

# Model static structure factors and pair-correlation functions for the unpolarized homogeneous electron gas

Giovanni B. Bachelet<sup>a</sup>, Paola Gori-Giorgi<sup>b,c</sup>, Francesco Sacchetti<sup>c,d</sup>

<sup>a</sup>*Dipartimento di Fisica and Unità INFM, Università di Roma "La Sapienza",  
Piazzale Aldo Moro 2, 00185 Rome, Italy*

<sup>b</sup>*Department of Physics and Quantum Theory Group, Tulane University,  
New Orleans, Louisiana 70118, USA*

<sup>c</sup>*Unità INFM di Perugia, Via A. Pascoli 1, 06123 Perugia, Italy*

<sup>d</sup>*Dipartimento di Fisica, Università di Perugia, Via A. Pascoli 1, 06123 Perugia, Italy*

**Abstract.** We present a simple and accurate model for the electron static structure factors (and corresponding pair-correlation functions) for the 3D unpolarized homogeneous electron gas. This model stems from a combination of analytic constraints and fitting procedures to quantum Monte Carlo data. We also identify the correct long-range behavior of the pair-correlation function and of its spin-resolved components. Finally, we use our fitting strategy for extracting other quantities from QMC simulations, namely the spin-resolved contributions to the correlation energy and the static local fields (the latter ones according to the Singwi, Tosi, Land, and Sjölander scheme) which are given in this work as analytic functions of both the momentum transfer and the electronic density.

## INTRODUCTION

Binding and structural energies of many real molecules and materials are well described by the Density Functional Theory (DFT) [1], which turns an interacting many-electron system into a non-interacting system subject to an external self-consistent field, and yields extremely accurate predictions for equilibrium geometries, vibrational frequencies and other relevant physical and chemical properties of both existing and yet-to-be-synthesized compounds. This includes, after the advent of the Car-Parrinello method, real-time atomic trajectories, and thus phase transitions, the liquid state and chemical reactions [2]. DFT needs, however, approximate density functionals for the so-called *exchange-correlation energy*. The major part of such approximate functionals are built up starting from the results obtained for a model system, the homogeneous electron gas. The homogeneous electron gas

is a solid whose positive ionic charges are smeared throughout the whole crystal volume to yield a shapeless, uniform positive background (whence the nickname of *jellium*). The model, by ignoring the ionic lattice which makes real materials different from one another, allows the theorists to concentrate on key aspects of the electron-electron interaction. It thus provides a mine of information for solid-state and many-body theorists [3]. In spite of its simplicity, the jellium model is not analytically solvable, and the most reliable results for the quantities of direct interest for DFT calculations are obtained by quantum Monte Carlo (QMC) simulations [4–9], which provide results in the form of a discrete data set. To build up approximate exchange-correlation potentials that are *local* functionals of the electronic density, one just needs to know the ground-state energy of jellium as a function of the electronic density (and of the spin polarization for spin-polarized systems). To this purpose, QMC data for the correlation energy of jellium have been fitted using suitable functional forms which fulfill most of the known exact limits [10–13]. If one wishes to go beyond this local density approximation (LDA), the electronic pair-correlation functions of jellium are generally needed [14–18]. The pair-correlation functions describe spatial correlations between electrons of a prescribed spin orientation. The knowledge of these functions has its own interest, since they provide a quantitative and intuitive description of the two-body properties of the system. Moreover, as said, to build up *semilocal* and *nonlocal* exchange-correlation energy density functionals, the pair-correlation functions of the jellium model must generally be known as a function of both the interelectronic distance and the electronic density (and of the spin polarization for spin-polarized systems). As a consequence several authors, over the last 20 years, have proposed ingenious expressions for this or related functions [17,19–27].

There are motivations for resuming and improving over these efforts. A first motivation is the availability, from very recent quantum Monte Carlo (QMC) simulations [9], of a wealth of new numerical results for the pair-correlation functions and their Fourier transforms (the static structure factors) of jellium<sup>1</sup>. None of the previous models provides an accurate interpolation of these new QMC data, especially at the densities of practical interest for DFT calculations. Since at these densities QMC should provide the best estimate for these functions, it is important to make QMC data available for DFT calculations. This amounts to providing analytic functions of both the inter-electronic distance and the electronic density which fulfill all the exact limits and have enough free parameters to accurately fit the QMC data, in analogy to what has been done in the past for the correlation energy. A second motivation comes from the observation that most of the previous models were not spin resolved (i.e. parallel- and antiparallel-spin cases were not treated separately), none fulfilled all the known exact properties, and none was given in analytic, closed form in both real and reciprocal space. As we shall see, the last feature is crucial in order to include in the functional form all the exact

---

<sup>1</sup>) The pair-correlation functions and static structure factors are independently extracted by QMC simulations, see Ref. [6].

constraints in a very straightforward way.

This paper is organized as follows. A first section is devoted to define the spin-resolved pair-correlation functions and static structure factors. We then analyze the exact limits of these functions for small and large arguments, and discuss the high-density limit of the corresponding correlation energy. Then, we describe a new, simple strategy to provide analytic pair-correlation functions and static structure factors which accurately interpolate the QMC data, fulfill most of the exact limits, and are closed-form in both real and reciprocal space. Finally, we show that this strategy, as a byproduct, allows to extract quantities from QMC simulations that are in general not available, namely the spin-resolved contributions to the correlation energy and the static local field factors in the STLS [28] scheme, which are given in this work as analytic functions of both the momentum transfer and the electronic density. Hartree atomic units are used throughout this work.

## DEFINITIONS

For an electronic system the pair-correlation function  $g_{\sigma_1\sigma_2}(\mathbf{r}_1, \mathbf{r}_2)$ , if  $n_\sigma(\mathbf{r})$  is the density of electrons with spin  $\sigma = \uparrow$  or  $\downarrow$ , is defined by

$$n_{\sigma_1}(\mathbf{r}_1)n_{\sigma_2}(\mathbf{r}_2)g_{\sigma_1\sigma_2}(\mathbf{r}_1, \mathbf{r}_2) = \langle \Phi | \psi_{\sigma_1}^\dagger(\mathbf{r}_1)\psi_{\sigma_2}^\dagger(\mathbf{r}_2)\psi_{\sigma_2}(\mathbf{r}_2)\psi_{\sigma_1}(\mathbf{r}_1) | \Phi \rangle \quad (1)$$

and is thus related to the probability of finding two electrons of prescribed spin orientations at positions  $\mathbf{r}_1$  and  $\mathbf{r}_2$ . The normalization of  $g$  is such that the expected number of electrons of spin  $\sigma_2$  in the volume  $dV$  at  $\mathbf{r}_2$  when another electron of spin  $\sigma_1$  is known to be at  $\mathbf{r}_1$  is given by

$$dN(\mathbf{r}_2\sigma_2|\mathbf{r}_1\sigma_1) = n_{\sigma_2}(\mathbf{r}_2)g_{\sigma_1\sigma_2}(\mathbf{r}_1, \mathbf{r}_2)dV; \quad (2)$$

the lack of any correlation amounts, then, to the condition  $g_{\sigma_1\sigma_2}(\mathbf{r}_1, \mathbf{r}_2) = 1$ . In the spin-unpolarized jellium the electronic spin density  $n_\uparrow(\mathbf{r}) = n_\downarrow(\mathbf{r}) = n/2 = (8\pi r_s^3/3)^{-1}$  is uniform in space<sup>2</sup>(i.e. independent of  $\mathbf{r}$ ), so  $g_{\sigma_1\sigma_2}(\mathbf{r}_1, \mathbf{r}_2)$  only depends on the distance between the two electrons  $r = |\mathbf{r}_1 - \mathbf{r}_2|$ .

The static structure factor  $S(q)$  is an "experimental" quantity, well-known to whoever is familiar with scattering theory. It is directly related to the Fourier transform of the pair-correlation function, and provides information on  $g(r)$ . A good pair-correlation function model should always correspond to a good static structure factor and vice versa. For an unpolarized homogeneous electron gas, after introducing the Fermi wavevector  $q_F = (3\pi^2 n)^{1/3} = \alpha/r_s$ , with  $\alpha = (9\pi/4)^{1/3}$ , the scaled variables  $\rho = q_F r$  and  $k = q/q_F$  are often convenient. With these variables the static structure factors are written as

<sup>2</sup> In what follows we won't be concerned with spatially nonuniform phases of jellium (although these phases are also of great interest: see e.g. J. A. Tuszyński, J. M. Dixon, and N. H. March, Phys. Rev. E **58**, 318 (1998), or Refs. [9] and [29]).

$$S_{\uparrow\downarrow}(k) = \frac{2}{3\pi} \int_0^\infty d\rho [g_{\uparrow\downarrow}(\rho) - 1] \rho^2 \frac{\sin(k\rho)}{k\rho} \quad (3)$$

$$S_{\uparrow\uparrow}(k) = 1 + \frac{2}{3\pi} \int_0^\infty d\rho [g_{\uparrow\uparrow}(\rho) - 1] \rho^2 \frac{\sin(k\rho)}{k\rho} \quad (4)$$

and the total pair-correlation function and static structure factor are given by  $g = (g_{\uparrow\uparrow} + g_{\uparrow\downarrow})/2$  and  $S = S_{\uparrow\uparrow} + S_{\uparrow\downarrow}$ . The functions  $g_{\sigma_1\sigma_2}$  and  $S_{\sigma_1\sigma_2}$  are usually split into exchange and correlation according to:

$$g_{\uparrow\downarrow}(\rho; r_s) = 1 + g_{\uparrow\downarrow}^c(\rho; r_s) \quad (5)$$

$$g_{\uparrow\uparrow}(\rho; r_s) = g_{ex}(\rho) + g_{\uparrow\uparrow}^c(\rho; r_s) \quad (6)$$

$$S_{\uparrow\downarrow}(k; r_s) = S_{\uparrow\downarrow}^c(k; r_s) \quad (7)$$

$$S_{\uparrow\uparrow}(k; r_s) = S_{ex}(k) + S_{\uparrow\uparrow}^c(k; r_s) \quad (8)$$

where the exchange functions, given by the Hartree-Fock approximation, are equal to:

$$g_{ex}(\rho) = 1 - 9 \left( \frac{\sin \rho - \rho \cos \rho}{\rho^3} \right)^2 \quad (9)$$

$$S_{ex}(k) = \begin{cases} 3k/4 - k^3/16 & \text{for } k \leq 2 \\ 1 & \text{for } k > 2 \end{cases} \quad (10)$$

The electron-electron potential energy is, as known, given by the sum of repulsive two-body Coulomb terms:

$$U = \frac{1}{2} \sum_{i \neq j}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (11)$$

Its ground-state expectation value (per electron), in a homogeneous electron gas of density  $r_s$ , is given by the following integral over the pair-correlation function:

$$\langle U \rangle_{r_s} = \frac{3}{2\alpha^2 r_s} \int_0^\infty [g(\rho; r_s) - 1] \rho d\rho. \quad (12)$$

By the virial theorem [30] and the usual definition of the correlation energy  $\epsilon_c$  as total electronic energy minus Hartree-Fock energy, one obtains the known relation between  $g^c(\rho; r_s)$  and  $\epsilon_c$ :

$$\epsilon_c = \frac{3}{2\alpha^2 r_s^2} \int_0^\infty d\rho \rho \int_0^{r_s} dr'_s [g^c(\rho; r'_s) - 1]. \quad (13)$$

The same relation can be obtained in a more general way [14] by the Hellmann-Feynman theorem and the coupling-constant average of  $g^c(\rho; r_s)$ , which, for the homogeneous system is just the average over  $r_s$ :

$$\bar{g}^c(\rho; r_s) = \frac{1}{r_s} \int_0^{r_s} g^c(\rho; r'_s) dr'_s. \quad (14)$$

The function  $\bar{g}^c(\rho; r_s)$  is directly related to the correlation hole [14,25] of the electron gas.

## EXACT LIMITS

The quantum Monte Carlo data for  $g_{\sigma_1\sigma_2}(\rho)$  and  $S_{\sigma_1\sigma_2}(k)$  are available for a discrete set of inter-electronic distances  $\rho \in [\rho_{\min}, \rho_{\max}]$ , momentum transfers  $k \in [k_{\min}, k_{\max}]$ , and densities  $r_s$ . In order to provide a reliable extrapolation of the QMC data outside the finite range  $[\rho_{\min}, \rho_{\max}]$  (or  $[k_{\min}, k_{\max}]$ ), it is crucial to impose to the fitting functional forms the exact behavior for small and large arguments. In this section we report these exact limits. Some of them are well known, while others were not emphasized before our work. They should be included in any model for the correlation holes of jellium.

### Pair-correlation functions near $r = 0$

The behavior of  $g_{\sigma_1\sigma_2}(r; r_s)$  in the  $r \rightarrow 0$  limit is well known and can be directly obtained from the many-body Schrödinger equation when two electrons approach each other (cusp conditions) [19,31,32]:

$$\left. \frac{\partial}{\partial r} g_{\uparrow\downarrow}(r; r_s) \right|_{r \rightarrow 0} = g_{\uparrow\downarrow}(r \rightarrow 0; r_s) \neq 0 \quad (15)$$

$$\left. \frac{\partial}{\partial r} g_{\uparrow\uparrow}(r; r_s) \right|_{r \rightarrow 0} = g_{\uparrow\uparrow}(r \rightarrow 0; r_s) = 0 \quad (16)$$

$$\left. \frac{\partial^3}{\partial r^3} g_{\uparrow\uparrow}(r; r_s) \right|_{r \rightarrow 0} = \frac{3}{2} \frac{\partial^2}{\partial r^2} g_{\uparrow\uparrow}(r; r_s) \Big|_{r \rightarrow 0} \neq 0. \quad (17)$$

Eqs. (15)-(17) hold for any 3D-system of  $N$  fermions interacting via the two-body repulsive Coulomb potential.

### Structure factors near $q = 0$

The conservation of particles in the system implies the relations:

$$S_{\uparrow\downarrow}(q \rightarrow 0; r_s) = S_{\uparrow\uparrow}(q \rightarrow 0; r_s) = 0. \quad (18)$$

The asymmetry between the definitions (3) and (4) leads to the two well-known sum rules for  $g_{\uparrow\downarrow}$  and  $g_{\uparrow\uparrow}$  (see for instance Ref. [19]). The long-wavelength behavior of the total static structure factor  $S = S_{\uparrow\uparrow} + S_{\uparrow\downarrow}$  is well known and is determined by the plasmon contribution, proportional to  $q^2$ , and by the single-pair and multi-pair quasiparticle-quasihole excitation contributions, proportional to  $q^5$  and  $q^4$  respectively [33,34]:

$$S(q \rightarrow 0; r_s) = S_{\uparrow\uparrow}(q \rightarrow 0; r_s) + S_{\uparrow\downarrow}(q \rightarrow 0; r_s) = \frac{q^2}{2\omega_p(r_s)} + Cq^4 + \mathcal{O}(q^5), \quad (19)$$

where  $\omega_p(r_s) = \sqrt{3/r_s^3}$  is the classical plasma frequency. The small- $q$  behavior of the spin-resolved static structure factors seems, instead, less known. It can be deduced by considering the magnetic structure factor, a quantity related to the spin response function to an external magnetic field and defined as

$$\tilde{S} = S_{\uparrow\uparrow} - S_{\uparrow\downarrow}. \quad (20)$$

In the random-phase approximation (RPA) (see e.g. Ref. [33]) the small- $q$  limit of  $\tilde{S}$  is obtained by the following simple argument [13,35]. RPA only takes into account the first-order exchange process (i.e. the Hartree-Fock term) and the highest-order direct processes. Since direct processes occur between both parallel- and antiparallel-spin pairs, in the unpolarized gas they are equally split between  $\uparrow\uparrow$  and  $\uparrow\downarrow$ . Thus, at any  $q$ , the difference  $S_{\uparrow\uparrow} - S_{\uparrow\downarrow}$  is, within RPA, equal to the first-order exchange term, i.e. Eq. (10). Hence we have:

$$\tilde{S}^{\text{RPA}}(k \rightarrow 0) = \frac{3}{4}k - \frac{k^3}{16} + \mathcal{O}(k^4). \quad (21)$$

In the small- $k$  limit (which, since  $k = q/q_F$ , can be achieved either by  $q \rightarrow 0$  or by  $r_s \rightarrow 0$ ), RPA is known to give exact results for the total  $\uparrow\uparrow + \uparrow\downarrow$  correlation [33,36–38]. However, as far as magnetic correlations are considered, RPA is the same as the Hartree-Fock approximation, and the limit of Eq. (21) could be violated in the exact case [39]. A recent study shows [40] that the appropriate corrections to RPA do not change the linear behavior  $\tilde{S}(k \rightarrow 0) \propto k$ ; they just slightly modify the coefficient of the linear term w.r.t the RPA value of  $3/4$  (and also the coefficient of the cubic term w.r.t the RPA value of  $-1/16$ ) in the above Eq. (21). In the following equations we will, for the sake of completeness, indicate these corrections as  $c_1$  and  $c_3$ , but in our fitting procedure we set them equal to zero, since, at least in the parameter range of our interest, the RPA limit appears to adequately describe the physics of the spin resolution at small  $k$  [13,41]. In the paramagnetic gas, the parallel- and antiparallel-spin contribution to the plasma mode is the same, so the  $\propto q^2$  term in Eq. (19) is equally split between  $\uparrow\uparrow$  and  $\uparrow\downarrow$ . Putting together Eq. (19) and (21) we thus obtain the small- $k$  expansion of the spin-resolved static structure factors,

$$S_{\uparrow\downarrow}|_{k \rightarrow 0} = -\left(\frac{3}{8} + \frac{c_1}{2}\right)k + \frac{q_F^2 k^2}{4\omega_p(r_s)} + \left(\frac{1}{32} + \frac{c_3}{2}\right)k^3 + \mathcal{O}(k^4) \quad (22)$$

$$S_{\uparrow\uparrow}|_{k \rightarrow 0} = \left(\frac{3}{8} + \frac{c_1}{2}\right)k + \frac{q_F^2 k^2}{4\omega_p(r_s)} - \left(\frac{1}{32} + \frac{c_3}{2}\right)k^3 + \mathcal{O}(k^4), \quad (23)$$

Notice that the RPA fulfills Eq. (19) within  $\mathcal{O}(k^4)$ , since no term  $\propto k^3$  appears in the total  $S^{\text{RPA}}$ .

## Pair-correlation functions for $r \rightarrow \infty$

The long-range behavior of the pair-correlation functions can be obtained from the small- $k$  behavior of the static structure factors, by means of simple properties of the spherical Fourier transforms. To be more precise, the  $r \rightarrow \infty$  behavior of  $g_{\sigma_1\sigma_2}$  is determined by the odd powers in the small- $k$  expansion of  $S_{\sigma_1\sigma_2}$ . Following the procedure already used in Refs. [19,31], we thus obtain for the total pair-correlation function

$$g(\rho \rightarrow \infty) - 1 \propto \frac{1}{\rho^8}. \quad (24)$$

The  $\rho^{-8}$  behavior is determined by the  $k^5$  term in the small- $k$  expansion of the total  $S$ . Notice that the widely-used Perdew-Wang model [25,41] does not fulfill this exact limit. Their real-space correlation hole decays as  $\rho^{-5}$ , and thus corresponds to a wrong small- $k$  behavior of  $S(k)$  proportional to  $k^2 \ln k$ . Using again the properties of the spherical Fourier transforms, from Eqs. (22) and (23) one can easily write down the long-range decay of the spin-resolved pair-correlation functions:

$$g_{\uparrow\downarrow}|_{\rho \rightarrow \infty} = 1 + \frac{1}{\rho^4} \left( \frac{9}{4} + 3c_1 \right) + \frac{1}{\rho^6} \left( \frac{9}{4} + 36c_3 \right) + \mathcal{O} \left( \frac{1}{\rho^8} \right) \quad (25)$$

$$g_{\uparrow\uparrow}|_{\rho \rightarrow \infty} = 1 - \frac{1}{\rho^4} \left( \frac{9}{4} + 3c_1 \right) - \frac{1}{\rho^6} \left( \frac{9}{4} + 36c_3 \right) + \mathcal{O} \left( \frac{1}{\rho^8} \right). \quad (26)$$

## Static structure factors for $k \rightarrow \infty$

The large- $k$  behavior of  $S_{\sigma_1\sigma_2}$  has been determined in Refs. [19,31], by means of Eqs. (15), (16) and (17). It is equal to

$$S_{\uparrow\downarrow}(k \rightarrow \infty) \propto \frac{1}{k^4} \quad (27)$$

$$S_{\uparrow\uparrow}(k \rightarrow \infty) - 1 \propto \frac{1}{k^6}. \quad (28)$$

## High-density limit of the corresponding correlation energies

Starting from Eq. (13) we can define the spin-resolved contributions to the correlation energy such that  $\epsilon_c = \epsilon_c^{\uparrow\downarrow} + \epsilon_c^{\uparrow\uparrow}$ :

$$\epsilon_c^{\sigma_1\sigma_2} = \frac{3}{4\alpha r_s^2} \int_0^{r_s} dr'_s \int_0^\infty d\rho \rho g_{\sigma_1\sigma_2}^c(\rho; r'_s). \quad (29)$$

Then, conditions on the high-density expansion of  $g_{\sigma_1\sigma_2}^c$  can be written down using the well-known limit  $\epsilon_c(r_s \rightarrow 0) = A \ln r_s + B + \mathcal{O}(r_s \ln r_s)$  [12,37,42–46]:

$$\frac{3}{4\alpha^2} \int_0^\infty g_{\sigma_1\sigma_2}^c(\rho; r_s) \rho d\rho|_{r_s \rightarrow 0} = r_s [2A_{\sigma_1\sigma_2} \ln r_s + (A_{\sigma_1\sigma_2} + 2B_{\sigma_1\sigma_2})]. \quad (30)$$

The spin-resolved high-density coefficients,  $A_{\sigma_1\sigma_2}$  and  $B_{\sigma_1\sigma_2}$ , are recovered by applying the same argument which yielded Eq. (21). The logarithmic divergent term in the  $r_s \rightarrow 0$  expansion of  $\epsilon_c$  arises by a direct process, and is thus equally split between  $\uparrow\downarrow$  and  $\uparrow\uparrow$  in the unpolarized gas. The constant term  $B$  is the sum of two contributions: a second-order exchange term,  $B_{exc}^{(2)}$ , which only concerns the  $\uparrow\uparrow$  part, and a direct term,  $B_d$ , which is, instead, equally split (in the unpolarized gas) between  $\uparrow\uparrow$  and  $\uparrow\downarrow$ . Hence,

$$A_{\uparrow\downarrow} = A_{\uparrow\uparrow} = \frac{1}{2}A \quad (31)$$

$$B_{\uparrow\downarrow} = \frac{B_d}{2} \quad (32)$$

$$B_{\uparrow\uparrow} = \frac{B_d}{2} + B_{exc}^{(2)}. \quad (33)$$

Both  $B_{exc}^{(2)}$  and  $B_d$  have been evaluated exactly [44,45].

## A NEW STRATEGY

We briefly recall our simple functional form [13] for the correlation part of the spin-resolved functions  $g_{\sigma_1\sigma_2}$  and  $S_{\sigma_1\sigma_2}$ , which automatically fulfills all the above limits, has enough free parameters to allow for an accurate fit of the new QMC data [9], and is analytic and closed-form in both real and reciprocal space.

### Antiparallel spins

For the  $\uparrow\downarrow$  part, in reciprocal space, a simple function with the desired properties is

$$S_{\uparrow\downarrow}^c(k; r_s) = e^{-b^{\uparrow\downarrow}(r_s)k} \sum_{n=1}^6 c_n^{\uparrow\downarrow}(r_s) k^n + \frac{\alpha_6^{\uparrow\downarrow}(r_s) k^8 + \alpha_4^{\uparrow\downarrow}(r_s) k^{10}}{[(a^{\uparrow\downarrow})^2 + k^2]^7}. \quad (34)$$

This function has the correct small- $k$  and large- $k$  behavior, and corresponds in real space to a similar form [13], since the first term in the r.h.s. is the spherical Fourier transform of the second one. The parameters  $b^{\uparrow\downarrow}$ ,  $c_n^{\uparrow\downarrow}$ ,  $a^{\uparrow\downarrow}$  and  $\alpha_n^{\uparrow\downarrow}$  will be determined as functions of  $r_s$  by means of the exact constraints and of a fitting procedure to QMC data [13]. Few, very simple equations are enough to make Eq. (34) fulfill the small- and large- $k$  limits:

$$c_1^{\uparrow\downarrow} = -\frac{3}{8} \quad (35)$$



$$c_2^{\uparrow\downarrow} = b^{\uparrow\downarrow} c_1^{\uparrow\downarrow} + \frac{q_F^2}{4\omega_p} \quad (36)$$

$$c_3^{\uparrow\downarrow} = (b^{\uparrow\downarrow})^2 \frac{c_1^{\uparrow\downarrow}}{2} + b^{\uparrow\downarrow} \frac{q_F^2}{4\omega_p} + \frac{1}{32} \quad (37)$$

$$\alpha_6^{\uparrow\downarrow} = (a^{\uparrow\downarrow})^3 \left\{ \alpha_4^{\uparrow\downarrow} \left( \frac{11}{a^{\uparrow\downarrow}} - \frac{512}{21} q_F \right) - \frac{2048}{21\pi} \left[ \frac{1}{3} + \sum_{n=1}^6 c_n^{\uparrow\downarrow} \frac{(n+2)!}{(b^{\uparrow\downarrow})^{n+3}} \right] \right\}. \quad (38)$$

One of the advantages of an analytic form both in real and reciprocal space is that we always deal with local rather integral properties. The Eqs. (35) and (37), as mentioned before and already done in Ref. [13], amount to choosing the simple RPA small- $k$  limit for the spin-resolved static structure factors by setting  $c_1 = c_3 = 0$  in Eq. (22). In the high-density limit, the correlation-energy constraint of Eq. (30) translates into the following conditions:

$$\alpha_4^{\uparrow\downarrow}(r_s \rightarrow 0) = \frac{1 + k_1 r_s \ln r_s + k_2 r_s + \mathcal{O}(r_s^2 \ln r_s)}{-3\pi q_F/4} \quad (39)$$

$$b^{\uparrow\downarrow}(r_s \rightarrow 0) = \left( \frac{4}{9\pi} \right)^{1/3} \pi \sqrt{\frac{3}{r_s}} + \mathcal{O}(r_s^0) \quad (40)$$

$$a^{\uparrow\downarrow}(r_s \rightarrow 0) = \text{const.} + \mathcal{O}(r_s) \equiv a^{\uparrow\downarrow} + \mathcal{O}(r_s) \quad (41)$$

where  $k_1$  and  $k_2$  depend on  $A_{\uparrow\downarrow}$ ,  $B_{\uparrow\downarrow}$  and  $a^{\uparrow\downarrow}$ :

$$k_1 = \frac{18\pi(a^{\uparrow\downarrow})^2}{\alpha} A_{\uparrow\downarrow} \quad (42)$$

$$k_2 = \frac{729}{64} \frac{(a^{\uparrow\downarrow})^2}{\alpha^4} - \frac{21}{64} \frac{1}{a^{\uparrow\downarrow}\alpha} + \frac{9(a^{\uparrow\downarrow})^2\pi}{2\alpha} (A_{\uparrow\downarrow} + 2B_{\uparrow\downarrow}). \quad (43)$$

Unfortunately, when the exact high-density limit of the correlation energy is imposed to Eq. (34), the exact  $r_s \rightarrow 0$  limit of the pair-correlation function at zero-interelectronic distance is not recovered. Evidently, the simple functional form of Eq. (34) does not correctly describe the short-range behavior of the Coulomb hole at very high densities. However, as long as our pair-correlation functions fulfill the high-density expansion of the energy, this drawback (which only affects densities  $r_s \lesssim 0.1$ ) is not energetically important.

## Parallel spins

For the correlation part of the  $\uparrow\uparrow$  static structure factor we basically use the same functional form used for the antiparallel-spin case,

$$S_{\uparrow\uparrow}^c(k; r_s) = e^{-b^{\uparrow\uparrow}(r_s)k} \sum_{n=1}^6 c_n^{\uparrow\uparrow}(r_s) k^n + \frac{\alpha_{10}^{\uparrow\uparrow}(r_s) k^8 + \alpha_8^{\uparrow\uparrow}(r_s) k^{10} + \alpha_6^{\uparrow\uparrow}(r_s) k^{12}}{[(a^{\uparrow\uparrow})^2 + k^2]^9}. \quad (44)$$

Only the large- $k$  part is different with respect to the  $\uparrow\downarrow$  case in order to reproduce the exact behavior of Eq. (28) and fulfill the Pauli principle. All the exact conditions are easily imposed as in the  $\uparrow\downarrow$  case (see Ref. [13] for more details).

## Fit to QMC data

After imposing all the exact constraints, we are left with 6 free parameters for the  $\uparrow\downarrow$  part and another 6 for the  $\uparrow\uparrow$ . We now have to find out how these free parameters depend on  $r_s$ . For each available density in the range  $0.8 \leq r_s \leq 10$  (i.e.  $r_s = 0.8, 1, 2, 3, 4, 5, 8$  and  $10$ ) we performed a best fit of the 6 free parameters to the QMC data [9], separately provided for the  $\uparrow\downarrow$  and the  $\uparrow\uparrow$  parts, and for real- and reciprocal-space pair-correlation functions and structure factors, respectively. The  $r_s$  dependence of the parameters turns out to be quite smooth, monotonic, and well described by the following functional forms (which also take into account the exact high-density limit of Eqs. (39)-(41) and guarantee the exact low-density expansion of the resulting correlation energy [4,10-12,47]  $d_1 r_s^{-1} + d_2 r_s^{-3/2}$ ):

$$\alpha_4^{\uparrow\downarrow}(r_s) = \frac{4 \left[ 1 - k_1(a^{\uparrow\downarrow}) r_s \ln \left( 1 + \tilde{k}_2(a^{\uparrow\downarrow})/r_s \right) \right]}{3\pi q_F (1 + k_3 r_s^2)} \quad (45)$$

$$\alpha_6^{\uparrow\uparrow}(r_s) = \frac{8 \left[ 1 - p_1(a^{\uparrow\uparrow}) r_s \ln \left( 1 + p_2(a^{\uparrow\uparrow})/r_s \right) \right]}{5\pi q_F (1 + p_3 r_s^2)} \quad (46)$$

$$a^{\sigma_1\sigma_2}(r_s) = a^{\sigma_1\sigma_2} \quad (47)$$

$$b^{\sigma_1\sigma_2}(r_s) = \left( \frac{4}{9\pi} \right)^{1/3} \pi \sqrt{\frac{3}{r_s}} + b_1^{\sigma_1\sigma_2} \quad (48)$$

$$c_n^{\sigma_1\sigma_2}(r_s) = \frac{\lambda_n^{\sigma_1\sigma_2} + \gamma_n^{\sigma_1\sigma_2} r_s}{1 + r_s^{3/2}} \quad n = 4, 5, 6 \quad (49)$$

where  $k_1(a^{\uparrow\downarrow})$  is given by Eq. (42), and  $\tilde{k}_2(a^{\uparrow\downarrow})$ ,  $p_1(a^{\uparrow\uparrow})$  and  $p_2(a^{\uparrow\uparrow})$  are equal to:

$$\tilde{k}_2(a^{\uparrow\downarrow}) = \exp \left[ \frac{7}{384\pi (a^{\uparrow\downarrow})^3 A_{\uparrow\downarrow}} - \frac{81}{128\pi \alpha^3 A_{\uparrow\downarrow}} - \frac{B_{\uparrow\downarrow}}{A_{\uparrow\downarrow}} - \frac{1}{2} \right] \quad (50)$$

$$p_1(a^{\uparrow\uparrow}) = \frac{33\pi A_{\uparrow\uparrow} (a^{\uparrow\uparrow})^4}{\alpha} \quad (51)$$

$$p_2(a^{\uparrow\uparrow}) = \exp \left[ \frac{7}{960\pi (a^{\uparrow\uparrow})^5 A_{\uparrow\uparrow}} - \frac{81}{128\pi \alpha^3 A_{\uparrow\uparrow}} - \frac{B_{\uparrow\uparrow}}{A_{\uparrow\uparrow}} - \frac{1}{2} \right]. \quad (52)$$

We are now left with 9 constants for  $\uparrow\downarrow$  and 9 constants for  $\uparrow\uparrow$ , that we fix by a two-dimensional best fit to the QMC data [9] in real and reciprocal space [13] (9368+9368 data points). We thus obtain analytic expressions for  $g$  and  $S$  that are very reliable and accurate in the whole density range  $r_s \in [0.8, 10]$  (see Figs. 1 and 3 of Ref. [13]).

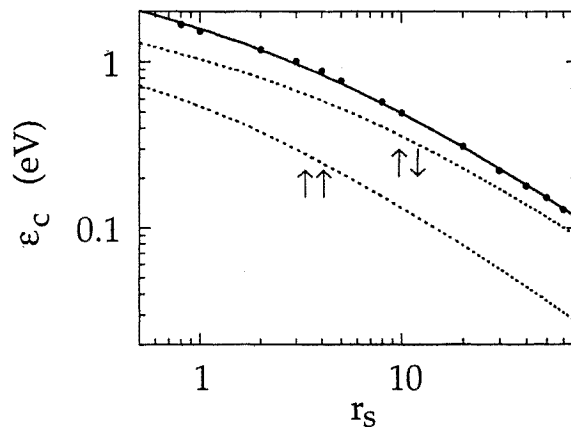
## EXTRACTING OTHER QUANTITIES FROM QMC SIMULATIONS

The new strategy we have just described allows to extract from QMC simulations quantities that are usually not available, i.e. the spin-resolved contributions to the

correlation energy and the static electric and magnetic local fields in the STLS [28] scheme.

### Spin-resolved correlation energies

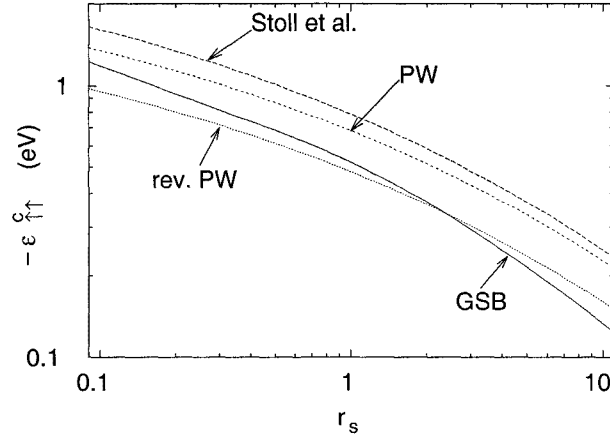
The correlation energy obtained by integrating our  $g$  [see Eq. (13)] is reported in Fig 1, together with the corresponding QMC data [9]. Its  $\uparrow\uparrow$  and  $\uparrow\downarrow$  contributions ( $\epsilon_c = \epsilon_c^{\uparrow\downarrow} + \epsilon_c^{\uparrow\uparrow}$ ) are also separately shown. As expected [33], correlations are dominated by  $\uparrow\downarrow$  interactions. Our total correlation energies are in agreement with QMC data within 5% (the maximum absolute error is 3.4 mRy); this accuracy is the same as the one reached by fitting other popular interpolation formulas [10–12] to the new QMC data of Ortiz, Harris and Ballone [9] (see Ref. [13]). Notice that our model pair-correlation function breaks down for  $r_s > 10$  [13], yet it gives very good correlation energies even at higher  $r_s$  values. This is due to the optimal choice of the  $r_s$  dependence of our free parameters, which also includes the low-density expansion of  $\epsilon_c$ . The spin-resolved contributions to the correlation



**FIGURE 1.** Total (solid) and spin-resolved (dashed) correlation energy obtained by the pair-correlation functions of Ref. [13]. QMC data [9] are also shown as dots.

energy, shown in Fig. 1, should be reliable in the density range  $r_s \leq 10$ , since they are obtained by integrating the corresponding QMC pair-correlation functions. This is the only way to extract the  $\uparrow\downarrow$  and  $\uparrow\uparrow$  contributions to  $\epsilon_c$  from QMC data. For  $r_s > 10$  we cannot expect our spin-resolved contributions to be as reliable as for  $r_s \leq 10$ , since at these very low densities they do not correspond to good pair-correlation functions. In Fig. 2 we compare our parallel-spin part of the correlation energy with three corresponding scaling guesses: Perdew-Wang in both its original version [25] [ $\epsilon_c^{\uparrow\uparrow}(r_s, \zeta = 0) = \epsilon_c(r_s, \zeta = 1)/2^{1/3}$ , where  $\zeta = |n_\uparrow - n_\downarrow|/n$ ], and its revised version [41] obtained by imposing to the orig-

inal form our Eq. (21) [ $\epsilon_c^{\uparrow\uparrow}(r_s, \zeta = 0) = \epsilon_c(r_s, \zeta = 1)/2^{5/6}$ ], and Stoll *et al.* [48] [ $\epsilon_c^{\uparrow\uparrow}(r_s, \zeta = 0) = \epsilon_c(2^{1/3}r_s, \zeta = 1)$ ]. Both the original PW [25] and the Stoll *et al.* [48] approximations overestimate the  $\uparrow\uparrow$  contribution to the correlation energy. As  $r_s$  increases, the PW and Stoll *et al.* approximations tend to the same limit, which is rather different from our result. In comparison, the revised PW [41] model does much better, even if it underestimates by  $\sim 22\%$  the  $\uparrow\uparrow$  correlation energy at  $r_s = 0$ , and overestimates it by an amount which increases with  $r_s$  (e.g. 3% at  $r_s = 3$ , 21% at  $r_s = 10$ ).



**FIGURE 2.** Our parallel-spin contribution to the total correlation energy [13] (GSB) compared to the Perdew-Wang [25] (PW), the revised Perdew-Wang [41] (rev. PW), and the Stoll *et al.* [48] approximations.  $\epsilon_c(r_s, \zeta = 1)$  is from Ref. [12].

## Static local fields in the STLS scheme

Local fields are introduced to take into account corrections to the random-phase approximation. The electric and magnetic response functions are, in fact, usually written as

$$\epsilon(q, \omega)^{-1} = 1 + \frac{v_q \chi_0(q, \omega)}{1 + [G(q, \omega) - 1] v_q \chi_0(q, \omega)} \quad (53)$$

$$\tilde{\chi}(q, \omega) = -g^2 \mu_B^2 \frac{\chi_0(q, \omega)}{1 + \tilde{G}(q, \omega) v_q \chi_0(q, \omega)}, \quad (54)$$

where  $\chi_0$  is the Lindhard response function for the noninteracting gas,  $v_q = 4\pi/q^2$ ,  $G$  and  $\tilde{G}$  are respectively the electric and the magnetic local fields,  $g$  is the electron gyromagnetic factor and  $\mu_B$  is the Bohr magneton. The RPA amounts to  $G =$

$\tilde{G} = 0$ , while the Hartree-Fock approximation to  $G = 1$  and  $\tilde{G} = 0$ . In the static approximation  $G$  and  $\tilde{G}$  only depend on  $q$ . In the scheme of Singwi *et al.* [28] (STLS)  $G(q)$  and  $\tilde{G}(q)$  are respectively given as functions of the total and the magnetic structure factors. Of course, the strength of the STLS theory comes mainly from its self-consistency requirement through the fluctuation dissipation theorem, and its application out of context is not justified. However, it is useful to have  $G(q)$  and  $\tilde{G}(q)$  which are compatible with simulations according to different recipes. In Refs. [49] and [50] it has been shown that the STLS relation between  $G$  and  $S$  can be usefully rewritten in terms of the first derivative of the pair-correlation function  $g(\rho)$ , as follows

$$G(k; r_s) = 1 - g(\rho = 0; r_s) - \int_0^\infty d\rho \left[ \frac{\partial g(\rho; r_s)}{\partial \rho} \right] \frac{\sin k\rho}{k\rho}, \quad (55)$$

where again we have used the scaled variables  $\rho = q_F r$  and  $k = q/q_F$ . As in the case of the pair-correlation functions, we can divide the electric  $G(k; r_s)$  into an exchange-only contribution  $G_{\text{ex}}(k)$  and a Coulomb-correlation contribution  $G_c(k; r_s)$ , which, in turn, can be split into its parallel- and antiparallel-spin parts,

$$G(k; r_s) = G_{\text{ex}}(k) + G_c^{\uparrow\uparrow}(k; r_s) + G_c^{\uparrow\downarrow}(k; r_s), \quad (56)$$

and then we have

$$\tilde{G}(k; r_s) = G_{\text{ex}}(k) + G_c^{\uparrow\uparrow}(k; r_s) - G_c^{\uparrow\downarrow}(k; r_s). \quad (57)$$

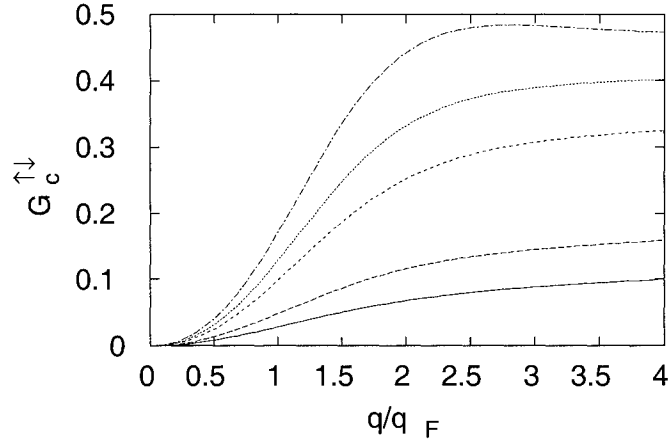
Within the STLS scheme,  $G_{\text{ex}}$ ,  $G_c^{\uparrow\uparrow}$  and  $G_c^{\uparrow\downarrow}$  can be obtained by inserting in Eq. (55) the corresponding pair-correlation functions  $\frac{1}{2}g_{\text{ex}}(\rho)$ ,  $\frac{1}{2}g_{\uparrow\uparrow}^c(\rho; r_s)$  and  $\frac{1}{2}g_{\uparrow\downarrow}^c(\rho; r_s)$ . The so-obtained exchange-only result is well-known [28],

$$G_{\text{ex}}(k) = \frac{3}{4} \left[ \left( \frac{k}{5} - \frac{k^3}{8} - \frac{6}{35} \frac{1}{k} \right) \ln \left| \frac{k+2}{k-2} \right| + \left( \frac{k^6}{560} - \frac{k^4}{20} \right) \ln \frac{|k^2-4|}{k^2} + \frac{k^4}{140} + \frac{11}{35}k^2 + \frac{6}{35} \right]. \quad (58)$$

But now, by means of the accurate pair-correlation functions presented in the previous sections, even the correlation contributions can be obtained in an analytic form. When the Fourier transforms of Eqs. (34) and (44) are inserted into Eq. (55) we obtain

$$G_c^{\uparrow\downarrow}(k) = \frac{1}{2} + \frac{3\pi}{8} q_F \alpha_4^{\uparrow\downarrow} + \alpha_4^{\uparrow\downarrow} F_4^{\uparrow\downarrow}(a^{\uparrow\downarrow}, k) + \alpha_6^{\uparrow\downarrow} F_6^{\uparrow\downarrow}(a^{\uparrow\downarrow}, k) + \frac{3}{k} \sum_{n=1}^6 c_n^{\uparrow\downarrow} (-1)^{n+1} \frac{\partial^{n+1}}{\partial (b^{\uparrow\downarrow})^{n+1}} A(b^{\uparrow\downarrow}, k), \quad (59)$$

$$G_c^{\uparrow\uparrow}(k) = \alpha_6^{\uparrow\uparrow} F_6^{\uparrow\uparrow}(a^{\uparrow\uparrow}, k) + \alpha_8^{\uparrow\uparrow} F_8^{\uparrow\uparrow}(a^{\uparrow\uparrow}, k) + \alpha_{10}^{\uparrow\uparrow} F_{10}^{\uparrow\uparrow}(a^{\uparrow\uparrow}, k) + \frac{3}{k} \sum_{n=1}^6 c_n^{\uparrow\uparrow} (-1)^{n+1} \frac{\partial^{n+1}}{\partial (b^{\uparrow\uparrow})^{n+1}} A(b^{\uparrow\uparrow}, k) \quad (60)$$



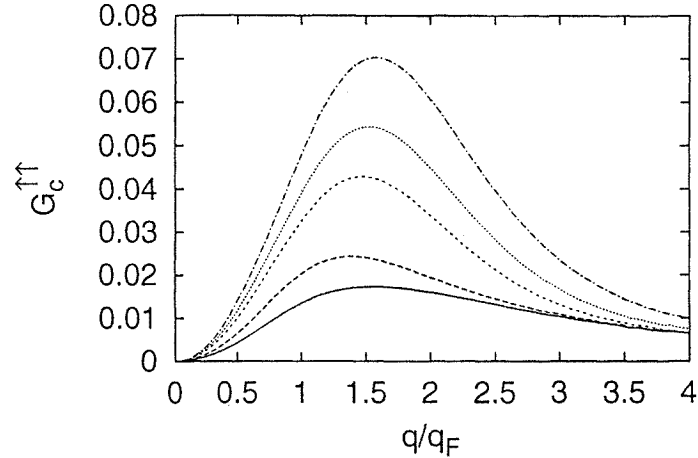
**FIGURE 3.** Antiparallel-spin part of  $G_c(k)$ . Solid line:  $r_s = 0.5$ ; long-dashed:  $r_s = 1$ ; short-dashed:  $r_s = 3$ ; dotted:  $r_s = 5$ ; dash-dotted:  $r_s = 10$ .

where  $\alpha_n^{\sigma\sigma'}$  ( $r_s$ ),  $c_n^{\sigma\sigma'}$  ( $r_s$ ),  $a^{\sigma\sigma'}$  and  $b^{\sigma\sigma'}$  ( $r_s$ ) are given in Eqs. (45)-(49) and in Ref. [13], and

$$\begin{aligned}
 F_4^{\uparrow\downarrow}(a, k) &= \frac{\pi}{8} \left[ \frac{3}{k} \arctan\left(\frac{k}{a}\right) - \frac{a}{2560 (a^2 + k^2)^5} (4215 a^8 + 18620 a^6 k^2 \right. \\
 &\quad \left. + 31418 a^4 k^4 + 24220 a^2 k^6 + 7335 k^8) \right] \\
 F_6^{\uparrow\downarrow}(a, k) &= \frac{\pi (315 a^8 + 1540 a^6 k^2 + 2970 a^4 k^4 + 2772 a^2 k^6 + 1155 k^8)}{20480 a (a^2 + k^2)^5} \\
 F_6^{\uparrow\uparrow}(a, k) &= \frac{3\pi}{917504 a (a^2 + k^2)^7} (3003 a^{12} + 20790 a^{10} k^2 + 100100 a^6 k^6 \\
 &\quad + 61425 a^8 k^4 + 15015 k^{12} + 54054 a^2 k^{10} + 96525 a^4 k^8) \\
 F_8^{\uparrow\uparrow}(a, k) &= \frac{\pi}{917504 a^3 (a^2 + k^2)^7} (2079 a^{12} + 3003 k^{12} + 14238 a^{10} k^2 \\
 &\quad + 41405 a^8 k^4 + 65780 a^6 k^6 + 60489 a^4 k^8 + 30030 a^2 k^{10}) \\
 F_{10}^{\uparrow\downarrow}(a, k) &= \frac{\pi}{4587520 a^5 (a^2 + k^2)^7} (4725 a^{12} + 3465 k^{12} + 31850 a^{10} k^2 \\
 &\quad + 90335 a^8 k^4 + 137148 a^6 k^6 + 113091 a^4 k^8 + 27258 a^2 k^{10}) \\
 A(b, k) &= \frac{e^{-bk} \text{Ei}(bk) (1 + bk) - e^{bk} \text{Ei}(-bk) (1 - bk)}{4 b^3},
 \end{aligned}$$

and  $\text{Ei}(t)$  is the standard exponential integral function. With respect to the expression of Bretonnet and Boulahbak [50] our Eqs. (59) and (60) have the advantage

of being analytic functions not only of the momentum transfer  $k$  but also of the electronic density  $r_s$ , while their equation only holds for few  $r_s$  values (namely  $r_s = 1, 3, 5$  and  $10$ ). In Figs. 3 and 4 we report our analytic spin-resolved contributions to the correlation part of  $G(k)$ .



**FIGURE 4.** Parallel-spin part of  $G_c(k)$ . Solid line:  $r_s = 0.5$ ; long-dashed:  $r_s = 1$ ; short-dashed:  $r_s = 3$ ; dotted:  $r_s = 5$ ; dash-dotted:  $r_s = 10$ .

## CONCLUSIONS

We have recalled a recent closed-form expression for the pair-correlation functions and the structure factors of the unpolarized homogeneous electron gas, discussed some of its peculiar analytic properties and presented new analytic formulae for the corresponding static local fields within the STLS scheme. Further work on the small- $k$  limit of the structure factors is underway [40]; a Fortran code computing our model functions is available upon request ([Giovanni.Bachelet@roma1.infn.it](mailto:Giovanni.Bachelet@roma1.infn.it)).

## ACKNOWLEDGMENTS

We are very grateful to P. Ballone for making available to us prior to publication the numerical results of Ref. [9], on which this work is based. PGG gratefully acknowledges the *Fondazione Angelo Della Riccia* (Firenze, Italy) and the U.S. National Science Foundation (Grant No. DMR98-10620) for financial support. GBB is grateful to M.P. Tosi, D.M. Ceperley, and G. Senatore for useful comments, to S. De Palo for a critical reading of this manuscript, and to the Italian MURST (Grant No. 9902263788) for financial support.

## REFERENCES

1. Hohenberg, P., and Kohn, W., *Phys. Rev.* **136**, B864 (1964); Kohn, W., and Sham, L. J., *Phys. Rev.* **140**, A1133 (1965); Mermin, N. D., *Phys. Rev.* **137A**, 1441 (1965); Gunnarsson, O., and Lundqvist, B. I., *Phys. Rev. B* **13**, 4724 (1976).
2. see e.g. Parr, R. G., and Yang, W., *Density-Functional Theory of Atoms and Molecules*, Oxford Science, Oxford, 1989; for further examples of its present capabilities see Car, R., in *Monte Carlo and Molecular Dynamics of Condensed Matter Systems*, edited by K. Binder and G. Ciccotti, Conference Proceedings **49**, SIF, Bologna, 1996; Boero, M., Parrinello, M., and Terakura, K., *J. Am. Chem. Soc.* **120**, 2746 (1998).
3. see e.g. Singwi, K. S., and Tosi, M. P., *Solid State Physics* **36**, 177 (1981); also, Hindgren, M., and Almladh, C.-O., *Phys. Rev. B* **56**, 12832 (1997), and references therein.
4. Ceperley, D. M., *Phys. Rev. B* **18**, 3126 (1978); Ceperley, D. M., and Alder, B. J., *Phys. Rev. Lett.* **45**, 566 (1980).
5. Pickett, W. E., and Broughton, J. Q., *Phys. Rev. B* **48**, 14859 (1993).
6. Ortiz, G., and Ballone, P., *Phys. Rev. B* **50**, 1391 (1994); *ibid.* **56**, 9970 (1997).
7. Moroni, S., Ceperley, D. M., and Senatore, G., *Phys. Rev. Lett.* **69**, 1837 (1992); *ibid.* **75**, 826 (1995).
8. Kwon, Y., Ceperley, D. M., and Martin, R. M., *Phys. Rev. B* **58**, 6800 (1998).
9. Ortiz, G., Harris, M., and Ballone, P., *Phys. Rev. Lett.* **82**, 5317 (1999).
10. Perdew, J. P., and Zunger, A., *Phys. Rev. B* **23**, 5048, (1981).
11. Vosko, S. H., Wilk, L., and Nusair, M., *Can. J. Phys.* **58**, 1200 (1980).
12. Perdew, J. P., and Wang, Y., *Phys. Rev. B* **45**, 13244 (1992).
13. Gori-Giorgi, P., Sacchetti, F., and Bachelet, G. B., *Phys. Rev. B* **61**, 7353 (2000).
14. Gunnarsson, O., Jonson, M., and Lundqvist, B. I., *Phys. Rev. B* **20**, 3136 (1979).
15. Perdew, J. P., in *Electronic Structure of Solids '91*, edited by P. Ziesche and H. Eschrig, Akademie Verlag, Berlin, 1991; Perdew, J. P., Burke, K., and Wang, Y., *Phys. Rev. B* **54**, 16533 (1996).
16. Gunnarsson, O., Jonson, M., and Lundqvist, B. I., *Phys. Lett. A* **59**, 177 (1976).
17. Chacón, E., and Tarazona, P., *Phys. Rev. B* **37**, 4013 (1988).
18. Dobson, J. F., *J. Phys. C* **4**, 7877 (1992); *J. Chem. Phys.* **94**, 4328 (1991); *ibid.* **98**, 8870 (1993).
19. Rajagopal, A. K., Kimball, J. C., and Banerjee, M., *Phys. Rev. B* **18**, 2339 (1978).
20. Yamashita, I., and Ichimaru, S., *Phys. Rev. B* **29**, 673 (1984).
21. Contini, V., Mazzone, G., and Sacchetti, F., *Phys. Rev. B* **33**, 712 (1986).
22. Lee, C., Yang, W., and Parr, R. G., *Phys. Rev. B* **37**, 785 (1988).
23. Becke, A. D., *J. Chem. Phys.* **88**, 1053 (1988).
24. Valone, S. M., *Phys. Rev. B* **44**, 1509 (1991).
25. Perdew, J. P., and Wang, Y., *Phys. Rev. B* **46**, 12947 (1992); *ibid.* **56**, 7018 (1997).
26. Gritsenko, O. V., Rubio, A., Balbás, L. C., and Alonso, J. A., *Phys. Rev. A* **47**, 1811 (1993).
27. Proynov, E. I., and Salahub, D. R., *Phys. Rev. B* **49**, 7874 (1994).
28. Singwi, K. S., Tosi, M. P., Land, R. H., and Sjölander, A., *Phys. Rev.* **176**, 589



- (1968).
29. Wigner, E., *Phys. Rev.* **46**, 1002 (1934); *Trans. Faraday Soc.* **34**, 678 (1938).
  30. March, N. H., *Phys. Rev.* **110**, 604 (1958); Argyres, P. N., *Phys. Rev.* **154**, 410 (1967); Iwamoto, N., *Phys. Rev. B* **38**, 4277 (1988); Kleinman, L., *Phys. Rev. B* **43**, 3918 (1991).
  31. Kimball, J. C., *Phys. Rev. A* **7**, 1648 (1973); *J. Phys. A* **8**, 1513 (1975).
  32. Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., and Stremnitzer, H., *Phys. Rev. Lett.* **68**, 3857 (1992).
  33. Pines, D., and Nozières, P., *Theory of Quantum Liquids*, Benjamin, New York, 1966.
  34. Iwamoto, N., *Phys. Rev. A* **33**, 1940 (1986).
  35. Gori-Giorgi, P., Sacchetti, F., and Bachelet, G. B., *Physica A* **280**, 199 (2000).
  36. Wang, Y., and Perdew, J. P., *Phys. Rev. B* **44**, 13298 (1991).
  37. Gell-Mann, M., and Brueckner, K. A., *Phys. Rev.* **106**, 364 (1957).
  38. Nozières, P., and Pines, D., *Phys. Rev.* **111**, 442 (1958).
  39. We are indebted to M.P. Tosi and D.M. Ceperley for independently bringing this point to our attention.
  40. Gori-Giorgi, P., in preparation.
  41. Schmidt, K., Kurth, S., Tao, J., and Perdew, J. P., *Phys. Rev. B* **62**, 2227 (2000).
  42. Carr, W. J. Jr., and Maradudin, A. A., *Phys. Rev.* **133** A371 (1964).
  43. Wang, Y., and Perdew, J. P., *Phys. Rev. B* **43**, 8911 (1991).
  44. Hoffman, G. G., *Phys. Rev. B* **45**, 8730 (1992).
  45. Onsager, L., Mittag, L., and Stephen, M. J., *Ann. Phys. (N. Y.)* **18**, 71 (1966).
  46. Endo, T., Horiuchi, M., Takada, Y., and Yasuhara, H., *Phys. Rev. B* **59**, 7367 (1999).
  47. Aguilera-Navarro, V. C., Baker, G. A. Jr., and de Llano, M., *Phys. Rev. B* **32**, 4502 (1985).
  48. Stoll, H., Pavlidou, C. M. E., and Preuss, H., *Theor. Chim. Acta* **49**, 143 (1978); Stoll, H., Golka, E., and Preuss, H., *ibid.* **55**, 29 (1980).
  49. Shaw, R. W., *J. Phys. C* **3**, 1140 (1970).
  50. Bretonnet, J. L., and Boulahbak, M., *Phys. Rev. B* **53**, 6859 (1996).