Analytic static structure factors and pair–correlation functions for the unpolarized homogeneous electron gas

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We propose a simple and accurate model for the electron static structure factors (and corresponding pair–correlation functions) of the 3D unpolarized homogeneous electron gas. Our spin–resolved pair–correlation function is built up with a combination of analytic constraints and fitting procedures to quantum Monte Carlo data, and, in comparison to previous attempts (i) fulfills more known integral and differential properties of the exact pair–correlation function, (ii) is analytic both in real and in reciprocal space, and (iii) accurately interpolates the newest, extensive diffusion–Monte Carlo data of Ortiz, Harris and Ballone [Phys. Rev. Lett. 82, 5317 (1999)]. This can be of interest for the study of electron correlations of real materials and for the construction of new exchange and correlation energy functionals.

I. INTRODUCTION

The homogeneous electron gas, a model solid whose positive ionic charges are smeared throughout the whole crystal volume to yield a shapeless, uniform positive background (whence the nickname of jellium) has provided, since the very start of quantum mechanics, a key conceptual reference and a mine of information for solid–state and many–body theorists. Initially it was mostly regarded as an approximation of the true distribution of valence electrons in simple metals, since, in spite of its crudity, it could already account for some of their experimental properties. Although the importance of valence–charge inhomogeneities in real materials was soon recognized (and described first by perturbation and later by self–consistent pseudopotential theory), the homogeneous electron gas stood by itself, over the decades, as an independent active field of theoretical investigation. One reason for this continued interest is that 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. Another reason for caring about such an unrealistic system resides in its connection to the inhomogeneous electron gas: not only does the jellium model represent an obvious–limit, but also, through the Density Functional Theory and its Local Density Approximation, it links to a popular and very successful description of real materials. For the latter reason, from the simplest Hartree–Fock approximation to the pioneering QMC simulations, almost any theory of jellium, its electron correlations and its pair–correlation functions has also implied an improved understanding and construction of Kohn–Sham energy functionals.

In this context our work aims at a new simple analytic expression for the pair–correlation function of the homogeneous electron gas, which describes the spatial correlations of electron pairs with prescribed spin orientations. A good model pair–correlation function and static structure factor has its own interest; its availability over a wide density range is crucial for new developments and applications of the Density Functional Theory, through the construction of ab initio exchange and correlation energy functionals in generalized gradient approximations and in other beyond–LDA schemes. As a consequence, over the last 20 years, several authors already proposed ingenious expressions for this or related functions. A first motivation for resuming and improving over previous efforts is the availability, from recent quantum Monte Carlo (QMC) simulations of a wealth of new numerical results for the pair–correlation functions and static structure factors of jellium. A second motivation comes from the observation that most of the previous models were not spin–resolved and all of them neither fulfilled all the known exact properties, nor were given in analytic, closed form both in real and reciprocal space. Our goal is thus to give a new, spin–resolved expression for the pair–correlation function which is analytic both in real and reciprocal space, automatically incorporates more exact properties than any previous expression, and contains enough free parameters to fit the new QMC results.

We recall the exact properties of the pair–correlation function for the unpolarized jellium in Sec. I. The three subsequent sections are devoted to a description of our general strategy (Sec. II) and of the resulting functional form for the antiparallel– (Sec. III) and parallel–spin (Sec. V) pair–correlation functions. In Sec. VI we describe our fitting procedure to QMC data. Once the exact constraints are imposed, 18 free parameters (9 for antiparallel spins and 9 for parallel spins) are enough to yield extremely accurate two–dimensional fits of the $\approx 9000 + 9000$ new QMC data points as a function of the interelectronic distance $r$ and the density parameter $\rho_s$ in the relevant density range $\rho_s \leq 10$. Our results are discussed and compared with the widely used Perdew–Wang model in Sec. VII.
In Sec. VIII we report the correlation energy which corresponds to our model pair–correlation function and we find that its agreement with the QMC energies, not targeted by our fitting procedure, is as good (~ 5%) as the most popular interpolation formulae for the correlation energy. The last Sec. IX is devoted to conclusions and perspectives.

II. EXACT PROPERTIES

We briefly recall many known properties of the pair correlation function of the unpolarized homogeneous electron gas. Its integral properties (sum rules) will be rewritten in terms of \( \sigma \) and is thus related to the probability of finding two electrons of spin \( \sigma \) at positions \( r_1 \) and \( r_2 \). The normalization of \( g \) is such that the expected number of electrons of spin \( \sigma_2 \) in the volume \( dV \) at \( r_2 \) when another electron of spin \( \sigma_1 \) is known to be at \( r_1 \) is given by

\[
\frac{dN(r_2 | r_1; \sigma_1)}{dV} = n_{\sigma_2}(r_2) g_{\sigma_1\sigma_2}(r_1, r_2) \quad \text{(2)}
\]

and is thus related to the probability of finding two electrons of prescribed spin orientations at positions \( r_1 \) and \( r_2 \). The normalization of \( g \) is such that the expected number of electrons of spin \( \sigma_2 \) in the volume \( dV \) at \( r_2 \) when another electron of spin \( \sigma_1 \) is known to be at \( r_1 \) is given by

\[
n_{\sigma_1}(r_1)n_{\sigma_2}(r_2)g_{\sigma_1\sigma_2}(r_1, r_2) = \langle \Phi | \psi_{\sigma_1}(r_1) \psi_{\sigma_2}(r_2) | \psi_{\sigma_1}(r_1) \rangle \Phi \quad \text{(1)}
\]

A. Definitions

For an electronic system the pair–correlation function \( g_{\sigma_1\sigma_2}(r_1, r_2) \), if \( n_{\sigma}(r) \) is the density of electrons with spin \( \sigma = \uparrow \) or \( \downarrow \), is defined by

\[
n_{\sigma_1}(r_1)n_{\sigma_2}(r_2)g_{\sigma_1\sigma_2}(r_1, r_2) = \langle \Phi | \psi_{\sigma_1}(r_1) \psi_{\sigma_2}(r_2) | \psi_{\sigma_1}(r_1) \rangle \Phi \quad \text{(1)}
\]

and is thus related to the probability of finding two electrons of prescribed spin orientations at positions \( r_1 \) and \( r_2 \). The normalization of \( g \) is such that the expected number of electrons of spin \( \sigma_2 \) in the volume \( dV \) at \( r_2 \) when another electron of spin \( \sigma_1 \) is known to be at \( r_1 \) is given by

\[
S(\rho; r_s) = \frac{1}{2} \left[ g_{\uparrow\uparrow}(\rho; r_s) + g_{\downarrow\downarrow}(\rho; r_s) \right] \quad \text{(5)}
\]

and is thus related to the probability of finding two electrons of spin \( \sigma \) at positions \( r_1 \) and \( r_2 \). The normalization of \( g \) is such that the expected number of electrons of spin \( \sigma_2 \) in the volume \( dV \) at \( r_2 \) when another electron of spin \( \sigma_1 \) is known to be at \( r_1 \) is given by

\[
S(k; r_s) = S_{\uparrow\uparrow}(k; r_s) + S_{\downarrow\downarrow}(k; r_s). \quad \text{(6)}
\]

B. Pair–correlation function near \( r = 0 \)

The behavior of \( g_{\sigma_1\sigma_2}(r; r_s) \) in the \( r \to 0 \) limit can be directly obtained from the many–body Schrödinger equation when two electrons approach each other (cusp conditions)

\[
\frac{\partial}{\partial r} g_{\uparrow\downarrow}(r; r_s) \bigg|_{r \to 0} = g_{\uparrow\downarrow}(r \to 0; r_s) \neq 0 \quad \text{(7)}
\]

\[
\frac{\partial}{\partial r} g_{\uparrow\uparrow}(r; r_s) \bigg|_{r \to 0} = g_{\uparrow\uparrow}(r \to 0; r_s) = 0 \quad \text{(8)}
\]

\[
\frac{\partial^2}{\partial r^2} g_{\uparrow\downarrow}(r; r_s) \bigg|_{r \to 0} = 0 \quad \text{(9)}
\]

Eqs. (7)–(9) hold for any 3D–system of \( N \) fermions interacting via the two–body repulsive Coulomb potential.

C. Structure factor near \( q = 0 \)

The conservation of particles in the system implies the relations:

\[
S_{\uparrow\downarrow}(q \to 0; r_s) = S_{\uparrow\uparrow}(q \to 0; r_s) = 0. \quad \text{(10)}
\]

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. 23).

The long–wavelength behavior of the total static structure factor of Eq. (3) is determined by the plasmon contribution, proportional to \( q^2 \), and by the single–pair and multipair quasiparticle–quasihole excitation contributions, proportional to \( q^2 \) and \( q^4 \) respectively.

\[
S(q \to 0; r_s) = \frac{q^2}{2 \omega_p(r_s)} + C q^4 + O(q^5) \quad \text{(11)}
\]

where \( \omega_p(r_s) = \sqrt{3/\pi} \) is the classical plasma frequency. In the paramagnetic gas, the parallel and antiparallel–spin contribution to the plasma mode is the same. Moreover, to build up model functions for the spin–resolved \( S_{\sigma_1\sigma_2} \), it’s crucial to include the following property of the so–called magnetic structure factor \( S_{\uparrow\downarrow} - S_{\downarrow\uparrow} \):

\[
S_{\uparrow\downarrow} - S_{\downarrow\uparrow} \bigg|_{k \to 0} = \frac{3}{4} k^3 - \frac{k^5}{16} + O(k^4) \quad \text{(12)}
\]

where the scaled variable \( k = q/q_F \) has been used. Eq. (12) is valid in the framework of the random–phase
approximation \( (\text{RPA}) \) and can be obtained from a series expansion of \( S_{\text{RPA}}^>(k) \) near \( k = 0 \) (Ref. 38), and from the corresponding expansion of the total \( S_{\text{RPA}} \) (see for instance Ref. 37). Since in the \( k \to 0 \) limit RPA is exact \( 33,34,37 \) we expect Eq. (12) to hold for the exact structure factor as well. From Eqs. (11) and (12) we can write the small-\( k \) expansion of \( S_{\uparrow \uparrow} \): 

\[
S_{\uparrow \uparrow}|_{k \to 0} = - \frac{3}{8} k + \frac{\alpha^2}{4 \omega_p(r_s)} k^2 + \frac{k^3}{32} + O(k^4) \tag{13}
\]

\[
S_{\uparrow \uparrow}|_{k \to 0} = \frac{3}{8} k + \frac{\alpha^2}{4 \omega_p(r_s)} k^2 - \frac{k^3}{32} + O(k^4). \tag{14}
\]

D. Correlation energy

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

\[
U = \frac{1}{2} \sum_{i \neq j}^N \frac{1}{|r_i - r_j|}. \tag{15}
\]

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

\[
\langle U \rangle_{r_s} = \frac{3}{2 \alpha^2 r_s} \int_0^\infty [g(\rho; r_s) - 1] \rho \, d\rho. \tag{16}
\]

By the virial theorem \( 34 \) and the usual definition of the correlation energy \( \epsilon_c \) as total electronic energy minus Hartree–Fock energy, we have:

\[
\langle U \rangle_{r_s} = \frac{3}{2 \alpha^2 r_s} \int_0^\infty \left[ \frac{3 g_F}{4 \pi} + \frac{1}{r_s} \frac{d}{d r_s} \left( r_s^2 \epsilon_c(r_s) \right) \right] \tag{17}
\]

Putting together Eqs. (16) and (17) one obtains the known relation between \( g_\chi(\rho; r_s) \) and the exchange and correlation energy:

\[
\epsilon_{xc} = - \frac{3 g_F}{4 \pi} + \epsilon_c = - \frac{3}{2 \alpha^2 r_s} \int_0^\infty \rho \, d\rho \int_0^{r_s} \left[ g(\rho; r_s') - 1 \right] \tag{18}
\]

The same relation can be obtained in a more general way \( 33 \) by the Hellmann–Feynman theorem and the coupling–constant average of \( g(\rho; r_s) \), which, for the homogenous system is just the average over \( r_s \):

\[
\overline{g}(\rho; r_s) = \frac{1}{r_s} \int_0^{r_s} g(\rho; r_s') \, dr_s'. \tag{19}
\]

The function \( \overline{g}(\rho; r_s) \) is directly related to the exchange and correlation hole \( 34 \) of the electron gas.

We have recalled these relations because we will later check our analytical expressions for \( g(\rho; r_s) \) against available energy data, and also because, among other constraints, we want our functional form of \( g(\rho; r_s) \) to be consistent with the high–density limit of \( \epsilon_c(r_s) \):

\[
\epsilon_c(r_s \to 0) = A \ln r_s + B + C r_s \ln r_s + D r_s \tag{20}
\]

where \( A, B, C \) and \( D \) are known constants.\( 38,39 \)

\[
A = (1 - \ln 2)/\pi^2, \quad B = -0.0469205, \quad C = 0.0092292, \quad D = -0.01,
\]

and the next leading term is \( O(r_s^2 \ln r_s) \).

III. GENERAL STRATEGY

We study the antiparallel and parallel–spin correlation functions both in real and reciprocal space and we split them, as usually, into exchange and correlation according to:

\[
g_{\uparrow \downarrow}(\rho; r_s) = 1 + g_{\uparrow \downarrow}^c(\rho; r_s) \tag{21}
\]

\[
g_{\uparrow \downarrow}(\rho; r_s) = g_{\uparrow \downarrow}^{\chi}(\rho; r_s) \tag{22}
\]

\[
S_{\uparrow \downarrow}(k; r_s) = S_{\uparrow \downarrow}^c(k; r_s) \tag{23}
\]

\[
S_{\uparrow \downarrow}(k; r_s) = S_{\uparrow \downarrow}^{\chi}(k; r_s) \tag{24}
\]

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

\[
g_{\uparrow \downarrow}^{\chi}(\rho; r_s) = 1 - \left( \frac{\sin \rho - \rho \cos \rho}{\rho^3} \right)^2 \tag{25}
\]

\[
S_{\uparrow \downarrow}^{\chi}(k; r_s) = \left\{ \begin{array}{ll}
3 k^4/4 - k^2/16 & \text{for } k \leq 2 \\
1 & \text{for } k > 2 
\end{array} \right. \tag{26}
\]

and our model only concerns the correlation part. Putting together Eqs. (1), (11), (23), (24) and (26) one finds a well–known result: in the total \( S = S_{\uparrow \downarrow} + S_{\uparrow \downarrow}^{\chi} \) the linear term of \( S_{\uparrow \downarrow}^{\chi} \) dominates its small–\( k \) behavior (and corresponds to a large–\( \rho \) leading term \( \propto 1/\rho^2 \) of \( g_{\uparrow \downarrow}^{\chi} \)) exactly cancels the small–\( k \) leading term of the correlation part \( S_{\uparrow \downarrow}^c + S_{\uparrow \downarrow}^{\chi} \). This property has been incorporated in several previous functional forms for the total \( g \), as the widely used Perdew–Wang model (hereafter PW) where, however, the \( k^2 \) coefficient in the small–\( k \) expansion of \( S(k) \) is slightly different from the exact one [Eq. (13)], because of spurious \( k^2 \) contributions from their \( \langle g_{\uparrow \downarrow} \rangle \) [Eq. (19) of Ref. 29] and from their short–range part of \( g_{\uparrow \downarrow} \) [Eq. (37) of Ref. 29].

The \( k \to 0 \) limit of Eq. (12) seems, instead, to be less known: even the best–to–date spin–resolved PW model does not incorporate such a non–trivial analytic property, which can alternatively be expressed as \( S_{\uparrow \downarrow}^c \) being identical to \( S_{\uparrow \downarrow}^c \) in the the small–\( k \) limit and corresponds to a visible feature of the magnetic structure factor (see Sec. VII). Our goal is to produce simple and practical analytical functional forms for \( S_{\uparrow \downarrow}^c(k; r_s) \) and \( S_{\uparrow \downarrow}^{\chi}(k; r_s) \) and hence \( g_{\uparrow \downarrow}^c(\rho; r_s) \) and \( g_{\uparrow \downarrow}^{\chi}(\rho; r_s) \) which satisfy all the physical properties of Sec. II and have enough variational flexibility to accurately interpolate the QMC data of Ortiz, Harris and Ballone.\( 34 \)
IV. ANTIPARALLEL SPINS

A. Functional form

In reciprocal space our functional form is simply written as:

\[
S_{\uparrow \downarrow}^r(k; r_s) = \exp \left[ -b_{\uparrow \downarrow}^{r}(r_s) k \right] \sum_{n=1}^{6} c_{n\uparrow \downarrow}^{r}(r_s) k^n + \frac{\alpha_{\uparrow \downarrow}^{r}(r_s) k^8 + \alpha_{\downarrow \uparrow}^{r}(r_s) k^{10}}{[(\alpha_{\uparrow \downarrow}^{r})^2 + k^2]^2}; \tag{27}
\]

as mentioned, the corresponding \( g_{\uparrow \downarrow}^{r} \) amounts to a linear combination of the same kind of functions in real space see App. A, Eq. (A1)). Two types of functions appear in Eq. (27): the first one, an exponential cut–off times a truncated power series, fully characterizes the long–wavelength behavior of \( S \), while the second one entirely determines its large–k expansion. The leading term as \( k \to \infty \) is of order \( k^{-4} \), as exactly known from the cusp condition \[ \frac{\partial}{\partial \rho} g^{\uparrow \downarrow}_{\uparrow \downarrow}(\rho; r_s) \big|_{\rho \to 0} = -3\pi \frac{4}{q}\alpha_{\uparrow \downarrow}^{r}(r_s) \tag{28} \]

\[
g^{\uparrow \downarrow}_{\uparrow \downarrow}(\rho = 0; r_s) = -\frac{3\pi}{4} qF(r_s)\alpha_{\uparrow \downarrow}^{r}(r_s). \tag{29} \]

B. Physical constraints

The \( k \to 0 \) conditions of Subsec. IV C are easily imposed:

\[
c_{1\uparrow}^{r} = -\frac{3}{8} \tag{30} \]

\[
c_{2\uparrow}^{r} = b_{\uparrow \downarrow}^{r} c_{1\uparrow}^{r} + \frac{q^2}{4\omega p} \tag{31} \]

\[
c_{3\uparrow}^{r} = \left( b_{\uparrow \downarrow}^{r} \right)^2 \frac{c_{1\uparrow}^{r}}{2} + b_{\uparrow \downarrow}^{r} \frac{q^2}{4\omega p} + \frac{1}{32}. \tag{32} \]

The cusp condition of Eq. (8) fixes a simple relation between \( \alpha_{6\uparrow}^{r} \) and the other parameters:

\[
\alpha_{6\uparrow}^{r} = (a_{\uparrow \downarrow}^{r})^3 \left\{ \alpha_{4\uparrow}^{r} \left( \frac{11}{a_{\uparrow \downarrow}^{r}} - \frac{512}{21} qF \right) - \frac{2048}{21\pi} \sum_{n=1}^{6} c_{n\uparrow \downarrow}^{r} \frac{(n+2)!}{(b_{\uparrow \downarrow}^{r})^{n+3}} \right\} \tag{33} \]

After imposing all the \( \uparrow \downarrow \) physical conditions, our model [Eq. (27)] is left with 6 free parameters: the two exponential cut–offs \( a_{\uparrow \downarrow}^{r} \) in real space and \( b_{\uparrow \downarrow}^{r} \) in reciprocal space, the parameter \( \alpha_{4\uparrow}^{r} \), which determines the short–range behavior of \( g(r) \), and the 3 linear parameters \( c_{4\uparrow}^{r} \), \( c_{5\uparrow}^{r} \) and \( c_{6\uparrow}^{r} \), which will be used to further increase the variational flexibility and fit the numerical \( g_{\uparrow \downarrow}^{r} \) obtained from QMC simulations. The dependence of these free parameters on \( r_s \) will be determined according to the strategy summarized in Sec. IV C and detailed in the following Subsec. IV C and Sec. IV A.
C. High–density expansion

As anticipated in Subsec. III, we want our pair–correlation function such that its $\updownarrow$ and $\uparrow\uparrow$ contributions automatically fulfill the high–density limit of the correlation energy. We thus fix the $r_s \to 0$ limit of our free parameters by means of Eqs. (11), (17) and (24). Our antiparallel contribution to the expectation value of the potential energy $U = U_{\uparrow\downarrow} + U_{\uparrow\uparrow}$ is simply given by:

$$U_{\uparrow\downarrow} = \frac{g_F}{\pi} \sum_{n=1}^{6} \left( \frac{\sigma_{\uparrow\downarrow}}{(b_{\uparrow\downarrow})^{n+1}} \right) + \frac{g_F}{2048} \left[ \frac{7\sigma_{\uparrow\downarrow}}{(a_{\uparrow\downarrow})^{n+1}} + \frac{21\sigma_{\uparrow\uparrow}}{(a_{\uparrow\uparrow})^{n+1}} \right].$$ (34)

In the high–density limit, the correlation–energy constraint of Eq. (20) translates into the following condition on $(U_{\uparrow\downarrow})_{r_s \to 0}$:

$$\langle U_{\uparrow\downarrow} \rangle_{r_s \to 0} = 2A_{\uparrow\downarrow} \ln r_s + (A_{\uparrow\downarrow} + 2B_{\uparrow\downarrow}) \ln r_s + O(r_s \ln r_s)$$ (35)

where, comparing to Eq. (24), $A_{\uparrow\downarrow}$ is simply given by $\frac{1}{2} A$. To determine $B_{\uparrow\downarrow}$ we recall that the constant $B$ in Eq. (21) is the sum of two contributions: a second–order exchange term, $B_{\uparrow\downarrow}^{(2)}$, which only concerns the $\uparrow\downarrow$ part, and a direct term, $B_d$, which is, instead, equally split (in the unpolarized gas) between $\uparrow\downarrow$ and $\uparrow\downarrow$. Hence, $B_{\uparrow\downarrow} = B_{\uparrow\downarrow}^{(2)}$. Both $B_{\uparrow\downarrow}^{(2)}$ and $B_d$ have been evaluated exactly.

Provided that the 3 linear parameters $c_{\uparrow\downarrow}$, $c_{\uparrow\downarrow}^{\uparrow\downarrow}$ and $c_{\uparrow\downarrow}^{\uparrow\uparrow}$ remain finite as $r_s \to 0$, the exact high–density limit of Eq. (35) amounts to the following conditions:

$$\alpha_{\uparrow\downarrow}^{\uparrow\downarrow} (r_s \to 0) = \frac{1}{3} + k_1 r_s \ln r_s + k_2 r_s + O(r_s^2 \ln r_s)$$ (36)

$$b_{\uparrow\downarrow}^{\uparrow\downarrow} (r_s \to 0) = \left( \frac{4}{9r_s} \right) \frac{1}{1/3} \pi \frac{3}{r_s} + O(r_s^0)$$ (37)

$$a_{\uparrow\downarrow}^{\uparrow\downarrow} (r_s \to 0) = \text{const.} + O(r_s) \equiv a_{\uparrow\downarrow}^{\uparrow\downarrow} + O(r_s)$$ (38)

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

$$k_1 = \frac{18\pi (a_{\uparrow\downarrow})^2}{\alpha} A_{\uparrow\downarrow}$$ (39)

$$k_2 = \frac{729 (a_{\uparrow\downarrow})^2}{64 \alpha^2} - \frac{21}{64} \frac{1}{a_{\uparrow\downarrow}^2} + \frac{9 (a_{\uparrow\downarrow})^2}{2 \alpha} (A_{\uparrow\downarrow} + 2B_{\uparrow\downarrow}).$$ (40)

Inserting Eq. (36) into Eq. (29) we see that in our model, once the high–density expansion of $g_c(r_s)$ is fixed, the $r_s \to 0$ limit of $g(\rho = 0; r_s)$ is also fixed to the form $1 + C r_s \ln r_s + O(r_s)$. The corresponding exact form is, up to orders $r_s^2$, $1 + C_1 r_s + C_2 r_s^2 \ln r_s$, thus slightly different from our. Evidently, the simple functional form of Eq. (27) does not correctly describe the short–range behavior of the Coulomb hole at very high densities. It is worthwhile to point out that this contradiction is due to the exponential cut–off times a truncated power series in real space [Eq. (23)], and emerges when the cusp condition of Eq. (2) is imposed to it. The relevance of this limitation, which only concerns densities $r_s \lesssim 0.1$, will be discussed in next Sec. IV.

V. PARALLEL SPINS

A. Functional form

For the high–density part of the $\uparrow\uparrow$ pair–distribution function we apply the same strategy used for the antiparallel–spin case. In reciprocal space we thus have:

$$S_{\uparrow\uparrow}^{\uparrow\uparrow} (k; r_s) = \exp \left[ -\beta \left( (a_{\uparrow\uparrow})^2 + k^2 \right) \right]$$ (41)

which again corresponds, in real space, to a linear combination of the same kind of functions [see App. A, Eq. (A2)]. The long–wavelength term has the same form as the $\uparrow\downarrow$ part. The large–$k$ term describes the short–range behavior of $g_{\uparrow\uparrow}$: the cusp condition of Eq. (2) tells us that, as $k \to \infty$, the leading term of $S_{\uparrow\uparrow}^{\uparrow\uparrow}$ must be of order $k^{-6}$. With respect to the $\uparrow\downarrow$ case, one more parameter is needed for the large–$k$ term to satisfy the Pauli principle. As in the antiparallel–spin case, the short–range properties of $g_{\uparrow\uparrow}$ are characterized by the $\alpha_{\uparrow\uparrow}$ parameter:

$$\left. \frac{\partial^3}{\partial \rho^3} g_{\uparrow\uparrow}^{\uparrow\uparrow} (\rho; r_s) \right|_{r_s \to 0} = \frac{3 \pi}{8} \alpha_{\uparrow\uparrow} (r_s)$$ (42)

$$\left. \frac{\partial^2}{\partial \rho^2} g_{\uparrow\uparrow}^{\uparrow\uparrow} (\rho; r_s) \right|_{r_s \to 0} = \frac{\pi}{4} g_F (r_s) \alpha_{\uparrow\uparrow} (r_s).$$ (43)

B. Physical constraints

The small–$k$ properties imply, for the $\uparrow\uparrow$ case, identical constraints as for the $\uparrow\downarrow$ case [see Eqs. (31), (33) and (32)].

The Pauli principle and the cusp condition of Eqs. (2) and (3) fix the dependence of $\alpha_{\uparrow\uparrow}$ and $\alpha_{\uparrow\downarrow}^{\uparrow\uparrow}$ on the remaining parameters:

$$\alpha_{\uparrow\uparrow} = \frac{2048}{3\pi} (a_{\uparrow\uparrow})^2 \sum_{n=1}^{6} \frac{c_n^{\uparrow\uparrow}}{(b_{\uparrow\uparrow})^{n+3}} \left[ (n+2)! - 5(n+4)! \right] \left( \frac{(a_{\uparrow\uparrow})^{n+3}}{(b_{\uparrow\uparrow})^{n+3}} \right)$$

$$+ \frac{4096}{3\pi} (a_{\uparrow\uparrow})^3 - \frac{\alpha_{\uparrow\downarrow}^{\uparrow\uparrow}}{(a_{\uparrow\uparrow})^3} \left( \frac{2560g_F}{33} + \frac{26}{a_{\uparrow\uparrow}} \right)$$ (44)

$$\alpha_{\uparrow\downarrow}^{\uparrow\uparrow} = \frac{2048}{3\pi} (a_{\uparrow\uparrow})^2 \sum_{n=1}^{6} \frac{c_n^{\uparrow\uparrow}}{(b_{\uparrow\uparrow})^{n+3}} \left[ (n+4)! \right] \frac{(a_{\uparrow\uparrow})^2}{(b_{\uparrow\uparrow})^{n+3}} - \frac{13}{3} \right) (n+2)!.$$ (45)
\[-\frac{4096}{15\pi}(a^{\uparrow \downarrow})^5 + \frac{\alpha_{\uparrow \downarrow}^{\uparrow \downarrow}}{3}(a^{\uparrow \downarrow})^5 \left(\frac{143}{a^{\uparrow \downarrow}} + 512 q_F\right). \tag{45}\]

The cusp condition of Eq. (43) is not included in the PW model. As in the antiparallel-spin case, we have 6 free parameters: the exponential cut-off in real space, \(a^{\uparrow \downarrow}\), the exponential cut-off in reciprocal space, \(b^{\uparrow \downarrow}\), the \(\alpha_{\uparrow \downarrow}^{\uparrow \downarrow}\) parameter, which determines the short-range behavior of \(g^{\uparrow \downarrow}\), and the three linear parameters \(c_{\uparrow \uparrow}, c_{\uparrow \downarrow}\), and \(c_{\downarrow \downarrow}\), which are used to fit the oscillatory behavior of \(g^{\uparrow \downarrow}\).

C. High-density expansion

The contribution to the expectation value of the potential energy due to the correlation part of our \(g^{\uparrow \downarrow}\) (\(U^{\uparrow \downarrow} = -3 q_F / 4 \pi + U_c^{\uparrow \downarrow}\)) is:

\[
U_c^{\uparrow \downarrow} = \frac{q_F}{\pi} \sum_{n=1}^6 \frac{\alpha_{\uparrow \downarrow}^{\uparrow \downarrow}}{(a^{\uparrow \downarrow})^n} + \frac{q_F}{65536} \left[ \frac{35 \alpha_{\uparrow \downarrow}^{\uparrow \downarrow}}{(a^{\uparrow \downarrow})^6} + \frac{45 \alpha_{\uparrow \downarrow}^{\uparrow \downarrow}}{(a^{\uparrow \downarrow})^3} \right] + \frac{99 \alpha_{\uparrow \downarrow}^{\uparrow \downarrow}}{(a^{\uparrow \downarrow})^5} \tag{46}\]

As \(r_s \to 0\), the condition on \(U^{\uparrow \downarrow}\) is identical to Eq. (53), where \(A^{\uparrow \downarrow} = \frac{1}{2} A\), and \(B^{\uparrow \downarrow} = B_{\uparrow \downarrow}^{(2)} + \frac{1}{2} B_d\). As in the \(\uparrow \downarrow\) case, the exact \(r_s \to 0\) expansion of \(U^{\uparrow \downarrow}\) implies for the two exponential cut-offs in real (\(a^{\uparrow \downarrow}\)) and reciprocal space (\(b^{\uparrow \downarrow}\)) identical conditions as Eqs. (27) and (28). For \(\alpha_{\uparrow \downarrow}^{\uparrow \downarrow}\) the condition is similar to Eq. (30):

\[
\alpha_{\uparrow \downarrow}^{\uparrow \downarrow}(r_s \to 0) = \frac{4}{\pi q_F} \left[ \frac{3}{5} + p_1 r_s \ln r_s + p_2 r_s + O(r_s^2 \ln r_s) \right], \tag{47}\]

where \(p_1\) and \(p_2\) depend on \(A^{\uparrow \downarrow}, B^{\uparrow \downarrow}\) and \(a^{\uparrow \downarrow}\) through equations similar to Eqs. (23) and (40). From Eqs. (43) and (47) one can see that, as expected, when \(r_s \to 0\), \(g_{\uparrow \downarrow}^{\uparrow \downarrow}(\rho = 0)\) goes to the Hartree–Fock value 2/5. As in the antiparallel-spin case, the high-density limit of the correlation energy fixes the \(r_s \to 0\) expansion of \(g_{\uparrow \downarrow}^{\uparrow \downarrow}(\rho = 0; r_s \to 0)\). The exact \(g_{\uparrow \downarrow}^{\uparrow \downarrow}(\rho = 0; r_s \to 0)\) should have the form \(2/5 + O(r_s)\), while our functional form gives \(2/5 + O(r_s \ln r_s)\). Again, we find that in real space the simple exponential cut-off times a truncated power series [Eq. (A2)] does not correctly describe the short range Coulomb interactions at very high densities.

VI. FIT TO QMC DATA

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\(]^2\) separately for the \(\uparrow \downarrow\) and the \(\uparrow \uparrow\) parts. The \(r_s\) dependence of the parameters turns out to be quite smooth and monotonic and well described by the following functional forms (which also take into account the exact high-density limit of Eqs. (39)–(38) and (13) and guarantee the exact low-density expansion of the resulting correlation energy\(]^3\)\(d_1 r_s^{-1} + d_2 r_s^{-3/2}\) of:

\[
\begin{align*}
\alpha_{\uparrow \downarrow}^{\uparrow \downarrow}(r_s) &= -\frac{4}{3\pi q_F} \ln \frac{1 + k_1(a^{\uparrow \downarrow}) r_s}{r_s} \\
\alpha_{\uparrow \downarrow}^{\uparrow \downarrow}(r_s) &= \frac{8}{5\pi q_F} \ln \frac{(1 + p_1(a^{\uparrow \downarrow}) r_s)(1 + p_2(a^{\uparrow \downarrow}) r_s)}{r_s} \\
\alpha_{\uparrow \downarrow}^{\uparrow \downarrow}(r_s) &= \frac{99}{5\pi q_F} \ln \frac{(1 + p_1(a^{\uparrow \downarrow}) r_s)(1 + p_2(a^{\uparrow \downarrow}) r_s)}{r_s} \tag{48}\end{align*}
\]

The 9 constants for \(\uparrow \downarrow\) and the 9 constants for \(\uparrow \uparrow\) have been fixed by a two-dimensional best fit to the QMC data in real and reciprocal space (9368+9368 data points). The efficiency of our interpolation scheme has been tested by performing preliminary fits in which some of the available \(r_s\) were not included and then verifying that the interpolated \(g\) and \(S\) were in good agreement with the corresponding QMC quantities for the excluded \(r_s\). Since this was always the case, we included all the available \(r_s\) in order to have optimal values for our final parameters. We thus expect our \(g\) and \(S\) to be very reliable and accurate in the whole density range \(r_s \in [0.8, 10]\).

The optimal 9 parameters which define our best antiparallel-spin model are: \(a^{\uparrow \downarrow} = 0.838, k_3 = 0.141, b_1^{\uparrow \downarrow} = 3.27, \lambda_4^{\uparrow \downarrow} = -78, \gamma_4^{\uparrow \downarrow} = 28, \lambda_5^{\uparrow \downarrow} = 216, \gamma_5^{\uparrow \downarrow} = -124, \lambda_6^{\uparrow \downarrow} = -140, \gamma_6^{\uparrow \downarrow} = 55, \) and the other 9 parameters for the parallel-spin part are: \(a^{\uparrow \uparrow} = 1.32, p_3 = 0.015, b_1^{\uparrow \uparrow} = 3.47, \lambda_4^{\uparrow \uparrow} = 98, \gamma_4^{\uparrow \uparrow} = -36, \lambda_5^{\uparrow \uparrow} = -295, \gamma_5^{\uparrow \uparrow} = 74, \lambda_6^{\uparrow \uparrow} = 170, \gamma_6^{\uparrow \downarrow} = -13.\)
VII. RESULTS IN REAL AND RECIPROCAL SPACE

After fixing the 9+9 parameters which fully specify our model, we are now ready to present, in Fig. 1, our real-space pair–correlation function $g_{\sigma_1\sigma_2}$, shown as a solid line, as a function of the scaled variable $r/r_s$. This is done for the 8 values of $r_s$ for which QMC results, shown as solid dots, were available. The best-to-date model correlation function of Perdew–Wang (PW) is also shown for comparison as a dashed line. Perdew and Wang interpolated the total pair–correlation function $g(r)$ between its short–range limit, dominated by the on-top value and cusp, and the nonoscillatory part of its long–range limit. Their interpolation, controlled by normalization and analytic constraints and fitting procedure nicely interpolates the QMC data, filtering out their noise. In reciprocal space it becomes clear that the long–range of the PW spin–resolved model is not exact. Moreover, as said in Sec. II, the PW total static structure factor does not recover, as $q \to 0$, the exact plasma frequency in its leading $q^2/2\omega_p$ term. This is visible for $r_s = 8$ and 10.

VIII. CORRELATION ENERGY

A. Spin–unresolved

The correlation energy obtained by integrating our $g$ [see Eq. (18)] is reported in Fig. 4, together with the corresponding QMC data. Its $\uparrow\uparrow$ and $\downarrow\downarrow$ contributions ($\epsilon_c = \epsilon_{\uparrow\downarrow} + \epsilon_{\downarrow\uparrow}$) are also separately shown. As expected, 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). Notice that, even if our model pair–distribution function breaks down for $r_s > 10$, 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 $\epsilon_c$.

To have an idea of the accuracy of our correlation energies, we performed best fits of the QMC data of Ortiz, Harris and Balon (hereafter OHB) based on other popular interpolation formulae for $\epsilon_c(r_s)$, i. e. the Perdew–Zunger (PZ), the Vosko–Wilk–Nusair (VWN) and the Perdew–Wang (PW2, to distinguish it from the pair–correlation model) functional forms. The new QMC data for the correlation energy of the unpolarized jellium are available for a large set of $r_s$: 0.8, 1, 2, 3, 4, 5, 8, 10, 20, 30, 40, 50 and 60. The results are the followings: with the PZ formula one obtains a rather good fit (within 3%), but a wrong negative coefficient for the high–density term $\epsilon_c(r_s \ln r_s)$, an unpleasant feature already pointed out in Ref. [11]. Moreover, the PZ energy has a discontinuity in its second derivative at $r_s = 1$, an unpleasant feature for whoever is interested in the corresponding pair–correlation function, related to the first
derivative of $\epsilon_c$.

The VWN form efficiently interpolates the OHB data (2.7% maximum relative error; 1.5 mRy maximum absolute error) only if the free parameter $x_0$ of the VWN formula has a positive value, which however implies an unphysical logarithmic divergence at finite $r_s$ ($\sim 0.6$). If $x_0$ is constrained to be negative, then the fit provided by the VWN form is not better than ours (5.2% maximum relative error; 3.4 mRy maximum absolute error).

The fit accomplished with the PW2 form is not very accurate (see also Ref. 10): 7% maximum relative error, 3.4 mRy maximum absolute error. Moreover, the optimal fit parameter $\beta_1$ of PW2 form turns out to be negative (see also Ref. 10), thus leading to a negative coefficient for the low–density expansion term $r_s^{-3/2}$ and to the violation of the Ferrel condition.

We can conclude that the correlation energies vs. $r_s$, which directly emerge from our pair–correlation functions, although not targeted by our fits, are rather good.

The main inaccuracies of the popular correlation–energy models just reviewed are located in the high–density region, where at first sight the QMC results cannot be reconciled with the exact $r_s \to 0$ limiting behavior. This discrepancy can be related to the combined impact of fixed–node approximation and infinite–size extrapolation (which would match the finding that, for $r_s \leq 2$, Monte Carlo simulations based on different nodes and size–scaling rules Refs. 3 and 12 obtain somewhat different energies); it should be kept in mind, however, that the exact high–density expansion only holds for $r_s \to 0$, and could, in principle, start dominating the correlation energy at smaller $r_s$ values than implicitly assumed by the existing models.

An alternative correlation–energy model, not related to our pair–correlation function but capable of an excellent interpolation of the QMC energies of Refs. 11 and 13 including those at high density, can be obtained by a minor generalization of the PW2 form. Such a generalization keeps its exact $r_s \to 0$ limit, improves some of its original analytic properties, and appears flexible enough to interpolate different sets of high–density QMC data. We separately present it in our Appendix B.

### IX. CONCLUSIONS AND PERSPECTIVES

We have proposed a new, analytic, spin–resolved, static structure factor and pair–correlation function for the unpolarized jellium which works in the density range $r_s \leq 10$. Our model functions fulfill a wealth of known analytic properties of their exact counterparts, nicely interpolate the most recent and complete QMC data of Ortiz, Harris and Ballone, and consistently yield accurate correlation energies. They can be of interest to build up beyond-LDA exchange–correlation energy density functionals for the magnetic response of the unpolarized homogeneous electron gas and also, within the theory developed in Refs. 58, for the $e–e$ correlation in real materials. As a byproduct, we have obtained two correlation energy models which work well in the entire $r_s < \infty$ density range.

In further developments we plan to extend our procedure to the partially polarized jellium and to lower densities ($r_s > 10$). A small Fortran code aimed at the numerical evaluation of our functions [Eqs. (27), (11), (A1), (A2), (B1)] can be obtained upon request to Giovanni.Bachelet@roma1.infn.it.

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APPENDIX A: PAIR–CORRELATION FUNCTIONS IN REAL SPACE

The expressions of Eqs. (22) and (31) correspond in real space to:
\[
g_{\uparrow\downarrow}(r; s) = \frac{\pi e^{-a\uparrow\downarrow r}}{480} \left\{ \frac{a_{\uparrow\downarrow}}{a_{\uparrow\downarrow}^3} \left[ \frac{10395}{64} a_{\uparrow\downarrow} + \frac{12645}{64} a_{\uparrow\downarrow}^2 + \frac{585}{64} (a_{\uparrow\downarrow})^2 - \frac{705}{64} (a_{\uparrow\downarrow})^3 + \frac{45}{64} (a_{\uparrow\downarrow})^4 - \frac{(a_{\uparrow\downarrow})^5}{64} \right] + \frac{a_{\downarrow\uparrow}}{a_{\downarrow\uparrow}^3} \left[ \frac{945}{64} a_{\downarrow\uparrow} + \frac{945}{64} a_{\downarrow\uparrow}^2 - \frac{315}{16} (a_{\downarrow\uparrow})^2 + \frac{345}{64} (a_{\downarrow\uparrow})^3 - \frac{33}{64} (a_{\downarrow\uparrow})^4 + \frac{(a_{\downarrow\uparrow})^5}{64} \right] \right\} + \\
+ 3 \sum_{n=1}^{6} c_{n}^{\uparrow\downarrow} (-1)^{n+1} \frac{\partial^{n+1}}{\partial (b_{\uparrow\downarrow})^{n+1}} \left[ \frac{1}{\rho^2 + (b_{\uparrow\downarrow})^2} \right] (A1)
\]
\[
g_{\uparrow\uparrow}(r; s) = \frac{\pi e^{-a\uparrow\uparrow r}}{6881280} \left\{ \frac{a_{\uparrow\uparrow}}{(a_{\uparrow\uparrow})^3} \left[ \frac{135135}{135135} a_{\uparrow\uparrow}^5 + 270270 (a_{\uparrow\uparrow})^2 + 14765 (a_{\uparrow\uparrow})^3 - 20370 (a_{\uparrow\uparrow})^4 + \right. \\
+ 1722 (a_{\uparrow\uparrow})^5 - 68 (a_{\uparrow\uparrow})^6 + (a_{\uparrow\uparrow})^7 \right\} + \frac{a_{\downarrow\downarrow}}{(a_{\downarrow\downarrow})^3} \left[ -31185 - 31185 a_{\downarrow\downarrow} + 6930 (a_{\downarrow\downarrow})^2 + 17325 (a_{\downarrow\downarrow})^3 + \\
- 6930 (a_{\downarrow\downarrow})^4 + 938 (a_{\downarrow\downarrow})^5 - 52 (a_{\downarrow\downarrow})^6 + (a_{\downarrow\downarrow})^7 \right] + \frac{a_{\downarrow\downarrow}}{(a_{\downarrow\downarrow})^3} \left[ 14175 + 14175 a_{\downarrow\downarrow} + 1890 (a_{\downarrow\downarrow})^2 + \\
- 2835 (a_{\downarrow\downarrow})^3 - 82 (a_{\downarrow\downarrow})^4 + 378 (a_{\downarrow\downarrow})^5 - 36 (a_{\downarrow\downarrow})^6 + (a_{\downarrow\downarrow})^7 \right] \right\} + \\
+ 3 \sum_{n=1}^{6} c_{n}^{\uparrow\uparrow} (-1)^{n+1} \frac{\partial^{n+1}}{\partial (b_{\uparrow\downarrow})^{n+1}} \left[ \frac{1}{\rho^2 + (b_{\uparrow\downarrow})^2} \right] (A2)
\]

APPENDIX B: OPTIMAL FIT TO THE QMC CORRELATION ENERGY

Since the Perdew–Wang\(^3\) (PW2) form is simple and physically motivated, we slightly modify it by introducing one more free parameter which grants us enough flexibility to accurately fit the new data by Ortiz, Harris and Ballone.\(^4\)

We also include the exact correlation energy at the highest densities and avoids undesired effects on the low–density regime (such as a negative coefficient for the \(r_{s}^{-3/2}\) term). The parameters \(A\), \(\beta_1\), \(\beta_2\), \(\beta_3\) and \(\alpha_1\) are fixed by imposing the high–density expansion of Eq. (B1): \(\alpha_1 = C/A\), \(\beta_1 = 0.5/A \exp(0.5B/A)\), \(\beta_2 = 2A\beta_1^2\) and \(\beta_3 = 0.5\beta_1(8\beta_1^2 A^4 - CB + DA)/A^2\). A best fit to new QMC data\(^5\) gives the following 4 free parameters: \(\alpha_2 = 5\), \(\beta_4 = 45\), \(\beta_5 = 32\), \(\beta_6 = 12.7\). The resulting low–density expansion is \(-0.39/r_{s} + 0.99/r_{s}^{3/2}\). The maximum absolute error is 1.6 mRy, while the maximum relative error is 2.4%.

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the gaussian cut-off used by several authors in real or reciprocal space would, instead, give rise to unpleasant non-closed form expressions for the spherical Fourier transform of odd powers of g(r) [and/or S(q)], since

\[
\int_0^\infty e^{-ar^2} \sin(qr) \, dr = \frac{\pi}{2a} \sum_{n=1}^{\infty} \frac{1}{(2n-1)(2n-1)^2} \left( \frac{a^2}{2} \right)^{n-1}
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we hear from J. P. Perdew that he and his collaborators are presently working on a better estimate for the spin resolution of the PW pair–correlation function.

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FIG. 1. Spin–resolved pair–correlation function of the unpolarized homogeneous electron gas plotted against the electron separation $r$ scaled by the density parameter $r_s$ for eight different values of $r_s$ between $r_s = 0$ and $r_s = 10$. Solid line: this work; dots: QMC data; dashed line: Perdew–Wang model.
FIG. 2. Antiparallel–spin correlation function at zero interelectronic distance plotted against the density parameter $r_s$. Solid line: this work; dashed line: electron–electron ladder evaluation. In the inset the exact high–density expansion is also shown as dots.
FIG. 3. Static structure factor and magnetic structure factor of the unpolarized jellium plotted against the wavevector $q$ scaled by the Fermi wavevector $q_F$ for the same eight $r_s$ values as Fig. 1. Solid line: this work; dots: QMC data; dashed line: Perdew–Wang model.
FIG. 4. Total (solid) and spin–resolved (dashed) correlation energy of the unpolarized homogenous electron gas plotted against the density parameter $r_s$. QMC data are also shown as dots.

FIG. 5. Our parallel-spin contribution to the total correlation energy compared to the Perdew–Wang and Stoll et al. approximations. $\epsilon_{c}(r_s, \zeta = 1)$ is from Ref. [41].