abscissa. One can make the same comments as those for Fig. 2. First OB-UI and UI (self-consistent) are in good agreement for long-range wavelengths (from $q=0$ to $q\approx 2k_F$) and for the short-range wavelength limit ($q\rightarrow\infty$) (see Table I). As regards the intermediate range, the sharp logarithmic singularity at $q=2k_F$ is enhanced in the self-consistent calculation. On the other hand in our Monte Carlo–based work (OB-UI), the minimum is deeper than the one corresponding to the self-consistent calculation. Once again our fitting expression [Eq. (32)] reproduces very accurately OB-UI obtained numerically in the whole q range.

Finally, our results are collected in Fig. 4 and are compared to the Toigo-Woodruff[25] (TW) density-independent LFC which was obtained numerically in a ''first-principles calculations.'' One remarks on the singular behavior of the OB-STLS curve in the short-range limit in connection with the STLS inconsistency. All LFC curves except OB-STLS are in good agreement in the short range from $q=0$ to $q\approx 0.5k_F$. Furthermore, we observe that OB-VS agrees with TW in the range $q=0$ to $q\approx k_F$.

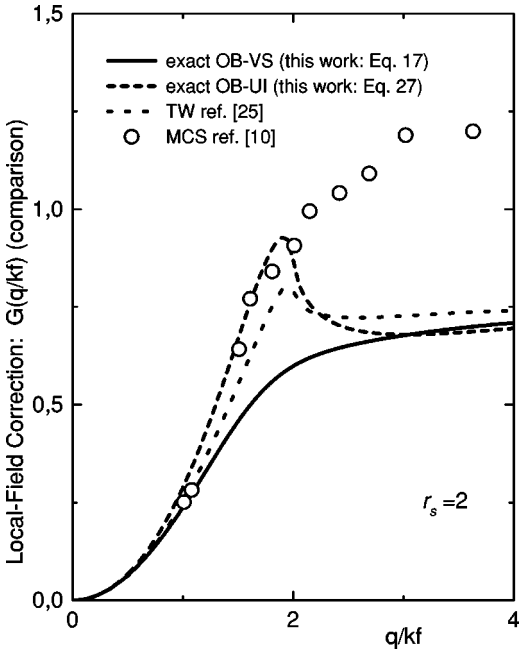

FIG. 5. Our exact Monte Carlo–derived results are grouped together to be compared to the LFC curve (open circles) obtained by Moroni *et al.* (Ref. 10) (MCS) from extensive diffusion Monte Carlo simulations with 38, 54, and 66 particles and within the density-density (linear-) response function: OB-VS (continuous line) and OB-UI (short-dashed line). The Toigo-Woodruf (Ref. 25) (TW) function is also reported (dotted line).

One common feature of the foregoing LFC's lies in the fact that they have a finite limit behavior at large q. On the contrary, Fig. 5 reveals the monotonic increase of the LFC given by Moroni *et al.*[10] (MCS). This noticeable feature suggests that the MCS results may be in agreement with the q^2-limit behavior foreseen by Holas.[13] As has been emphasized previously, this typical behavior is in keeping with the ''kinetic correlation effect'' whose contribution is included in MCS results and neglected in the other LFC's. Indeed, the LFC of MCS is extracted directly from the ''full density-density response function'' [10] obtained by extensive diffusion Monte Carlo simulations with 38, 54, and 66 particles. The ''kinetic correlation effect'' part of the LFC function, denoted as G_n by Richardson and Ashcroft,[11] vanishes at small q values and is substantial at q values roughly beyond $2k_F$ (Fig. 3 of Ref. 11). It follows that MCS results are significantly larger than those of the LFC considered previously at $q \gtrsim k_F$ for OB-VS or at $q \gtrsim 2k_F$ for OB-UI. Otherwise, our OB-VS curve agrees well with the quantum Monte Carlo–derived LFC obtained by MCS between $q \approx 0$ and $q \approx k_F$ and our OB-UI curve is in good agreement with MCS results between $q \approx 0$ and $q \approx 2k_F$.

IV. CONCLUSION

From Monte Carlo results presented in the literature by Ortiz and Ballone, we carried out numerically the local-field correction using three schemes within the so-called ''equation of motion'' formalism. Each of them corresponds to the manner for truncating the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy of the kinetic equation. We indicate the origin of some inaccuracies in earlier published work. We discuss precisely the domain of validity of the classical formalism. Finally, we give a simple analytical expression to implement the calculations in VS and UI schemes which furthermore captures the main physical features given by Monte Carlo simulation.

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[1] D.C. Marinescu and I. Tifrea, Phys. Rev. B **65**, 113201 (2002).
[2] F. Perrot and M.W.C. Dharma-Wardana, Phys. Rev. B **62**, 16 536 (2000).
[3] P. Gori-Giorgi, F. Sacchetti, and G.B. Bachelet, Phys. Rev. B **61**, 7353 (2000).
[4] G. Ortiz, M. Harris, and P. Ballone, Phys. Rev. Lett. **82**, 5317 (1999).
[5] B. Tanatar and N. Mutluay, Eur. Phys. J. B **1**, 409 (1998).
[6] G. Ortiz and P. Ballone, Phys. Rev. B **50**, 1391 (1994); **56**, 9970 (1997).
[7] A. Gold, Z. Phys. B: Condens. Matter **103**, 491 (1997).
[8] M. Boulahbak, J.-F. Wax, N. Jakse, and J.L. Bretonnet, J. Phys.: Condens. Matter **9**, 4017 (1997).
[9] J.L. Bretonnet and M. Boulahbak, Phys. Rev. B **53**, 6859 (1996).
[10] S. Moroni, D.M. Ceperley, and G. Senatore, Phys. Rev. Lett. **75**, 689 (1995).
[11] C.F. Richardson and N.W. Ashcroft, Phys. Rev. B **50**, 8170 (1994).
[12] B. Farid, V. Heine, G.E. Engel, and I.J. Robertson, Phys. Rev. B **48**, 11 602 (1993).
[13] A. Holas, in *Strongly Coupled Plasma Physics*, edited by F.J. Rogers and H.E. De Witt (Plenum, New York, 1987).
[14] J.P. Hansen and I.R. McDonald, *Theory of Simple Liquids* (Academic, New York, 1986).
[15] S. Ichimaru, Rev. Mod. Phys. **54**, 1017 (1982).
[16] J.P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[17] K. Utsumi and S. Ichimaru, Phys. Rev. B **22**, 5203 (1980).
[18] G. Niklasson, Phys. Rev. B **10**, 3052 (1974).
[19] J.C. Kimball, Phys. Rev. A **7**, 1648 (1973); J. Phys. A **8**, 1543 (1973).
[20] P. Vashista and K.S. Singwi, Phys. Rev. B **6**, 875 (1972).
[21] H. Yasuhara, Solid State Commun. **11**, 1481 (1972).
[22] R.W. Shaw, Jr., J. Phys. C **3**, 1140 (1970).
[23] K.S. Singwi, A. Sjölander, M.P. Tosi, and R.H. Land, Phys. Rev. B **1**, 1044 (1970).
[24] K.S. Singwi, M.P. Tosi, R.H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).
[25] F. Toigo and T.O. Woodruff, Phys. Rev. B **2**, 3958 (1970); **4**, 4312 (1971).
[26] D. Pines and P. Nozières, *Theory of Quantum Liquids* (Benjamin, New York, 1966).
[27] D.J.W. Geldart and S.H. Vosko, Can. J. Phys. **44**, 2137 (1966).
[28] L.J. Sham, Proc. R. Soc. London, Ser. A **283**, 33 (1965).
[29] J. Hubbard, Proc. R. Soc. London, Ser. A **243**, 336 (1957).