Homogeneous electron gas in arbitrary dimensions beyond the random phase approximation

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The ground state of the homogeneous electron gas is a cornerstone in quantum physics and chemistry. It is an archetypal system in the regime of slowly varying densities in which the exchange-correlation energy can be estimated with a myriad of methods. For high densities, the behavior of the energy is well-known for 1, 2, and 3 dimensions. Here, we extend this model to arbitrary integer dimensions, and compute its correlation energy beyond the random phase approximation (RPA), using the celebrated approach developed by Singwi, Tosi, Land, and Sjölander (STLS), which is known to be remarkably accurate in the description of the full electronic density response. For two and three dimensions, both in the paramagnetic and ferromagnetic ground states, STLS is capable of producing correlation energies in close agreement with Monte-Carlo values. For higher dimensions, we compare the results obtained for the correlation energy using the STLS method with the values previously obtained using RPA. We furthermore illustrate the importance of the plasmon contribution to STLS theory.

I. INTRODUCTION

The ground state of the homogeneous electron gas (HEG) has played a prominent role in the modelling and understanding of a wide range of interacting electronic systems [1]–[12]. It is one of the models of choice to develop, improve and benchmark many approximate approaches to the full many-electron problem, including some of the most popular exchange-correlation functionals of density functional theory (DFT) [13–16].

An important question about this model is the dependency of the correlation energy, and other physical quantities, on $D$, the dimension of the physical space in which the gas is embedded. Indeed, there is a wealth of experimental electronic setups in which one or two of the physical dimensions are much smaller than the remaining ones. They can thus be modeled as one- or two-dimensional quantum systems [17]–[20]. Furthermore, reduced dimensional systems often exhibit notable physical properties, ranging from Luttinger physics [21] to Moiré superlattices [22]. More recently, progress in the fabrication of artificial materials is paving the way for the realization of non-integer or synthetic dimensions, as fractal substrates (e.g., Sierpinski carpets of bulk Cu) confining electron gases [23]–[25] or synthetic materials that circumvent the von Neumann–Wigner theorem [26]–[27].

For the high-density spin-unpolarized HEG in $D = 1, 2, 3$, the energy per electron can be expanded in terms of $r_s$, the Wigner-Seitz radius, as follows [28]:

$$\epsilon_D(r_s \to 0) = a_D \frac{r_s^2}{r_s^D} - b_D \frac{r_s}{r_s^D} + c_D \ln r_s + O(r_s^D).$$  (1)

The constants $a_D$, $b_D$ and $c_D$ are independent of $r_s$, and their functional form in terms of the dimension $D$ is well known [8]. Quite remarkably, the logarithm that appears in Eq. (1) for the 3D case is due to the long range of the Coulomb repulsion, and cannot be obtained from standard second-order perturbation theory [29]. In a recent work [30], the HEG was extended to arbitrary integer dimensions. It was found a very different behavior for $D > 3$: the leading term of the correlation energy does not depend on the logarithm of $r_s$ [as in Eq. (1)], but instead scales polynomially as $c_D/r_s^{3-D}$, with the exponent $\gamma_D = (D - 3)/(D - 1)$. In the large-$D$ limit, the value of $c_D$ was found to depend linearly with the dimension. This result was originally obtained within the random-phase approximation (RPA) by summing all the ring diagrams to infinite order.

While RPA is known to be exact in the limit of the dense gas, includes long-range interactions automatically, and is applicable to systems where finite-order many-body perturbation theories break down [31], it has well-known deficiencies at metallic (intermediate) and low densities. Quantum Monte-Carlo (QMC) is an option for those regimes [12]–[32], but there are other high-quality approaches such as the celebrated Singwi, Tosi, Land, and Sjölander (STLS) method that provides results comparable to QMC [33]. This scheme is often surprisingly accurate in the description of the full electronic density response, and as such it is commonly used to investigate quasi-one-dimensional [34] and warm dense electron gases [35]–[38]. It has also inspired the development of new functional methods that explicitly retain the dynamical and non-local nature of electronic correlations, while properly accounting the exchange contribution [37]–[40].

The purpose of this paper is to calculate the correlation energy of the HEG for arbitrary integer dimensions (in particular for $D > 3$) with the STLS method. As expected, the value of this portion of the energy improves

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significant with respect to the RPA result (that tends to overcorrelate the gas). The remainder of this paper is organized as follows. In Section II we review the main STLS equations and rewrite them explicitly in arbitrary $D$ dimensions. As a result, we are able to compute the Lindhard polarizability, the structure factor as well as the so-called local field correction in the Hartree-Fock approximation, and provide explicit formulae for some representative systems. In Section III we explain how the correlation energy is computed in this scheme, and discuss the fully polarized case. In Sections V and VI we present and discuss our numerical results and our conclusions. Two Appendices that give further technical details on our calculations are presented at the end of the text.

II. STLS THEORY IN $D$ DIMENSIONS

In this section we review the main STLS equations and write them explicitly in arbitrary $D$ dimensions. We follow the standard notation, namely, $n$ is the $D$-dimensional particle density, $\Omega$ the volume occupied by the electronic gas, and $q_F$ the usual Fermi wavelength. The STLS theory departs from RPA (to include short-range correlation between electrons) by writing the two-particle density distribution $f_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}', t)$ as follows:

$$f_2(\mathbf{r}, \mathbf{p}, \mathbf{r}', \mathbf{p}', t) = f(\mathbf{r}, \mathbf{p}, t)f(\mathbf{r}', \mathbf{p}', t)g(\mathbf{r}-\mathbf{r}') , \quad (2)$$

where $f(\mathbf{r}, \mathbf{p}, t)$ is the one-particle phase-space density and $g(\mathbf{r})$ is the equilibrium, static pair distribution function. Eq. (2) can be seen as an ansatz that terminates the hierarchy that otherwise would write the two-particle distribution function in terms of the three-particle distribution function, and so on. This leads to the following density-density response function [33]:

$$\chi_D(q, \omega) = \frac{\chi_D^0(q, \omega)}{1 - \Phi(q)[1-G_D(q)]\chi_D^0(q, \omega)} . \quad (3)$$

Here $\chi_D^0(q, \omega)$ is the Lindhard polarizability, i.e., the inhomogeneous non-interacting density response function of an ideal Fermi gas in $D$ dimensions, $G_D(q)$ is the local field correction, and $\Phi(q)$ is the $D$-dimensional Fourier transform of the Coulomb potential:

$$\Phi(q) = \frac{(4\pi)^{D-1}}{q^{D-1}} \frac{\Gamma\left(\frac{D-1}{2}\right)}{q^{D-1}} , \quad (4)$$

where $\Gamma$ denotes the gamma function. The presence of $G_D(q)$ in Eq. (3) is the key feature of the STLS equations that gives the “beyond RPA” flavor to the theory. This local field correction is a direct result of the short-range correlation between the electrons. In arbitrary dimensions, it is given by:

$$G_D(q) = -\frac{1}{n} \int q' \cdot \frac{q^{D-3}}{q'^{D-1}} \left[S_D(q-q') - 1\right] \frac{q'D}{(2\pi)^D} , \quad (5)$$

with $S_D(q)$ being the structure factor. We can simplify this integral to a two-dimensional one by substituting $q-q'=t$ and using the fact that $S_D(q)=S_D(q)$ in homogeneous systems. Afterwards, we rewrite the integral using $D$-dimensional spherical coordinates, where $q$ is parallel to the $D^{th}$-axis, and integrate over all angles except the angle $\theta$ between $q$ and $t$ to obtain:

$$G_D(q) = -\frac{q^{D-3}}{(2\pi)^D} 2\pi \frac{2\pi^{D-1}}{\Gamma\left(\frac{D-1}{2}\right)} \int_0^{\pi} \int_0^\infty \left|S_D(t) - 1\right| \left|\frac{q^{D-1}}{q'^{D-1}} - \frac{qt\cos \theta}{t^{D-2}}\right| \frac{d\theta dt}{(q^2 + t^2 - 2qt\cos \theta)^{D-1}} . \quad (6)$$

Note in passing that in the 2D case we must use polar coordinates instead of the spherical coordinates and obtain:

$$G_2(q) = -\frac{1}{(2\pi)^2} \int_0^{\pi} \int_0^{2\pi} \left|S_2(t) - 1\right| \frac{q t \cos \theta}{(q^2 + t^2 - 2qt\cos \theta)^{1/2}} d\theta dt . \quad (7)$$

These equations, together with the equation for the dielectric function, $1/\epsilon_D(q, \omega) = 1 + \Phi(q)\chi_D(q, \omega)$, lead to an equation for the dielectric function within the STLS theory, namely:

$$\epsilon_D(q, \omega) = 1 - \frac{\Phi(q)\chi_D^{0}(q, \omega)}{1 + G_D(q)\Phi(q)\chi_D^{0}(q, \omega)} . \quad (8)$$

Finally, the relation between the structure factor and the dielectric function $\epsilon_D(q, \omega)$ (see, for instance, [41]) can be easily generalized for arbitrary dimensions:

$$S_D(q) = -\frac{1}{\pi n \Phi(q)} \int_0^{\infty} \text{Im}\left(\frac{1}{\epsilon_D(q, \omega)}\right) d\omega . \quad (9)$$

We can improve the readability of this equation by separating the contributions of the single-particle and plasmon excitations [42]:

$$S_D(q) = -\frac{1}{\pi n \Phi(q)} \int_{v_F}^{\infty} \frac{2}{\pi} \frac{\text{Im}\left(\frac{1}{\epsilon_D(q, \omega)}\right)}{\omega} d\omega + \frac{1}{\Phi(q)n} \frac{\partial \text{Re}\epsilon_D(q, \omega)}{\partial \omega} \left(\delta(\omega - \omega_p(q))\right) . \quad (10)$$

where $v_F$ is the Fermi velocity and $\omega_p(q)$ is the plasmon dispersion [43]. Equation 10, Eq. 6 and Eq. 8 form the core of the STLS set of equations. In this framework, they can be evaluated self-consistently. Notice, indeed, that $G_D(q)$ and $S_D(q)$ can be written symbolically as $G_D = F_1[S_D]$ and $S_D = F_2[G_D]$, indicating the existence of the mutual functional relations introduced above [40].

A. Real part of the Lindhard function for $D = 5, 7$

The expressions for $\chi_2^{0}(q, \omega)$ and $\chi_3^{0}(q, \omega)$ are widely known since long ago (see for instance [28]), but higher
The real part of $\chi^0_D(q, \omega)$ can be written explicitly as:

$$\text{Re} \chi^0_D(q, \omega) = \frac{2}{(2\pi)^D} \mathcal{P} \int \frac{\Theta(q_F - |p - \frac{1}{2}q|)\Theta(|p + \frac{1}{2}q| - q_F)}{\omega - p \cdot q} d^Dp$$

$$- \frac{2}{(2\pi)^D} \mathcal{P} \int \frac{\Theta(|p - \frac{1}{2}q| - q_F)\Theta(q_F - |p + \frac{1}{2}q|)}{\omega - p \cdot q} d^Dp,$$

where $\mathcal{P}$ denotes the principal value. By evaluating these integrals, it is possible to obtain analytical expressions for specific cases. For instance, for $D = 5$ and $D = 7$ one gets:

$$\text{Re} \chi^0_D(q, \omega) = \frac{q_F^3}{8\pi^4} \left\{ \frac{1}{96q^5} \left[ \left( \frac{3}{2} \left( \frac{q^2}{2} - 2\tilde{\omega} \right)^4 + 24q^4 - 12q^2 \left( \frac{q^2}{2} - 2\tilde{\omega} \right)^2 \right) \ln \left| \frac{2\tilde{q} - \tilde{q}^2 + 2\tilde{\omega}}{2\tilde{q} + \tilde{q}^2 - 2\tilde{\omega}} \right| 
+ \left( \frac{3}{2} \left( \frac{q^2}{2} + 2\tilde{\omega} \right)^4 + 24q^4 - 12q^2 \left( \frac{q^2}{2} + 2\tilde{\omega} \right)^2 \right) \ln \left| \frac{2\tilde{q} - \tilde{q}^2 - 2\tilde{\omega}}{2\tilde{q} + \tilde{q}^2 + 2\tilde{\omega}} \right| + 12q^2 - 16q^2 + 144q^4 \tilde{\omega}^2 \right] \right\}$$

and

$$\text{Re} \chi^0_D(q, \omega) = \frac{q_F^5}{368640\pi^4q^3} \left\{ \left[ 60(16q^4 + 3(\tilde{q}^2 + 2\tilde{\omega})^4 - 12(\tilde{q}^3 + 2\tilde{q}\tilde{\omega})^2) - \frac{15(\tilde{q}^2 + 2\tilde{\omega})^6}{q^2} \right] \ln \left| \frac{2\tilde{q} - \tilde{q}^2 + 2\tilde{\omega}}{2\tilde{q} + \tilde{q}^2 - 2\tilde{\omega}} \right| 
+ \left[ 60(16q^4 + 3(\tilde{q}^2 - 2\tilde{\omega})^4 - 12(\tilde{q}^3 - 2\tilde{q}\tilde{\omega})^2) - \frac{15(\tilde{q}^2 - 2\tilde{\omega})^6}{q^2} \right] \ln \left| \frac{2\tilde{q} - \tilde{q}^2 + 2\tilde{\omega}}{2\tilde{q} + \tilde{q}^2 - 2\tilde{\omega}} \right| 
- 120q^5 + 1280q^3(\tilde{q}^4 + 12\tilde{\omega}^2) - 120q(\tilde{q}^8 + 40q^4\tilde{\omega}^2 + 80q^2) \right\}.$$ 

A similar calculation gives a closed expression for the imaginary part:

$$\text{Im} \chi^0_D(q, \omega) = \begin{cases} 
\frac{h(D)}{q} \left[ (1 - \nu_2^2) D^{-1} - (1 - \nu_1^2) D^{-1} \right] & \text{if } \tilde{\omega} < \tilde{q} \frac{q^2}{2} 	ext{ and } \tilde{q} < 2 \\
0 & \text{if } \tilde{\omega} < \tilde{q} \frac{q^2}{2} \text{ and } \tilde{q} > 2 \\
\frac{h(D)}{q} \left[ 1 - \nu_2^2 \right] D^{-1} & \text{if } \tilde{q} \frac{q^2}{2} \leq \tilde{\omega} \leq \tilde{q} \frac{q^2}{2} \\
0 & \text{if } \tilde{\omega} > \tilde{q} \frac{q^2}{2} 
\end{cases}$$  

where $\tilde{q} = q/q_F$, $\tilde{\omega} = \omega/q_F^2$, $h(D) = q_F^{D-2} \left[ 2^{D-2}(D-1)\pi \frac{D-1}{2} \Gamma \left( \frac{D-1}{2} \right) \right]^{-1}$ and $\nu_\pm = \tilde{\omega}/\tilde{q} \pm 1/2$.

B. The Hartree-Fock approximation for the first iteration

For the first iteration, the original STLS theory uses the structure factor obtained from the Hartree-Fock calculation. We take the same approach here. Formally, the generalized $D$-dimensional structure factor is straightforward and reads:

$$S^{HF}_D(q) = 1 - \frac{2}{(2\pi)^D} \int_{k, k' \leq q_F} \delta(q - k' + k) d^Dk'd^Dk.$$
s. This eventually gives the relevant integration region as the intersection of two hyperspheres, as discussed in detail in Appendix B where we obtain the following expression:

\[ G_{D}^{\text{HF}}(q) = \frac{q^{D-3}}{q_{F}^{\sqrt{D} \pi}} \left( \frac{D}{2} + 1 \right) \int_{0}^{\pi} \int_{0}^{\pi} I_{s} I_{b} \left( D + 1, \frac{1}{2} \right) \times \left( q^{2} + q \cos \theta \right)^{D-1} \sin^{D-2} \theta \left( q^{2} + q^{2} + 2q \cos \theta \right)^{D-2} d\theta dt, \]  

with \( I_{s}(a, b) \) denoting the regularized incomplete beta function. The numerical evaluation of the local field correction as expressed in Eq. (16) is now a much simpler task. In fact, we present the lengthy analytical expression for \( G_{D}^{\text{HF}}(q) \) in Appendix B.

### III. ENERGY CONTRIBUTIONS

The calculation of the kinetic energy of the \( D \)-dimensional HEG is as straightforward as it is for \( D = 3 \). It is given by:

\[ E_{\text{kin}} = \frac{\sigma_{D}^{2}}{2(D + 2)} \frac{\Upsilon_{2}(\xi)}{r_{s}^{2}}, \]  

where \( \sigma_{D} = 2^{(D-1)/D} \Gamma(D/2 + 1)2^{D}/2 \).

\[ \Upsilon_{n}(\xi) = \frac{1}{2} \left[ (1 + \xi)^{D+n}/D + (1 - \xi)^{D+n}/D \right] \]

is the spin-scaling function, and \( \xi \) is the usual spin-polarization. The interaction energy per particle is given by the following expression:

\[ E_{\text{int}} = \frac{1}{\Omega} \sum_{q \neq 0} \Phi(q) \frac{1}{2} \left( S(q) - 1 \right) \]  

If we introduce the function \( \gamma(r_{s}) = -\frac{4}{q_{F}^{\sqrt{D} \pi}} \int_{0}^{\infty} |S(q) - 1| dq \) we can rewrite the energy of the unpolarized electron gas in Eq. (18) as:

\[ E_{\text{int}} = -\frac{2^{D-3}}{\sqrt{\pi}} \frac{D^{2} \Gamma(2 - 1/2)}{\Gamma(D/2)} \frac{D^{2-D} \gamma(r_{s})}{r_{s}}. \]

By using the adiabatic-connection formula, the total interaction energy per particle can be computed by using the formula \( \int_{0}^{\lambda} \alpha \E_{\text{int}}(\lambda r_{s}) \, d\lambda \), where \( \lambda \) is a coupling constant that represents the strength of the interaction. Therefore, the full ground-state energy of the unpolarized electron gas in the STLS theory can then be written as:

\[ E_{0} = \frac{\sigma_{D}^{2}}{2(D + 2)} \frac{\Upsilon_{2}(0)}{r_{s}^{2}} - E(D) \frac{1}{r_{s}^{2}} \int_{0}^{r_{s}} \gamma(r_{s}')dr_{s}', \]  

where \( E(D) \) is defined as:

\[ E(D) = \frac{2^{D-3}}{\sqrt{\pi}} \frac{D^{2} \Gamma(2 - 1/2)}{\Gamma(D/2)} \frac{D^{2-D}}{\pi} \Gamma(D/2). \]

To obtain the correlation energy we need to make use of the Hartree-Fock energy. While the kinetic energy is already calculated, the calculation of the exchange energy is not trivial. This was already calculated by two of us in Ref. [30]:

\[ E_{HF} = \frac{\alpha_{D}^{2}}{2(D + 2)} \frac{\Upsilon_{2}(\xi)}{r_{s}^{2}} - \frac{2\alpha_{D}^{2} r_{s}}{\pi(D^{2}-1) r_{s}}. \]

Since the correlation energy is defined as the difference between the ground-state energy and the ground-state Hartree-Fock energy, we get for the \( D \)-dimensional gas the following compact formula:

\[ E_{\text{corr}} = \frac{1}{r_{s}^{2}} \int_{0}^{r_{s}} \left[ -E(D) \gamma(r_{s}') + \frac{2\alpha_{D}^{2} \Upsilon_{1}(0)}{\pi(D^{2}-1)} \right] dr_{s}'. \]

This is the formula we are going to use for the calculation of the correlation energy.

### IV. THE FULLY POLARIZED CASE

The extension of the above equations for the fully polarized case is quite straightforward (for \( D = 3 \) see [45, 46]). The relation between the local field correction and the structure factor is given by:

\[ G_{D}^{\uparrow \uparrow}(q) = -\frac{1}{n} \int \frac{(q' \cdot q)p^{D-3}}{q^{D-1}} \left[ S_{D}^{\uparrow \uparrow}(q - q') - 1 \right] \frac{d^{D} q'}{(2\pi)^{D}}. \]

where \( S_{D}^{\uparrow \uparrow}(q - q') \) is the spin-resolved structure factor. The corresponding density-density response function is given by:

\[ \chi_{D}^{\uparrow \uparrow}(q, \omega) = \frac{\chi_{D}^{\uparrow \uparrow}(q, \omega)}{1 - \Phi(q)[1 - G_{D}^{\uparrow \uparrow}(q)]\chi_{D}^{0 \uparrow \uparrow}(q, \omega)}. \]

where \( \chi_{D}^{0 \uparrow \uparrow}(q, \omega) \) is the polarizability of the fully polarized non-interacting HEG that can be easily related with the spinless quantities \( \chi_{D}^{0 \uparrow \uparrow}(q, \omega) \) by a factor of \( 1/2 \) [28]. In addition, the Fermi wavelength should be re-scaled \( q_{F}^{\uparrow \uparrow} = 2^{1/D} q_{F} \). Finally, the fluctuation-dissipation theorem leads to:

\[ S_{D}^{\uparrow \uparrow}(q) = -\frac{1}{\pi n} \int_{0}^{\infty} \text{Im} \chi_{D}^{\uparrow \uparrow}(q, \omega) d\omega. \]

As a result, in the fully polarized case, the correlation energy is given by:

\[ E_{\text{corr}} = \frac{1}{r_{s}^{2}} \int_{0}^{r_{s}} \left[ -F(D) \gamma(r_{s}') + \frac{2\alpha_{D}^{2} \Upsilon_{1}(0)}{\pi(D^{2}-1)} \right] dr_{s}'. \]

where \( F(D) \) is a simple re-scaling of \( E(D) \) in Eq. (20):

\[ F(D) = 2^{1/D} E(D). \]
Starting from the expression for the local field correction in the Hartree-Fock approximation $G_{HF}^D(q)$ presented in section II B, we calculated $S_D(q)$ using Eq. (10). In this case $\omega(p)$ is obtained from the zero of the dielectric function $\epsilon(q, \omega)$, which in turn is given by Eq. (8). We then started the entire self-consistent cycle of the STLS equations. To improve the convergence of the iterative procedure we applied the following linear mixing:

$$\bar{G}_D^i(q) = G_D^i(q) - G_D^{i-1}(q) + \left( G_D^i(q) - G_D^{i-1}(q) \right) / a, \quad (28)$$

where $i$ is the iteration number and $a$ takes values between 1 and 3.5 (for the 5D and the 7D cases we used $a = 1.5$). At each iteration we calculated the quantity $\gamma(r_s)$ with the new structure factor $S_D(q)$. After 10 iterations we obtained convergence in $\gamma(r_s)$ within 0.1%. The value of $\gamma(r_s)$ at the end of the self-consistent calculation is then used to calculate the correlation energy using Eq. (22).

We first benchmarked our implementation for 2D and 3D. The results are presented in Fig. 1, where it can be seen that we recovered the original STLS results and obtained the celebrated agreement of STLS with the Quantum Monte-Carlo results [48, 49]. In the 2D case we also obtained similar results to the ones obtained previously by Jonson [47]. The decrease of the magnitude of the correlation energy in the paramagnetic case is consistent with the Quantum Monte-Carlo results [12].

Our new results for the HEG in 5D and 7D (for which we were able to compute analytically the Lindhard polarizability and the local field correction) in the paramagnetic and the ferromagnetic case are presented in Fig. 2a, 2b, 3a and 3b respectively. Those are compared with the RPA results previously obtained in Ref. [30]. It is a general result of our implementation that the STLS correlation energy decreases (in absolute value) in comparison with the one from RPA, which confirms that this latter approximation tends to over-correlate the gas, even in dimensions higher than 3. Yet, for high dimensions the general error of RPA is smaller, both in the ferromagnetic and the paramagnetic cases. The correlation energy is smaller in magnitude in the ferromagnetic case in comparison with the paramagnetic one in all the dimensions studied, the same behaviour found with the RPA. Furthermore, since the structure factor of STLS can be easily separated into the pair and the plasmonic contributions [41, 43], we investigated the plasmon contribution separately by calculating the correlation energy with and without it. We conclude that the plasmonic correction is more relevant for intermediate densities at all dimen-

V. NUMERICAL RESULTS

We corrected a small error in the numerical evaluation of the coefficients presented in Table I of Ref. [30] that however does not affect the main conclusions of that paper.
FIG. 3: Correlation energy of the fully polarized HEG in 5D and 7D expressed as a function of $r_s$. Our results for STLS are compared with the RPA results from Ref. [30].

For the sake of completeness we also present in Fig. 4 the values for the local field correction $G(q)$ we obtained for both paramagnetic and ferromagnetic gases for $D = 3, 5$, for a selected value of the density (i.e., $r_s = 2$). While the magnitude of the local correction is larger for the fully polarized gas, the global value diminishes for large dimensions in the whole domain of $q$.

VI. CONCLUSION AND OUTLOOK

In this paper we have extended the celebrated Singwi, Tosi, Land, and Sjölander (STLS) scheme for homogeneous electron gases (HEG) —whose accuracy to compute the full electronic density response is comparable to Quantum Monte-Carlo— to arbitrary integer dimensions. Our main motivation was to study the quality of the random phase approximation (RPA) results for the HEG in arbitrary integer dimensions. To that goal, we have provided new analytical formulae for the real and imaginary parts of the Lindhard polarizability and for the so-called local field correction of the STLS theory, that improves the RPA in the density-density response. From our results we can conclude that the algebraic properties of the correlation energy found in Ref. [30] are mainly valid in the high-density limit. Furthermore, in agreement with what is known in 2 and 3 dimensions, the RPA tends to over-correlate the gas also in the high dimensions studied here. We have shown the versatility of STLS to tackle arbitrary dimensions, which can potentially shed light into the more far-reaching problems of quantum many-body systems embedded in fractional or synthetic dimensions [23, 25, 50–52]. We believe the results of this paper can be an useful framework to improve our overall comprehension of Coulomb gases, and to develop a more coherent and unified dimensional approach to the correlation problem of those systems [20, 53–55].

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Appendix A: Calculation of the Lindhard polarizability in $D \geq 3$

To compute the Lindhard polarizability for dimensions larger than 3 we start by writing the one-particle density and the external potential as linear perturbations from equilibrium:

$$f(r, p, t) = f_0(p) + \lambda \delta f(r, p, t),$$
$$v(r, t) = v_0(r) + \lambda \delta v(r, t).$$ \hspace{1cm} (A1)

After substituting Eq. (A1) in Eq. 2 one obtains the following result for the induced charge density $\rho_{\text{ind}}(q, \omega)$:

$$\rho_{\text{ind}}(q, \omega) = \frac{\chi_0^D(q, \omega)}{1 - Q(q)[1 - \delta_D(q)]} \chi_0(q, \omega) \delta v(q, \omega),$$ \hspace{1cm} (A2)

where $\chi_0^D(q, \omega)$ is given by:

$$\chi_0^D(q, \omega) = -\lim_{\eta \to 0^+} \int \frac{q \cdot \nabla_p f_0(p)}{\omega + i\eta - p \cdot q} d^Dp.$$ \hspace{1cm} (A3)

By using the Taylor expansion: $f_0(p \pm \frac{1}{2}q) = f_0(p) \pm \frac{1}{2}q \cdot \nabla_p f_0(p) + \cdots$, we can then rewrite $\chi_0^D(q, \omega)$ as:

$$\chi_0^D(q, \omega) \approx \lim_{\eta \to 0^+} \int \frac{f_0(p - \frac{1}{2}q) - f_0(p + \frac{1}{2}q)}{\omega + i\eta - p \cdot q} d^Dp.$$ \hspace{1cm} (A4)

This is the Lindhard polarizability of a $D$-dimensional Fermi gas [56].

At $T = 0$ the equilibrium density reads

$$f_0(p \pm \frac{1}{2}q) = \frac{2}{(2\pi)^D} \Theta \left[ \frac{1}{2} \left(q_F^2 - |p \pm \frac{1}{2}q|^2 \right) \right] = \frac{2}{(2\pi)^D} \Theta(qF - |p \pm \frac{1}{2}q|).$$ \hspace{1cm} (A5)

Plugging these equations and the identity $\lim_{\eta \to 0^+} \int_{x-x_0}^{x-x_0} = \mathcal{P}\frac{1}{x-x_0} + i\pi \delta(x-x_0)$ into Eq. (A4) yields:

$$\chi_0^D(q, \omega) = \frac{2}{(2\pi)^D} \int \frac{\Theta(qF - |p - \frac{1}{2}q|) - \Theta(qF - |p + \frac{1}{2}q|)}{\omega - p \cdot q} d^Dp$$
$$- i\frac{2\pi}{(2\pi)^D} \int \left[ \Theta(qF - |p - \frac{1}{2}q|) - \Theta(qF - |p + \frac{1}{2}q|) \right] \delta(\omega - p \cdot q) d^Dp.$$ \hspace{1cm} (A6)

The real part of $\chi_0^D(q, \omega)$ can then be rewritten as:

$$\text{Re} \chi_0^D(q, \omega) = \frac{2}{(2\pi)^D} \int \frac{\Theta(qF - |p - \frac{1}{2}q|)\Theta(|p + \frac{1}{2}q|) - qF)}{\omega - p \cdot q} d^Dp$$
$$- \frac{2}{(2\pi)^D} \int \frac{\Theta(|p + \frac{1}{2}q|)}{\omega - p \cdot q} d^Dp.$$ \hspace{1cm} (A7)

The second integral can be rewritten with the substitution $p \to -p$ so that the expression of $\text{Re} \chi_0^D(q, \omega)$ reduces to just one single integral:

$$\text{Re} \chi_0^D(q, \omega) = \frac{2}{(2\pi)^D} \int \Theta(qF - |p - \frac{1}{2}q|)\Theta(|p + \frac{1}{2}q|) \left( \frac{1}{\omega - p \cdot q} - \frac{1}{\omega + p \cdot q} \right) d^Dp.$$ \hspace{1cm} (A8)

Utilizing the following property of the Heaviside step function: $\Theta(x) = 1 - \Theta(-x)$ and the symmetry of the integrand under the transformation $p \to -p$, $\text{Re} \chi_0^D(q, \omega)$ can be further simplified to:

$$\text{Re} \chi_0^D(q, \omega) = \frac{2}{(2\pi)^D} \int \Theta(qF - |p - \frac{1}{2}q|) \left( \frac{1}{\omega - p \cdot q} - \frac{1}{\omega + p \cdot q} \right) d^Dp.$$ \hspace{1cm} (A9)

This integral becomes dimensionless by putting $p - \frac{q}{2} = \tilde{k}$ and introducing the following substitutions $\tilde{q} = q/q_F$, $\tilde{k} = k/q_F$ and $\tilde{\omega} = \omega/q_F^2$:

$$\text{Re} \chi_0^D(q, \omega) = \frac{2q_F^{D-2}}{(2\pi)^D} \int \Theta(1 - \frac{1}{\tilde{k}}) \left( \frac{1}{\tilde{\omega} - \tilde{q} \cdot \tilde{k} - \frac{q^2}{2}} - \frac{1}{\tilde{\omega} + \tilde{q} \cdot \tilde{k} + \frac{q^2}{2}} \right) d^D\tilde{k}.$$ \hspace{1cm} (A10)
To solve this integral we choose $D$-dimensional spherical coordinates such that $\tilde{q}$ is parallel to the last axis:

\[
\text{Re} \chi^0_D(q, \omega) = \frac{q_F^{D-2}}{(2\pi)^{D-1}} \frac{2\pi^{D-1}}{\Gamma(D/2-1)} \int_0^1 \int_0^\pi \left( \frac{\tilde{k}^{D-1} \sin^{D-2} \theta}{\tilde{\omega} - \tilde{q} \cos \theta - \frac{\tilde{q}^2}{2}} - \frac{\tilde{k}^{D-1} \sin^{D-2} \theta}{\tilde{\omega} + \tilde{q} \cos \theta + \frac{\tilde{q}^2}{2}} \right) d\theta dk,
\]

where $\theta$ is the angle between $\tilde{q}$ and $\tilde{k}$. The full evaluation of this integral is quite involved. We just mention that this gives the known result for $D = 3$:

\[
\text{Re} \chi^0_3(q, \omega) = \frac{q_F^2}{2\pi^2} \left\{ -1 + \frac{1}{2\tilde{q}} \left[ 1 - \left( \frac{2\tilde{\omega} - \tilde{q}^2}{2\tilde{q}} \right)^2 \right] \ln \left| \frac{2\tilde{q} - \tilde{q}^2 + 2\tilde{\omega}}{2\tilde{q} + \tilde{q}^2 - 2\tilde{\omega}} \right| \right\}.
\]

A12

We provide the explicit results for $D = 5$ in [12] and $D = 7$ in [13].

The imaginary part of the Lindhard polarizability can be computed by using the same substitutions as in the calculation of $\text{Re} \chi^0_D(q, \omega)$:

\[
\text{Im} \chi^0_D(q, \omega) = -\frac{q_F^{D-2}}{(2\pi)^{D-1}} \int [\Theta(1 - \tilde{k}) - \Theta(1 - |\tilde{q} + \tilde{k}|)] \delta \left( \tilde{\omega} - \tilde{q} + \tilde{k} - \frac{\tilde{q}^2}{2} \right) d^D\tilde{k}.
\]

A13

Next we want to investigate the symmetry of $\text{Im} \chi^0_D(q, \omega)$. By considering $\text{Im} \chi^0_D(-q, -\omega)$ and substituting $\tilde{k}' = \tilde{k} - \tilde{q}$ we realize that $\text{Im} \chi^0_D(q, \omega) = -\text{Im} \chi^0_D(-q, -\omega)$. This symmetry allows us to restrict ourselves to case where $\omega > 0$. $\text{Im} \chi^0_D(q, \omega)$ can then be rewritten for positive $\omega$ as follows:

\[
\text{Im} \chi^0_D(q, \omega) = -\frac{q_F^{D-2}}{(2\pi)^{D-1}} \int \Theta(1 - \tilde{k}) \Theta(|\tilde{q} + \tilde{k}| - 1) \delta \left( \tilde{\omega} - \tilde{q} + \tilde{k} - \frac{\tilde{q}^2}{2} \right) d^D\tilde{k}.
\]

A14

There are 2 cases where the integrand is different from 0:

- $\left| \tilde{q} - \frac{\tilde{q}^2}{2} \right| \leq \tilde{\omega} \leq \tilde{q} + \frac{\tilde{q}^2}{2}$
- $\tilde{\omega} < \tilde{q} - \frac{\tilde{q}^2}{2}$, $\tilde{q} < 2$

The evaluation of both integrals is technically similar. Thus we just want to discuss the evaluation in the first case. The minimum value of $\tilde{k}$ in the first case is $\tilde{k}_{\text{min}} = \left| \tilde{\omega}/\tilde{q} - \tilde{q}/2 \right|$. Performing the integration over all angles except the angle $\theta$ between $\tilde{q}$ and $\tilde{k}$ and substituting $\cos \theta = t$ leads to:

\[
\text{Im} \chi^0_D(q, \omega) = -\frac{q_F^{D-2}}{(2\pi)^{D-1}} \frac{2\pi^{D-1}}{\Gamma(D/2-1)} \int_0^1 \int_0^1 \delta \left( \tilde{\omega} - \tilde{q} + \tilde{k} - \frac{\tilde{q}^2}{2} \right) \tilde{k}^{D-2}(1 - t^2)^{D-3} dtdk.
\]

A15

To evaluate it we should put $\tilde{\omega} = \tilde{q}^2/2 + \tilde{q} \tilde{k} \cos \theta \Rightarrow -1 \leq \tilde{\omega}/\tilde{q} - \tilde{q}/2 \tilde{k} \leq 1$, so that the integral over $t$ can be carried out easily. We obtain in this case the following result:

\[
\text{Im} \chi^0_D(q, \omega) = h(D) \frac{1}{q} \left[ 1 - \nu^2 \right]^{D-1}_2,
\]

A16

where we define $h(D) = q_F^{D-2} \left[ 2^{D-2}(D-1)\pi \frac{D-1}{2} \Gamma \left( \frac{D-1}{2} \right) \right]^{-1}$ and $\nu_\pm = \tilde{\omega}/\tilde{q} \pm \tilde{q}/2$.

In the second case, $\tilde{k}_{\text{min}} = \sqrt{1 - 2\tilde{\omega}}$ and we obtain the following result:

\[
\text{Im} \chi^0_D(q, \omega) = h(D) \frac{1}{q} \left[ (1 - \nu^2) \frac{D-1}{2} - (1 - \nu^2) \frac{D-1}{2} \right].
\]

A17

Eventually $\text{Im} \chi^0_D(q, \omega)$ reads as in Eq. (14).
Appendix B: The local field correction in the Hartree-Fock approximation

After the substitution \( s = (k + k')/2 \) and \( t = k - k' \) Eq. (15) becomes:

\[
G_{D}^{\text{HF}}(q) = \frac{2q^{D-3}}{(2\pi)^{2D/2}} \int_{|s| \leq q_{F}} ds \int_{|s+\frac{1}{2}| \leq q_{F}} \int_{|s-\frac{1}{2}| \leq q_{F}} \frac{q \cdot (q + t)}{|q + t|^{D-1}} dt ds. \tag{B1}
\]

Because the integrand only depends on \( q \) and \( t \), we can perform the integration over \( s \). This gives us the volume of the integration region and the integral becomes:

\[
G_{D}^{\text{HF}}(q) = \frac{2q^{D-3}}{(2\pi)^{2D/2}} \int dt \frac{q \cdot (q + t)}{|q + t|^{D-1}} \int ds \Theta(q_{F} - |s + \frac{1}{2}|) \Theta(q_{F} - |s - \frac{1}{2}|). \tag{B2}
\]

Thus we need to identify the region in hyperspace in which we are integrating. The region after the substitution is mathematically defined by \( |s + t/2| \leq q_{F} \) and \( |s - t/2| \leq q_{F} \) and therefore can be seen as the overlap region of two Fermi spheres in hyperspace (as shown by the colored region in Fig. 5). The centers of the spheres sit at a distance \( |t| \) from each other, the origin of \( s \) is the midpoint of the connecting line of two centers. The integration over \( s \) is the volume of this overlap region, which is the combined volumes of two identical hyperspherical caps. The volume of a \( D \)-dimensional hyperspherical cap was already calculated by Li [57]:

\[
\mathcal{V}_{D} = \frac{1}{2} V_{D}(r) I_{\sin^{2}\phi} \left( \frac{D + 1}{2}, \frac{1}{2} \right),
\]

where \( V_{D}(r) \) is the volume of a hypersphere with radius \( r \) in \( D \)-dimensional space, \( \phi \) is the angle between a vector and the positive \( D \)-th-axis of the sphere and \( I(x, y) \) is the regularized incomplete beta function. In our case it can easily be verified that \( \sin^{2}\phi = 1 - \frac{q^{2}}{4|t|} \) and \( V_{D}(r) = \pi^{D/2} q_{F}^{D} / \Gamma \left( \frac{D}{2} + 1 \right) \). As a result, \( G_{D}^{\text{HF}}(q) \) becomes:

\[
G_{D}^{\text{HF}}(q) = \frac{2q^{D-3}}{(2\pi)^{2D/2}} \frac{\pi^{D/2}}{\Gamma \left( \frac{D}{2} + 1 \right)} q_{F}^{D} \int_{1 - \frac{q^{2}}{4|t|}}^{1} \frac{q \cdot (q + t)}{|q + t|^{D-1}} dt. \tag{B3}
\]

By changing to \( D \)-dimensional spherical coordinates such that \( q \) is parallel to the \( D \)-th-axis and using the relation between the density and the Fermi wavelength \( q_{F} \) we obtain Eq. (16). For some cases this calculation can be done analytically. Here we provide the result for the 5D case:

\[
G_{5}^{\text{HF}}(q) = -\frac{5}{4928} \left( \frac{q}{q_{F}} \right)^{8} + \frac{25}{1232} \left( \frac{q}{q_{F}} \right)^{6} + \frac{1775}{7392} \left( \frac{q}{q_{F}} \right)^{4} - \frac{5}{66} \left( \frac{q}{q_{F}} \right)^{2} + \frac{25}{154} \left( \frac{q}{q_{F}} \right)^{3} \ln \left| \frac{q + 2q_{F}}{q - 2q_{F}} \right|
\]

\[
+ \left[ -\frac{15}{128} \left( \frac{q}{q_{F}} \right)^{5} + \frac{15}{224} \left( \frac{q}{q_{F}} \right)^{3} + \frac{5}{56} \left( \frac{q}{q_{F}} \right)^{2} - \frac{25}{154} \left( \frac{q_{F}}{q} \right) \right] \ln \left| \frac{q^{2} - 4q_{F}^{2}}{q^{2}} \right|. \tag{B4}
\]
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