

Analytic form of the correlation energy of the uniform electron gas

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An expression for the correlation energy density of the uniform electron gas is derived based on the adiabatic connection method. It covers with a single form the transition between high-density and low-density regions in the range $0.1 \leq r_s \leq 30$, parsing the entire spin-polarization range $0 \leq \xi \leq 1$. The pair-correlation function used to generate the result has been used previously to describe mainly finite systems. We argue that the universality implied by the short-wavelength hypothesis goes both ways, and a model that works well for finite systems may be adapted to describe the uniform electron gas as well.

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The uniform electron gas (UEG) is an important subject in the quest for accurate exchange and correlation functionals in density functional theory. Local (local spin density) [1,2] and semilocal [generalized gradient approximation (GGA) and meta GGA] [3–6] approximations were created from a detailed knowledge of the UEG properties. The success of these approximations for systems much different from the UEG can in part be explained by the short-wavelength hypothesis [7]. It suggests that some degree of universality may exist in the way electrons correlate in different systems, especially at short interelectronic distances. Alternatively, efficient functionals for atoms and molecules have been developed without referring to properties of the UEG [8–12]. In this Brief Report, we argue that the universality implied by the short-wavelength hypothesis goes both ways, and a model that works well for finite systems can be used to derive approximations for the UEG correlation energy. Some evidence along this line has been given previously [13].

Exact or nearly exact first-principles results are still in demand for the UEG correlation energy. Interpolations based on quantum Monte Carlo (QMC) data [14,15] combined with known exact limits and constraints have reached a reasonable accuracy [2,16–18], while feasible first-principles solutions are still lacking it.

In this Brief Report we use the adiabatic connection method [19–22], employing a spin-polarized, opposite-spin pair-correlation function (PCF) of Jastrow type, which depends on the coupling strength parameter λ :

$$g_{\uparrow\downarrow}^{(\lambda)}(r) = 1 - \exp(-k_{\uparrow\downarrow}^2 r^2) [2 - \Phi_{\uparrow\downarrow}^{(\lambda)}(2 + \lambda r)] - \exp(-2k_{\uparrow\downarrow}^2 r^2) \times \left[1 - \Phi_{\uparrow\downarrow}^{(\lambda)}(2 + \lambda r) + (\Phi_{\uparrow\downarrow}^{(\lambda)})^2 \left(1 + \lambda r + \frac{\lambda^2 r^2}{4} \right) \right], \quad (1)$$

where $r = |\mathbf{r}_1 - \mathbf{r}_2|$ is the interelectronic distance. This PCF obeys automatically the known opposite-spin, λ -dependent cusp condition [23] for any $k_{\uparrow\downarrow}$ and λ , and has the following cusp value:

$$\lim_{r \rightarrow 0} g_{\uparrow\downarrow}^{(\lambda)}(r) = [\Phi_{\uparrow\downarrow}^{(\lambda)}(k_{\uparrow\downarrow})]^2 > 0 \quad \text{for any } 0 \leq \lambda \leq 1. \quad (2)$$

In the noninteracting limit ($\lambda=0$), the opposite-spin correlation vanishes, which imposes the conditions

$$\lim_{\lambda=0} g_{\uparrow\downarrow}^{(\lambda)}(r) = 1, \quad \lim_{\lambda=0} \Phi_{\uparrow\downarrow}^{(\lambda)}(k_{\uparrow\downarrow}) = 1 \quad \text{for any } r, k_{\uparrow\downarrow}. \quad (3)$$

This kind of PCF has been used in the past to derive functionals mainly for finite systems [11,12,24].

The opposite-spin correlation energy density is next determined by the adiabatic connection formula (ACF) [20,22] applied to the considered case ($n=n_{\uparrow}+n_{\downarrow}$):

$$\varepsilon_c^{\text{opp}} = 2 \frac{n_{\uparrow} n_{\downarrow}}{n} \int_0^1 d\lambda \int_0^{\infty} r dr [g_{\uparrow\downarrow}^{(\lambda)}(r) - 1]. \quad (4)$$

To this end we have to specify the form of the cusp factor $\Phi_{\uparrow\downarrow}^{(\lambda)}(k_{\uparrow\downarrow})$. We deduce it from the exact PCF normalization condition, which in the case of the UEG reads (opposite spins only)

$$\int_0^{\infty} r^2 dr [g_{\uparrow\downarrow}^{(\lambda)}(r) - 1] = 0. \quad (5)$$

Solution of the above equation first at $\lambda=1$ with respect to $\Phi_{\uparrow\downarrow}$ gives

$$\Phi_{\uparrow\downarrow}^{(\lambda=1)}(k) = \frac{1}{2A(k)} \{-B(k) + [B(k)^2 - 4A(k)C]^{1/2}\}, \quad k \equiv k_{\uparrow\downarrow}, \quad (6)$$

$$A(k) = \frac{\sqrt{2}}{4} + \frac{3\sqrt{2}}{64k^2} + \frac{1}{2k\sqrt{\pi}}, \quad (7)$$

$$B(k) = \left(2 - \frac{\sqrt{2}}{2} \right) + \frac{3}{2k\sqrt{\pi}}, \quad C = \frac{\sqrt{2}}{4} - 2. \quad (8)$$

The form of $\Phi_{\uparrow\downarrow}^{(\lambda)}(k_{\uparrow\downarrow})$ at arbitrary λ is then obtained from Eq. (6) by the substitution $k_{\uparrow\downarrow} \rightarrow k_{\uparrow\downarrow}/\lambda$, following the coordinate-scaling rules of Levy [22]. This form of $\Phi_{\uparrow\downarrow}^{(\lambda)}$ obeys automatically the noninteracting limit, Eq. (3).

Next we solve analytically the ACF, Eq. (4), using Eq. (1) with the above form of $\Phi_{\uparrow\downarrow}^{(\lambda)}(k_{\uparrow\downarrow})$, Eq. (6). The resulting expression is decomposed into a sum of several different types of integral, each handled separately. After some tedious and lengthy algebra that we do not present here due to a lack of space, we arrive at the following expression for the opposite-spin correlation energy density, up to an arbitrary form of the correlation wave vector $k_{\uparrow\downarrow}$:

$$\varepsilon_c^{\text{opp}} = \frac{n_{\uparrow} n_{\downarrow}}{n} [Q_1^{\uparrow\downarrow}(k_{\uparrow\downarrow}) + Q_2^{\uparrow\downarrow}(k_{\uparrow\downarrow}) + Q_3^{\uparrow\downarrow}(k_{\uparrow\downarrow})], \quad (9)$$

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TABLE I. Selected results for ε_c (a.u.) at different r_s and ξ .

r_s	ξ	$-\varepsilon_c(r_s, \xi)^a$	$-\varepsilon_c(r_s, \xi)^b$	r_s	ξ	$-\varepsilon_c(r_s, \xi)^a$	$-\varepsilon_c(r_s, \xi)^b$
0.1	0.0	0.1209	0.1209	5.0	0.0	0.0282	0.0282
	0.4	0.1147	0.1145		0.4	0.0266	0.0267
	1.0	0.0626	0.0644		1.0	0.0154	0.0154
0.5	0.0	0.0766	0.0766	10.0	0.0	0.0186	0.0186
	0.4	0.0725	0.0725		0.4	0.0175	0.0176
	1.0	0.0402	0.0406		1.0	0.0105	0.0106
1.0	0.0	0.0598	0.0598	20.0	0.0	0.0115	0.0115
	0.4	0.0565	0.0565		0.4	0.0109	0.0109
	1.0	0.0316	0.0316		1.0	0.0068	0.0070
2.0	0.0	0.0448	0.0448	30.0	0.0	0.0085	0.0084
	0.4	0.0422	0.0423		0.4	0.0081	0.0080
	1.0	0.0239	0.0234		1.0	0.0051	0.0053
MAD							0.0002
MAPD ^c							0.80%

^aBenchmark results from Refs. [18,27].

^bResults of the present work using Eqs. (24) and (25).

^cThe mean deviations include also data for $r_s=3, 8,$ and $16,$ and $\xi=0.2, 0.6, 0.8,$ and 0.9 (not listed in the table).

$$Q_1^{\uparrow\downarrow}(k) = \frac{1}{D_1(k)} \left(-\arctan(a_2k + a_3) \frac{D_2(k)}{k} - \frac{D_3(k)}{k} \ln[D_1(k)] \right. \\ \left. + \frac{\ln(k)}{k} D_4(k) - a_4k + a_{12} + \frac{a_{14}}{k} + \frac{a_{18}}{k^2} \right), \quad (10)$$

$$Q_2^{\uparrow\downarrow}(k) = -\frac{c_1}{k} - \frac{c_2}{k^2} - \frac{c_3}{k} \ln(k) + \frac{c_4}{k} \ln[D_5(k)] + \frac{c_8}{k} \arctan \\ \times (a_2k + a_3) + \frac{c_9}{k} \ln(k + c_{10}) - \frac{c_{11}}{k} \ln[D_6(k)], \quad (11)$$

$$Q_3^{\uparrow\downarrow}(k) = \frac{c_{19}}{k} \arctan\left(\frac{c_{20}}{c_{21}k + c_{22}}\right) - \frac{c_{23}}{k} \operatorname{arctanh}\left[\frac{c_{24} + c_{25}k}{D_8(k)}\right] \\ - \frac{c_{15}}{k} \ln[D_7(k)] - \frac{c_{29}}{k^2} D_8(k), \quad (12)$$

where $D_i(k)$ are certain quadratic polynomials yielded by the algebra, and a_i, c_i are theoretical coefficients yielded by the algebra as well. All these are given in the Appendix.

The obtained form of $\varepsilon_c^{\text{opp}}$ is used next to model the parallel-spin correlation energy density

$$\varepsilon_c^{\text{par}} = (\varepsilon_c^{\uparrow\uparrow} + \varepsilon_c^{\downarrow\downarrow}). \quad (13)$$

We argue that the correlation among electrons with parallel spins, beyond and “after” the Fermi exchange, should be qualitatively similar to the correlation among electrons with opposite spins [24]. With this in mind, the parallel-spin correlation energy components $\varepsilon_c^{\sigma\sigma}$ are approximated as

$$\varepsilon_c^{\sigma\sigma} = \frac{n_\sigma^2}{2n} [Q_1^\sigma(k_\sigma) + Q_2^\sigma(k_\sigma) + Q_3^\sigma(k_\sigma)], \quad (14)$$

where the functions $Q_i(k_\sigma)$ have the same form as in Eqs. (10)–(12), but with different argument, the parallel-spin correlation wave vector. “Beyond and after the Fermi exchange” means here that the approximation for $\varepsilon_c^{\sigma\sigma}$ is reasonable only for $k_\sigma < k_{f\sigma}$, where $k_{f\sigma}$ is the local Fermi wave vector:

$$k_{f\sigma}(\vec{r}) = a'_x n_\sigma^{1/3}(\vec{r}) = a_x [n(\vec{r})(1 \pm \xi(\vec{r}))]^{1/3}, \quad (15)$$

$$\sigma = \uparrow (+), \quad \sigma = \downarrow (-),$$

$a'_x = (6\pi^2)^{1/3}$, $a_x = (3\pi^2/2)^{1/3}$, and ξ is the spin-polarization parameter,

$$n_\uparrow = \frac{1}{2}n(1 + \xi), \quad n_\downarrow = \frac{1}{2}n(1 - \xi). \quad (16)$$

A trial form of k_σ that obeys the condition $k_\sigma < k_{f\sigma}$ can be constructed in terms of effective screening functions multiplying the Fermi wave vector [25]:

$$k_\sigma(\vec{r}) = \alpha_{\text{eff}}(r_s, \xi) k_{f\sigma}, \quad (17)$$

where α_{eff} is a certain screening function to be specified. The opposite-spin wave vector is obtained following the Becke ansatz [8]:

$$k_{\uparrow\downarrow}(\vec{r}) = \beta_{\text{eff}}(r_s) \frac{2k_{f\uparrow}k_{f\downarrow}}{(k_{f\uparrow} + k_{f\downarrow})}, \quad (18)$$

where β_{eff} is yet another screening function. The screening functions are determined by fitting suitable trial forms of these to available literature benchmarks for the correlation energy components $\varepsilon_c^{\text{opp}}$ and $\varepsilon_c^{\text{par}}$ [18,27] in the density range $0.1 \leq r_s \leq 10$. Considering first $k_{\uparrow\downarrow}$, we use the following trial form of β_{eff} [25]:

$$\beta_{\text{eff}}(r_s) = \eta_1 + \eta_2 \exp(-\eta_3 r_s^{1/3}) r_s^{1/4} + \eta_4 \exp(-\eta_5 r_s^{1/3}) r_s^{1/3}. \quad (19)$$

The optimized coefficients η_i are given in the Appendix.

The parallel-spin screening factor is chosen here in the form

$$\alpha_{\text{eff}}(r_s, \xi) = \alpha_n(r_s) \alpha_\xi(r_s, \xi), \quad (20)$$

$$\alpha_n(r_s) = \eta_6 + \eta_7 \exp(-\eta_8 r_s^{1/3}) r_s^{2/3} + \eta_9 \exp(-\eta_{10} r_s^{1/3}) r_s^{1/3}, \quad (21)$$

$$\alpha_\xi(r_s, \xi) = \frac{2}{[(1 + \xi)^{s(r_s, \xi)} + (1 - \xi)^{s(r_s, \xi)}]}, \quad (22)$$

where the exponential factor $s(r_s, \xi)$ is optimized using Thiele’s interpolation technique [26]:

$$s(r_s, \xi) = f_r(r_s) f_s(\xi), \quad (23)$$

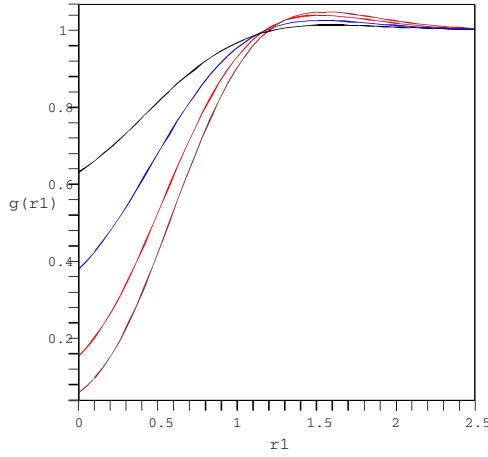


FIG. 1. (Color online) Opposite-spin PCF of spin-unpolarized UEG as a function of the dimensionless distance $r_1 = r/(r_s a_0)$. Curves from left to right: $r_s = 0.8, 2, 5,$ and 10 a.u.

$$f_r(r_s) = \frac{P_1(r_s)}{P_2(r_s)}, \quad P_1(r_s) = \sum_{i=0}^5 a_i r_s^i, \quad P_2(r_s) = \sum_{i=0}^4 b_i r_s^i, \quad (24)$$

$$f_s(\xi) = \frac{P_3(\xi)}{P_4(\xi)}, \quad P_3(\xi) = \sum_{i=0}^4 c_i \xi^i, \quad P_4(\xi) = \sum_{i=0}^3 d_i \xi^i. \quad (25)$$

All the coefficients above are given in the Appendix.

The final expression of the UEG correlation energy is a single formula that covers smoothly the transition from high-density to low-density regions for any given ξ in the density range $0.1 \leq r_s \leq 30$. Table I contains results for a few selected r_s and ξ sample values. The mean absolute percentage deviation (MAPD) with respect to literature benchmarks [18,27,28] is 0.80% within the density range $0.1 \leq r_s \leq 30$, parsing the whole spin-polarization range for each r_s . Regarding only the spin-compensated case, $\xi=0$, our model yields the correlation energy with MAPD of 0.24% in the same density range.

The present model relies substantially on the opposite-spin PCF, Eq. (1). The shape of this function is depicted in Fig. 1 for different values of r_s at $\xi=0$. The curves compare favorably with the few existing top-notch results for this function [30].

An important property governed by the opposite-spin PCF is the value of its cusp $g_{\uparrow\downarrow}(0)$. First-principles and QMC estimates have been reported in Refs. [29,31,32]. Table II contains sample values of $g_{\uparrow\downarrow}(0)$ at selected electron densities and spin polarizations. These are compared to available literature results (available mostly for $\xi=0$). In the high-density region the estimates of Rassolov *et al.* [29] are exact. Very close to these are the first-principles results of Gori-Giorgi *et al.* [31]. Our values are also close to theirs in this limit. More noticeable is the difference from the QMC-extrapolated results in this region. The QMC method is known to be less accurate at small and vanishing interelectronic distances in the high-density region [30,31]. Considering medium- and low-density regions, the QMC-based analytic model of Ref. [30] [the Gori-Giorgi-Sacchetti-Bochelet (GSB) model] involves a number of exact con-

TABLE II. Values of the cusp $g_{\uparrow\downarrow}(0)$ for different r_s and ξ .

r_s	ξ	GGP ^a	Y72 ^b	RPR99 ^c	GSB ^d	PW ^e
0.01	0.0	0.9927	0.9940	0.9927	0.9833	0.9923
	0.8					0.9902
0.1	0.0	0.9302	0.9360	0.9268	0.9040	0.9305
	0.8					0.9132
1.0	0.0	0.5145	0.5320		0.5860	0.5738
	0.8					0.5060
2.0	0.0	0.2879	0.3000		0.3752	0.3790
	0.8					0.3114
3.0	0.0	0.1680			0.2407	0.2682
	0.8					0.2103
5.0	0.0	0.0631	0.0660		0.1116	0.1532
	0.8					0.1132
10.0	0.0	0.0082	0.0080		0.0309	0.0575
	0.8					0.0397

^aResults from Eq. (30) of Ref. [31] (Gori-Giorgi-Perdew).

^bFirst principles results of Ref. [32] (Yasuhara 1972), within the ladder approximation to the electron-electron interaction.

^cExact high-density estimates of Ref. [29] (Rassolov-Pople-Ratner 1999).

^dQMC-extrapolated analytic results from Ref. [30].

^eResults of the present work (PW). r_s is multiplied by the Bohr radius a_0 before evaluating $g_{\uparrow\downarrow}(0)$ [see Eq. (5) of Ref. [28]].

straints and is expected to be accurate at least in the range ($0.8 \leq r_s \leq 10$) [30]. It is interesting that, in this range, our cusp values are systematically closer to the GSB results among the data presented in Table II.

Let us note in conclusion that a variety of functionals can in principle be generated from Eq. (9), depending on what form of the correlation wave vectors is used. We employ the screening concept to obtain a form that turns out to be suitable for the UEG case within certain limits. It yields a compact and accurate correlation energy expression in the range $0.1 \leq r_s \leq 30$ and the whole spin-polarization range. Exploration of lower-density regions, $r_s > 30$, would require dealing with UEG magnetic phase transitions [15,33], which is beyond the scope of this Brief Report.

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APPENDIX

The theoretical values of all coefficients a_i and c_i are listed in Table III. The forms of the polynomials $D_i(k)$ entering Eqs. (10)–(12) are

$$\begin{aligned} D_1 &= a_6 k^2 + a_7 k + a_8, & D_2 &= a_1 k^2 + a_{10} k + a_{16}, \\ D_3 &= a_5 k^2 + a_{13} k + a_{15}, & D_4 &= a_9 k^2 + a_{11} k + a_{17}, \\ D_5 &= c_5 k^2 + c_6 k + c_7, & D_6 &= c_{12} k^2 + c_{13} k + c_{14}, \\ D_7 &= c_{16} k^2 + c_{17} k + c_{18}, \\ D_8 &= (c_{26} k^2 + c_{27} k + c_{28})^{1/2}. \end{aligned}$$

The values of the fitting parameters in Eq. (19) are

$$\begin{aligned} \eta_1 &= 0.538\,074\,483\,500\,437, \\ \eta_2 &= -2.226\,094\,990\,985\,190, \end{aligned}$$

TABLE III. The coefficients a_i and c_i in Eqs. (10)–(12) and in the polynomials $D_i(k)$.

a_1	0.184 630 439 485 191	a_{17}	0.035 913 346 995 016	c_{15}	14.565 097 171 166 0
a_2	5.939 656 549 519 008	a_{18}	0.222 017 353 476 156	c_{16}	0.781 250 000 000 00
a_3	2.369 580 128 666 418	c_1	132.479 090 287 794	c_{17}	0.623 347 313 127 24
a_4	0.051 188 865 525 959	c_2	32.401 470 851 677 1	c_{18}	0.146 484 375 000 00
a_5	0.095 768 925 320 043	c_3	22.566 445 316 250 4	c_{19}	111.811 548 105 797 8
a_6	0.028 359 261 614 488	c_4	11.283 222 658 125 2	c_{20}	0.160 041 105 570 901
a_7	0.022 627 416 997 970	c_5	0.401 060 523 940 96	c_{21}	0.781 250 000 000 000
a_8	0.005 317 361 552 717	c_6	0.32	c_{22}	0.320 866 950 607 957
a_9	0.191 537 850 640 085	c_7	0.075 198 848 238 93	c_{23}	13.284 449 507 299 84
a_{10}	0.147 313 777 119 493	c_8	116.935 042 647 481	c_{24}	0.268 418 671 319 107
a_{11}	0.152 825 093 835 090	c_9	29.624 002 304 690 1	c_{25}	0.471 060 597 934 992
a_{12}	1.015 083 075 438 391	c_{10}	0.482 257 181 994 47	c_{26}	1/4
a_{13}	0.076 412 546 917 545	c_{11}	0.246 903 981 179 10	c_{27}	0.252 882 919 616 990
a_{14}	0.898 537 460 263 473	c_{12}	1/2	c_{28}	0.072 048 583 112 715
a_{15}	0.017 956 673 497 508	c_{13}	0.410 709 696 778 19	c_{29}	42.649 054 489 103 11
a_{16}	0.034 618 207 403 477	c_{14}	0.105 323 524 476 77		

$$\eta_3 = 0.837\ 303\ 782\ 322\ 808, \quad \eta_4 = 2.619\ 709\ 858\ 963\ 178,$$

$$\eta_5 = 1.036\ 657\ 594\ 643\ 520.$$

The values of the fitting parameters in Eqs. (21) are

$$\eta_6 = 0.410\ 811\ 466\ 521\ 28, \quad \eta_7 = 0.599\ 343\ 256\ 903\ 515,$$

$$\eta_8 = 1.709\ 394\ 768\ 021\ 68, \quad \eta_9 = 0.077\ 123\ 208\ 419\ 481,$$

$$\eta_{10} = 0.469\ 584\ 490\ 076\ 19.$$

The coefficients in Eqs. (24) and (25) read

$$a_5 = 0.000\ 293\ 039\ 144\ 178\ 338,$$

$$a_4 = 0.944\ 080\ 741\ 695\ 104\ 794,$$

$$a_3 = -23.824\ 237\ 216\ 837\ 930\ 2,$$

$$a_2 = 49.341\ 312\ 958\ 396\ 707\ 50,$$

$$a_1 = 24.005\ 021\ 512\ 787\ 114\ 40,$$

$$a_0 = -113.693\ 369\ 789\ 727\ 190,$$

$$b_4 = 1.0, \quad b_3 = -25.154\ 009\ 904\ 187\ 990,$$

$$b_2 = 54.403\ 433\ 137\ 390\ 836\ 6,$$

$$b_1 = 16.266\ 312\ 944\ 424\ 241\ 5,$$

$$b_0 = -109.742\ 634\ 932\ 169\ 10,$$

$$c_4 = -0.010\ 991\ 223\ 672\ 914\ 40,$$

$$c_3 = 0.580\ 344\ 063\ 812\ 247\ 980,$$

$$c_2 = -1.426\ 930\ 414\ 984\ 216\ 40,$$

$$c_1 = 1.180\ 131\ 465\ 463\ 191\ 050,$$

$$c_0 = -0.324\ 815\ 686\ 049\ 198\ 86,$$

$$d_3 = 1.0,$$

$$d_2 = -2.521\ 881\ 835\ 869\ 481\ 80,$$

$$d_1 = 2.097\ 085\ 058\ 834\ 907\ 36,$$

$$d_0 = -0.577\ 861\ 031\ 932\ 394\ 30.$$

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