Homogeneous electron gas in arbitrary dimensions

Robert Schlesier, Carlos L. Benavides-Riveros, and Miguel A. L. Marques

1Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany
2NR-ISM, Division of Ultrafast Processes in Materials (FLASHit), Area della Ricerca di Roma 1, Via Salaria Km 29.3, I-00016 Monterotondo Scalo, Italy

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The homogeneous electron gas is one of the most studied model systems in condensed-matter physics. It is also the basis of the large majority of approximations to the functionals of density-functional theory. As such, its exchange-correlation energy has been studied extensively, and it is well known for systems of one, two, and three dimensions. Here, we extend this model and compute the exchange and correlation energy, as a function of the Wigner-Seitz radius \( r_s \), for arbitrary dimension \( D \). We find a very different behavior for reduced dimensional spaces \( (D = 1 \text{ and } 2) \), our three-dimensional space, and for higher dimensions. In fact, for \( D > 3 \), the leading term of the correlation energy does not depend on the logarithm of \( r_s \) (as for \( D = 3 \)), but instead scales like a polynomial: \( -c_D/r_s^\gamma_D \), with the exponent \( \gamma_D = (D - 3)/(D - 1) \). In the large-\( D \) limit, the value of \( c_D \) is found to depend linearly on the dimension. In this limit, we also find that the concepts of exchange and correlation merge, sharing a common \( 1/r_s \) dependence.

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I. INTRODUCTION

The homogeneous electron gas (HEG) is one of the most fundamental models of condensed-matter theory [1]. Despite its apparent simplicity, it has played a crucial role in the development of electronic structure theory for almost a century [2–10]. In 1965, Kohn and Sham showed that the exchange and correlation energy of the HEG can be used to perform accurate many-body calculations for atoms, molecules, and solids [11]. Since then, the HEG is one of the systems of choice to develop, improve, and benchmark functionals in density-functional theory (DFT) [12].

In the \( D \)-dimensional HEG model, an infinite uniform gas of electrons fills an infinite \( D \)-dimensional cube. The negative charge is neutralized by a uniform positive background. Not surprisingly, simple metals (i.e., metal sodium) resemble quite well this paradigmatic system. While the exact kinetic energy and exchange energy were determined at the very beginning of quantum mechanics [13,14], the first analytical expression for the correlation energy had to wait until much later. This was obtained for high densities within the random-phase approximation (RPA) [15]. Now we also have available highly accurate numerical values for the correlation energy of the HEG, for \( D = 1 \) [16], 2 [17], and 3 [18,19], from Monte Carlo simulations.

For the spin-unpolarized HEG in \( D = 1 \), 2, and 3, the energy per electron reads, as a function of \( r_s \), the Wigner-Seitz radius \( r_s \):

\[
\varepsilon_D(r_s \to 0) = \frac{a_D}{r_s} - \frac{b_D}{r_s^3} + c_D \ln r_s + O(r_s^0),
\]

where \( a_D \), \( b_D \), and \( c_D \) are constants independent of \( r_s \). The first term on the right-hand side of (1) is the noninteracting kinetic energy term, while the second is the exchange one. The remaining terms represent the correlation energy. The values of the constants in (1) are known for \( D = 1 \), 2, and 3 [1]. The reconstruction of the series beyond the high-density regime is a fascinating field in itself, with gaps still remaining in our knowledge (see, for a recent review, Ref. [1]).

One of the most basic and essential concepts in science, the dimensional parameter \( D \) is usually investigated as it can yield remarkable insights into the physical 3D case [21–26]. There is a multitude of physical systems in which one or two of the physical dimensions are much smaller than the remaining ones. Such systems can often be modeled as one- and two-dimensional (with the 3D form of the Poisson equation for the Coulomb interaction), reducing their complexity while keeping the most important qualitative features of \( D = 3 \) [27–29]. Indeed, by a meaningful dimensional crossover, insights from 3D systems are useful to study and develop exchange-correlation potentials for lower-dimensional systems [30,31]. Furthermore, and perhaps more importantly, reduced dimensions often exhibit notable physical properties. For example, in one dimension we find Luttinger physics [32], while the synthesis of graphene [33] and related materials has opened the way to a myriad of novel physical effects in two dimensions [34]. In the large-\( D \) limit, by increasing the degrees of freedom, the quantum world reduces to a classical one [35]. Finally, recent progress in the fabrication of artificial 2D materials paved the way for the artificial realization of noninteger dimensions. Indeed, fractal substrates (e.g., Sierpiński carpets of bulk Cu) confining electron gases have already been reported, and the quantum states are found to exhibit also a fractal structure [36–38].

The main aim of this paper is to study the HEG in arbitrary dimensions. We assume that the integral form of the Coulomb interaction in three dimensions is valid at
arbitrary dimensions. Note that this is the usual assumption for gases with dimensions larger than 1. For \( D = 1 \) the usual Coulomb interaction leads to divergence, so it is usually softened [39]. Other interactions have also been proposed to study the crossover between 2D and 3D systems [31]. We consider the \( D \)-dimensional Cartesian space, which can be efficiently studied with the plane-wave basis set. Other, much more involved, types of geometries are important to study the strongly correlated (i.e., low-density) regime, as, for instance, hyperspheres. Unfortunately, due to the added complexity, that line of research has been limited to few electrons [40,41].

We will present analytic results for the \( D \)-dimensional HEG for the leading terms of the kinetic, exchange, and correlation energies. Our main result is that for \( D > 3 \) the ground-state energy of the HEG has a quite different behavior when compared to \( D = 3 \). Specifically, we will show that the energy for \( D > 3 \) exhibits the following expansion in terms of the Wigner-Seitz radius \( r_s \):

\[
\epsilon_D(r_s \to 0) \approx \frac{a_D}{r_s^2} \frac{b_D}{r_s} + \frac{c_D}{r_s^{1+\alpha}} + O(r_s^0),
\]

where \( \gamma_D = (D-3)/(D-1) \). To obtain this result we use the RPA, which is known to be exact in the limit of the dense gas. Incidentally, we note that the usefulness of the RPA in materials science goes well beyond the study of the HEG. In fact, the RPA provides an excellent framework for producing fully nonlocal exchange-correlation functionals, including long-range van der Waals interactions [42–44] and static electronic correlations [45]. To go beyond the RPA and to obtain accurate results for the mid- to low-density regime would require the use of Monte Carlo techniques [46] or other high-quality approaches such as the Singwi, Tosi, Land, and Sjölander method [47].

This paper is organized as follows. We discuss first the kinetic and exchange energy for the \( D \)-dimensional gas. Although the results are both known, we offer an alternative derivation for the exchange energy that is valid for integer and noninteger dimensions. We then compute the correlation energy for the HEG in arbitrary dimensions. The paper ends with a conclusion and two more technical Appendixes. Atomic units are used throughout.

**II. KINETIC AND EXCHANGE ENERGY**

We use \( k_\uparrow \) for the Fermi levels of the spin-up and spin-down channels, respectively. For convenience, we also define the quantity \( k_F^D \equiv (k_\uparrow^D + k_\downarrow^D)/2 \). The relations \( k_{\uparrow,\downarrow} \equiv k_\pm/k_F = (1 \pm \xi)D \) determine \( \xi \), the system’s spin polarization, lying between 0 and 1. The Wigner-Seitz radius is written as a function of the uniform density \( N/\Omega \) in the usual way:

\[
\frac{\Gamma(D/2 + 1)}{\pi^{D/2}} \frac{1}{r_s^D} = \frac{N}{\Omega}.
\]

Here \( \Gamma \) is the gamma function, \( N \) is the number of electrons, and \( \Omega \) is the volume occupied by the electrons.

At any dimension, the one-electron orbitals are plane waves and the ground-state energy of the HEG can be obtained by perturbation methods, yielding

\[
\epsilon_D(r_s, \xi) = \epsilon_D^\uparrow(r_s, \xi) + \epsilon_D^\downarrow(r_s, \xi) + \epsilon_D^\uparrow(r_s, \xi).
\]

where the noninteracting kinetic energy \( \epsilon_D^\uparrow(r_s, \xi) \) and the exchange energy \( \epsilon_D^\downarrow(r_s, \xi) \) are the zeroth- and first-order terms of the expansion. The correlation energy \( \epsilon_D^\uparrow(r_s, \xi) \) is computed from all higher orders.

The calculation of the kinetic energy for the HEG is a textbook problem, and we present only the result. By integrating the energy contribution of each electron along the Fermi sphere, one gets the following expression [1]:

\[
\epsilon_D^\uparrow(r_s, \xi) = \frac{a_D^2}{2r_s^2} \frac{\Upsilon_2(\xi)}{\sqrt{r_s^2}}.
\]

where \( a_D = 2^{(D-1)/D}\Gamma(D/2 + 1) \) and

\[
\Upsilon_2(\xi) = \xi^2 [(1 + \xi)^{D+n}/D + (1 - \xi)^{D+n}/D]
\]

is the spin-scaling function. The first prefactor for the spin-unpolarized case in Eqs. (1) and (2) is thus \( a_D = a_D^\uparrow D/2(D + 2) \). In the large-\( D \) limit (which is easily achieved by using Stirling’s formula) we have for this function a quadratic scaling with the dimension

\[
ad_{D \to \infty} = \frac{D^2}{2\pi^2} + \frac{\ln(\pi) + \text{ln}(D)}{\pi^2} D + O(D^0).
\]

Here \( e \) is Euler’s constant.

The standard calculation of the exchange energy can also be easily generalized to arbitrary dimensions. Indeed, the exchange energy per particle reads

\[
\epsilon_D^\uparrow = -\frac{\Omega}{2N} \sum_{\alpha=\uparrow,\downarrow} \int \frac{d^D p_1}{(2\pi)^D} \frac{d^D p_2}{(2\pi)^D} U(p_1 - p_2),
\]

where \( U(q) \) is the \( D \)-dimensional Fourier transform of the Coulomb potential. All angular integrals in the expression (7) are straightforward except the one for the angle between the momenta \( p_1 \) and \( p_2 \). The integrals within are symmetric under the interchange of \( p_1 \) and \( p_2 \), which can be used to factor out one of the integrals over the magnitude of the momenta. After these steps, one arrives at the expression

\[
\epsilon_D^\uparrow = \frac{\Omega}{2N} \sum_{D+1} \frac{(k_\uparrow^{D+1} + k_\downarrow^{D+1})}{(4\pi)^{D/2}} \frac{\Gamma(D/2 + 1)}{\Gamma(D/2 + 1)} I(D/2 + 1).
\]

where we introduced the integral

\[
I(a) = \int_0^1 \int_0^{1/2} \eta^{2a}(1 - \eta^2)^{p-1} d\eta d\eta.
\]

We were unable to evaluate analytically this integral for arbitrary values of \( a \). However, we use a special relation with respect to the variable \( \eta \) to construct a recursive relation. In Appendix A we perform this calculation in full detail, leading to the recursive formula

\[
I(a) - I(a + 1) = \frac{1}{a(a + 1)}.
\]

In the special cases \( a = 1/2, 1 \), the integral (9) can be performed analytically, resulting in \( I(a) = 1/a \) for all integral dimensions. Furthermore, one can evaluate the integral numerically on the interval \( a \in (0, 1] \), leading to the result \( I(a) = 1/a \) for all values of \( a \). Now one can substitute the Fermi momenta with the corresponding expressions depending on the spin polarization. One eventually obtains the result of
Ref. [48] for arbitrary integer and noninteger dimensions as well:
\[
\varepsilon_D^{(n)}(r_s, \xi) = -\frac{2a_D D}{\pi (D^2 - 1)} \ \Gamma_1(\xi) r_s^D.
\] (11)
Thus for the spin-unpolarized case in Eq. (1) we have \( b_D = 2a_D D / \pi (D^2 - 1) \). In the large-\( D \) limit, this term goes to a constant value:
\[
b_{D \to \infty} = \frac{2}{\pi} e^{\pi} + O(1/D).
\] (12)
Notice that from Eq. (11) one eventually deduces that the exchange energy scales as \( (N/\Omega)^{1/D+1} \), with the same exponent of the Lieb-Oxford bound for the indirect Coulomb energy in arbitrary dimensions [49,50].

III. CORRELATION ENERGY

The high-density correlation energy for the two- and three-dimensional HEG is well understood [1]. For instance, for \( D = 3 \) the correlation energy has the following expansion [51]:
\[
\varepsilon^c(\xi) = \sum_j \left[ \lambda_j(\xi) \ln(r_s) + \omega_j(\xi) \right] r_s^D.
\] (13)

For arbitrary dimensions in the high-density regime, we apply the known resummation technique for \( D = 3 \) and generalize accordingly to arbitrary dimensions. We follow closely the classical work of Gell-Mann and Brueckner [15]. Since the change of dimension does not modify the topology of the Feynman diagrams, the sum of all the ring diagrams of the same order \( n \) yields the usual form known from the RPA:
\[
E^{(n)} = (-1)^{n+1} \frac{\Omega}{2} \int \frac{d^D q}{(2\pi)^D} \left[ \frac{U(q)}{(2\pi)^D} \right]^n A_n(q),
\] (14)
where the functions
\[
A_n(q) = \frac{n!}{n} \prod_{k=1}^{n} \int_{-\infty}^{\infty} dt_k F_k(t_k) \delta \left( \sum_{k=1}^{n} k_0 \right)
\] (15)
integrate the propagators \( F_k(t) \), the \( n \)-th order energy contribution is exact. Remarkably, the constant ring diagram contributions of order greater than or equal to 2 diverge. The divergence occurs at low momentum \( q \). If one now focuses on the low momentum behavior of \( \varepsilon_D^{(n)}(r_s, \xi) \), it turns out that this quantity is independent of \( q \). Thus one can pull this factor out of the momentum integral if one stays close to the lower limit of the integration. After expanding the integral measure, one arrives at an integral that is proportional to \( 1/[q^{D-2}(q^{D-1})^{n-2}] \). Its integral diverges at the lower limit for all \( D > 2 \) and \( n > 2 \).

Since we are interested in high densities (i.e., \( r_s \to 0 \)), the only relevant parts are the low momentum domain of the \( q \ll 1 \) integral. We then drop all terms with \( q \) raised to a higher power. After these approximations are performed, we reach a relatively simple expression for \( \varepsilon_D^{(n)}(r_s, \xi) \):
\[
\varepsilon_D^{(n)}(r_s, \xi) = -\frac{1}{\pi} \ln(2) \ \Gamma_0(2, \xi) \ln(r_s) + O(\varepsilon_D^{(0)}).
\] (19)

with \( \varepsilon_D^{(0)}(u, \xi) = \int dt F_t(t) e^{iut} \). In the RPA, the total correlation energy per particle amounts naturally to the sum of all these contributions. At this stage, one can show that the individual ring diagram contributions of order greater than or equal to 2 diverge. The divergence occurs at low momentum \( q \). If one now focuses on the low momentum behavior of \( \varepsilon_D^{(n)}(r_s, \xi) \), it turns out that this quantity is independent of \( q \). Thus one can pull this factor out of the momentum integral if one stays close to the lower limit of the integration. After expanding the integral measure, one arrives at an integral that is proportional to \( 1/[q^{D-2}(q^{D-1})^{n-2}] \). Its integral diverges at the lower limit for all \( D > 2 \) and \( n > 2 \).

We can group the results for the RPA correlation energy in three different cases (see Appendix B):

(i) When \( D = 1 \) or \( D = 2 \) the leading contribution to the correlation energy is a constant term.

(ii) When \( D = 3 \) the leading term is the logarithmic correction known since 1950 [52]:
\[
\varepsilon_D^{(n)}(r_s, \xi) = -\frac{1}{\pi^3} \ln(2) \ \Gamma_0(2, \xi) \ln(r_s) + O(\varepsilon_D^{(0)}).
\] (20)

(iii) For \( D > 3 \), the contribution is
\[
\varepsilon_D^{(n)}(r_s, \xi) = -\frac{2D \Sigma_D}{\pi^3(D-1)} \frac{\Gamma(\frac{D-1}{2})}{4\pi r_s^{D-1}} \int_{-\infty}^{\infty} du \left[ \frac{1}{\pi^{D-1} u^{\frac{D-1}{2}} + \delta_0} \right] + \frac{D}{\pi^3(D-3)} \int_{-\infty}^{\infty} du \left[ \frac{1}{\pi^{D-1} u^{\frac{D-1}{2}} + \delta_0} \right] \ln(r_s).
\] (21)

where \( \Sigma_D \) is a special \( D \)-dependent series (see Appendix B) and \( \delta_0 \) regulates the full approximation such that the second-order energy contribution is exact. Remarkably, the constant
term in Eq. (21) does not diverge as \( D \to 3 \) from above, since \( \delta_D \) exhibits the same divergence with the opposite sign.

Our result then shows that for \( D > 3 \), the correlation behaves as

\[
\varepsilon^c_D(r_s, \xi) \sim r_s^{(3-D)/(D-1)}. \tag{22}
\]

We obtained numerically the prefactors \( c_D \) (see Fig. 1). In Table I we give explicitly the values up to \( D = 9 \). Notice that they are all negative, as expected for a correlation energy. In the large-\( D \) limit, they scale linearly with the dimension: \( c_D \to -D/2e\pi^2 + O(D^0) \). Finally, from Eq. (22) one obtains that in leading order the total correlation energy scales with the density as \((\Omega/N)(D^{D-3})/(D^{D-1})\).

For the sake of comparison, we can now evaluate the equilibrium density that minimizes the energy of the HEG. Interestingly, the larger the dimension, the larger is the equilibrium \( r_s \). For example, using only the exchange energy, we obtain the equilibrium \( r_s \) of 4.823 37 \( (D = 3) \), 9.340 01 \( (D = 4) \), and 15.1596 \( (D = 5) \). Including the RPA correction, these values are reduced to 3.828 65 \( (D = 3) \), 8.739 97 \( (D = 4) \), and 13.3068 \( (D = 5) \). This means that the large-dimension HEG is stable for very low density gases. Recall that \( r_s \) and the density are connected by the definition (3). Since the dimensional factor \( \Gamma(D/2 + 1)/\pi^{D/2} \) increases rapidly with the dimension, one can see that the equilibrium density decreases with the dimension but at a much slower pace than the increase of \( r_s \).

IV. CONCLUSION AND OUTLOOK

Recent progress in the physical realization of noninteger dimensions has stimulated the study of electronic gases in exotic dimensions, beyond the three-dimensional world that we are used to \textit{a priori}. In this paper, we studied the HEG in such situations, with special emphasis on the leading orders of the correlation energy.

From our results, we can extract some interesting algebraic properties of the correlation energy of the \( D \)-dimensional HEG. First, our physical world, with \( D = 3 \), stands out as completely different from either the reduced dimensions \( (1 \) or \( 2) \) or higher dimensions. For dimensions greater than 3, the leading dependence on \( r_s \) changes with the dimensionality, in contrast to the kinetic and exchange parts. Finally, for large dimensions the correlation energy goes as \( 1/r_s \), which is the same dependence as exchange. This means that for higher dimensions, the HEG no longer becomes weakly correlated for large densities, but it is equally correlated in the whole range of densities. We believe that this work on arbitrary dimensions can shed some light on the more far-reaching problems of the correlation energy for the HEG in fractional dimensions \([36,38,53–55]\) and its quantum-information properties \([56–60]\). This can also be a point of departure to develop a more coherent and unified dimensional approach to new exchange-correlation functionals within DFT. Indeed, for the cases of 2D and 3D, such a dimensional unification has already proved to be quite successful \([31]\).

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APPENDIX A: CALCULATION OF THE RECURSIVE RELATION FOR THE INTEGRAL \( I(a) \)

Let us define the auxiliary function \( f(c, b, u) \), which reads

\[
f(c, b, u) = \int_0^1 \frac{\eta^b}{\left(1 + \eta^2 - 2\eta u\right)^c} d\eta. \tag{A1}
\]

One can easily verify that this function satisfies the relation
It turns out to be useful if one first obtains the antiderivative of \( f \) (as a function of \( u \)), which is \( F(c, b, u) = f(c - 1, b - 1, u)/[2(c - 1)] \) and its derivative, \( f'(c, b, u) = 2cf(c + 1, b + 1, u) \), before one starts with the main calculation. Now, choosing \( b = 2a \) and \( c = a \), Eq. (A1) leads to the following expression:

\[
I(a) = 2^{-a} \int_{-1}^{1} \left( 1 + u \right)^{a-1} du + 2a \\
\times \int_{-1}^{1} (1 - u^2)^{a-1} f(a, 2a - 1, 2a - 2, u) du.
\]

The first term on the right-hand side is an easy integration giving \( 2/a \). Consider now the third term on the right-hand side. We can partially integrate this term, and under the condition \( a > 1 \), the boundary term vanishes. This results in

\[
-2a \int_{-1}^{1} \frac{d}{du} \left[ (1 - u^2)^{a-1} u \right] F(a, 2a - 1, u) du \\
= -\frac{a}{a-1} I(a-1) - \frac{a(1-2a)}{a-1} \\
\times \int_{-1}^{1} (1 - u^2)^{a-2} u f(a, 1, 2a, 3, u) du.
\]

Let us now come to the second term on the right-hand side of (A3). Here we partially integrate again. The boundary terms vanish also for \( a > 1 \). As before, we integrate \( f \) and differentiate the rest of the integrand to obtain the following expression:

\[
-(1 - 2a) \int_{-1}^{1} \frac{d}{du} \left[ (1 - u^2)^{a-1} u \right] F(a, 2a, u) du \\
= (1 - 2a) \int_{-1}^{1} (1 - u^2)^{a-2} u f(a, 1, 2a, 3, u). \tag{A4}
\]

Inserting these three results on the right-hand side of Eq. (A3), we obtain

\[
I(a) = \frac{2a}{a} + \frac{(1 - 2a) L(a) - aI(a - 1)}{a-1} \tag{A5}
\]

with

\[
L(a) = \int_{-1}^{1} (1 - u^2)^{a-2} (1 - u) f(a, 1, 2a, 3, u) - \frac{a}{2a} f(a, 1, 2a, 2, u) du.
\]

Now we use the relation (A1) again, but this time inserting \( c = a - 1 \) and \( b = 2a - 1 \), obtaining

\[
(2 - 2a)^2 - 2f(a - 1, 2a - 1, u) \\
= 2(a - 1) f(a - 1, 2a - 3, u) \\
- 2af(a - 1, 2a - 2, u). \tag{A6}
\]

If we multiply (A6) with \( u(1 - u^2)^{a-2} \) and integrate over \( u \) from \(-1\) to 1, we can see that the right-hand side is equal to \( 2L(a) \). After manipulating the left-hand side (partial integration of the second term; in this case we differentiate the function \( f \) and integrate the rest of the integrand), we get

\[
I(a) = -I(a) + (a - 2)/a, \quad \text{Eq. (A6)}
\]

and obtain

\[
I(a) = \frac{1}{(a - 1)^2} - \frac{a(a - 1) + (1 - 2a) I(a)}{a - 1} \\
\rightarrow I(a - 1) - I(a) = \frac{1}{a(a - 1)} \Rightarrow I(a) - I(a + 1) \\
= \frac{1}{a(a + 1)}. \tag{A7}
\]

Notice that for the partial integration steps, we assumed \( a > 1 \) to eliminate the boundary terms. Therefore, this expression only holds for \( a > 1 \). This is the relation we used in the main text of the paper.

**APPENDIX B: SUMMATION OF ALL RING DIAGRAMS**

We now derive the final formula for the correlation energy starting from the expression (17). If we insert in this expression our approximation for \( \epsilon \) and perform the angular \( q \) integrals, we obtain the following:

\[
\delta_{\beta} = \frac{2D}{\pi^2} \int_{-\infty}^{\infty} du R_{\beta 2}^{2a}(u, \xi) \int_{0}^{1} dq \frac{d}{dq^2} \\
\times \sum_{n=2}^{\infty} (-1)^n \left( \frac{4R_{\beta 2}(u, \xi) r_s}{a_D \pi q^{a_D - 1}} \right)^{n-2}. \tag{B1}
\]

In this expression, \( \delta_{\beta} \) regulates the approximation such that the second-order energy contribution is exact, namely,

\[
\delta_{\beta} = \epsilon_{\beta}^{(2)} + \frac{D}{\pi^2} \int_{-\infty}^{\infty} R_{\beta 2}(u, \xi) \frac{d}{du} \int_{0}^{1} dq \frac{d}{dq^2} \\
\times \int_{0}^{1} dq \sum_{n=2}^{\infty} (-1)^n \left( \frac{4R_{\beta 2}(u, \xi) r_s}{a_D \pi q^{a_D - 1}} \right)^{n-2}.
\]

where

\[
\Xi_{1}^{(D)}(q; k_1, k_1) = \frac{1}{4} \sum_{i,j=1}^{2} \int_{A_i} d^{D} p_1 d^{D} p_2 \\
\times \frac{k_{1 i}^{D-1} + k_{1 j}^{D-1}}{x + y} + \frac{2(k_{1 i} k_{1 j})^{D-1}}{x k_{1 i} + y k_{1 j}}.
\]
with \( A_{ij} = |(p_i| < k_j) \cap (|p_i + q| > k_i) \cap (|p_j| < k_j) \cap (|p_j + q| > k_j) \).

To simplify the notation, we define \( \beta_D(u, \xi) \equiv \frac{1}{q_{\alpha-1}} R_{\alpha-1}(u, \xi) \). Substituting this in Eq. (B1), we obtain

\[
\varepsilon_D \approx \delta_D - \frac{2D}{\pi} \int_0^\infty \frac{du}{(\beta_D(u, \xi)r_s)} \left[ \frac{\beta_D(u, \xi)r_s}{2} - \int_0^1 dq q^\alpha \ln \left( 1 + \frac{\beta_D(u, \xi)r_s}{q^{\alpha-1}} \right) \right] \quad (B2)
\]

\[
= \delta_D - \frac{2D}{\pi} \int_0^\infty \frac{du}{(\beta_D(u, \xi)r_s)} \left[ \frac{\beta_D(u, \xi)r_s}{2} - \int_0^1 dy \left( 1 + \frac{\beta_D(u, \xi)r_s}{y} \right) \right]. \quad (B3)
\]

We made the substitution \( y = q^{\alpha-1} \). Furthermore, we define the quantity \( \alpha \equiv 2D/\pi \). Unfortunately, since the latter is not in general an integer, we cannot solve this integral in a closed form. To evaluate it, we must expand the integrand in a Taylor series. To do this, we must separate the integral into two parts, where one part is smaller than and one part greater than \( \beta_D(u, \xi)r_s \). By doing so, one stays in the convergence radius of the corresponding series. Let us consider first the lower part of the interval, namely

\[
\int_0^{\beta_D(u, \xi)r_s} \frac{\alpha y^\alpha}{n} \ln \left( 1 + \frac{\beta_D(u, \xi)r_s}{y} \right) \frac{dy}{y} = \frac{\alpha}{2} \int_0^{\beta_D(u, \xi)r_s} y^{\alpha-1} \ln \left( 1 + \frac{\beta_D(u, \xi)r_s}{y} \right) dy \quad (B4)
\]

The second integral on the right-hand side of this equation can be easily done, yielding \( \frac{\beta_D(u, \xi)r_s}{\alpha + 1} \). The first integral on the right-hand side can be Taylor-expanded. After doing so, we arrive at

\[
\int_0^{\beta_D(u, \xi)r_s} y^{\alpha-1} \ln \left( 1 + \frac{\beta_D(u, \xi)r_s}{y} \right) dy = -\sum_{n=1}^{\infty} \frac{(-1)^n}{n} \int_0^{\beta_D(u, \xi)r_s} y^{\alpha+n} dy
\]

\[
= -\sum_{n=1}^{\infty} \frac{(-1)^n}{n} \frac{[\beta_D(u, \xi)r_s]^{\alpha+n}}{\alpha + n + 1}. \quad (B5)
\]

To perform the upper half of the integration interval, let us define \( \delta_{a,b} \) as the Kronecker delta and a related quantity \( \Delta_{a,b} = 1 - \delta_{a,b} \), which works as the complement of the Kronecker delta. With these definitions, we can expand and eventually calculate the integral

\[
\int_0^1 \frac{\alpha y^\alpha}{n} \ln \left( 1 + \frac{\beta_D(u, \xi)r_s}{y} \right) \frac{dy}{y} = -\frac{\alpha}{2} \sum_{n=1}^{\infty} \frac{[\beta_D(u, \xi)r_s]^n}{n} \int_0^{\beta_D(u, \xi)r_s} y^{\alpha-n} dy \quad (B6)
\]

Let us define \( \Sigma_D \equiv \sum_{n=1}^{\infty} \left( \frac{(-1)^n}{n}\frac{\Delta_{a,n+1}}{(a+1) - n} \right) \) and rewrite the content of the square brackets in Eq. (B3):

\[
\frac{\beta_D(u, \xi)r_s}{2} - \int_0^1 \frac{dy}{D - 1} y^{\frac{1}{\alpha-1}} \ln \left( 1 + \frac{\beta_D(u, \xi)r_s}{y} \right) \quad (B7)
\]

\[
\frac{\beta_D(u, \xi)r_s}{2} + \frac{\alpha}{2} \Sigma_D [\beta_D(u, \xi)r_s]^{a+1} - \frac{\alpha}{2} \sum_{n=1}^{\infty} \frac{[\beta_D(u, \xi)r_s]^n}{n} \ln [\beta_D(u, \xi)r_s] \quad (B8)
\]

Now let us take a closer look at \( \alpha = \frac{2D}{\pi} \). If we restrict our calculations to dimensions greater than 1, we have that \( \alpha \in (0, \infty) \). This means that \( \alpha + 1 \) is never 1, therefore we can drop the \( n = 1 \) term of the second series on the right-hand side of Eq. (B8). In contrast to this, the \( n = 1 \) term of the first series is always there and cancels the first term of the right-hand side in Eq. (B8). That allows us to simplify the above expression, and arrive at

\[
\frac{\beta_D(u, \xi)r_s}{2} - \int_0^1 \frac{dy}{D - 1} y^{\frac{1}{\alpha-1}} \ln \left( 1 + \frac{\beta_D(u, \xi)r_s}{y} \right) \quad (B9)
\]

\[
= \frac{\alpha}{2} \Sigma_D [\beta_D(u, \xi)r_s]^{a+1} + \frac{\alpha}{2} \sum_{n=1}^{\infty} \frac{\Delta_{a,n+1}}{(a + 1) - n} - \frac{\alpha}{2} \sum_{n=1}^{\infty} \frac{[\beta_D(u, \xi)r_s]^n}{n} \ln [\beta_D(u, \xi)r_s]. \quad (B10)
\]

Since we are only interested in terms that do not vanish when \( r_s \) approaches zero, we consider the expression \( \int_0^{\beta_D(u, \xi)r_s} y^{\alpha-1} \) times the equation above. If we now look in the limit of small \( r_s \), we can perform some simplifications: The first term vanishes for small radii if \( \alpha > 1 \), which leads to the step function in the next expression. Furthermore, the parts of the series will all vanish for small radii if and only if \( n > 2 \), which means that the series truncates at \( n = 2 \). Since it started from 2, the series has in this limit only one term, namely \( n = 2 \). Performing all these steps, we get the following closed expression:

\[
\frac{\alpha}{2} \Sigma_D [\beta_D(u, \xi)r_s]^{a+1} \Theta(1 - \alpha)
\]

\[
+ \frac{\alpha \Delta_{a,1}}{4(\alpha - 1)} - \frac{\alpha \Delta_{a,1}}{4} \ln [\beta_D(u, \xi)r_s]
\]

\[
= \frac{\Sigma_D [\beta_D(u, \xi)r_s]^{a+1}}{D - 1} \Theta(D - 3)
\]

\[
- \frac{\Delta_{3,D}}{2(D - 3)} - \frac{\Delta_{3,D}}{4} \ln [\beta_D(u, \xi)r_s]. \quad (B10)
\]
where we have substituted the definition of $\alpha$. The full expression for the correlation energy is then

$$
\varepsilon_{\text{D}}^c \approx \delta_D - \frac{2D\Sigma_D}{\pi^3(D-1)} \left( \frac{\alpha_D\pi}{4r_s} \right)^{\frac{D-1}{2}} \times \int_{-\infty}^{\infty} |R_{\text{D}}(u, \xi)|^{\frac{D-1}{2}} du \theta(D-3)
$$

$$
+ \int_{-\infty}^{\infty} \left[ \frac{D\Delta_3, D}{\pi^3(D-3)} + \frac{D\delta_3, D}{2\pi^3} \ln \left( \frac{4r_s}{\alpha_D\pi} R_{\text{D}}^{-1}(u, \xi) \right) \right] \times |R_{\text{D}}(u, \xi)|^2 du.
$$

(B11)

From this expression, one can learn directly the different behavior for $D < 3$, $D = 3$, and $D > 3$.


