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Spin resolved energy parametrization of a quasi-one-dimensional electron gas

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Abstract

By carrying out extensive lattice regularized diffusion Monte Carlo calculations, we study the spin and density dependence of the ground-state energy for a quasi-one-dimensional electron gas, with harmonic transverse confinement and long-range $1/r$ interactions. We present a parametrization of the exchange–correlation energy suitable for spin density functional calculations, which fulfils exact low and high density limits.

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1. Introduction

In this paper we present a parametrization for the exchange–correlation energy of a quasi-one-dimensional electron gas (1DEG) at arbitrary polarization. The electrons interact via a $\frac{1}{r}$ potential and are confined to a line by a transverse harmonic potential $v(r_{\perp}) = \frac{r_{\perp}^2}{4b^4}$, where b controls the thickness of the wire. Here and henceforth we use the effective Bohr radius $a_0^* = \frac{\hbar^2 \epsilon}{m^* e^2}$ as unit of length and the effective Rydberg $Ryd^* = \frac{e^2}{2\epsilon a_0^*}$ as unit of energy, where ϵ is the dielectric constant of the embedding medium and m^* is the effective electron mass. We can separate the transverse and longitudinal parts of the Hamiltonian by assuming that the electrons are in the ground state of the 2D harmonic oscillator in the transverse direction. This is a good approximation provided that $r_s \gg \frac{\pi b}{4}$, where r_s is the Wigner–Seitz radius. The above condition is met for low enough densities and thin enough wires. Thus, it is possible to

integrate out the perpendicular degrees of freedom and work with a strictly one-dimensional Hamiltonian with electrons interacting via an effective potential given by

$$V_b(x) = \frac{\sqrt{\pi}}{b} \exp\left(\frac{x^2}{4b^2}\right) \operatorname{erfc}\left(\frac{|x|}{2b}\right). \quad (1)$$

This potential has been widely used in previous works to model the 1DEG, and we refer the reader to [1] for a detailed description of the Hamiltonian we study and the variational wavefunction we use. Here, we employed the lattice regularized diffusion Monte Carlo (LRDMC) [2] algorithm to compute the ground-state energy of the system at different densities r_s and polarizations, ($\zeta \equiv (N^\uparrow - N^\downarrow)/N$). In one dimension, this method provides the exact energy within the statistical accuracy, since the nodes of the ground-state wavefunction are known exactly.

Despite the huge amount of work done for 1D systems with a $1/r$ interaction [1, 3–8], a spin density exchange–correlation functional is still lacking, and the Bethe ansatz solution is not available in this case. Fogler [9] derived an approximate mapping of the problem with a realistic Coulomb interaction onto exactly solvable models of mathematical physics, but the relation is valid only for ultra-thin wires and requires a careful matching between different regimes. The quantum Monte Carlo framework can provide a parametrization valid in all regimes, but so far a functional has been derived only for an unpolarized wire [1]. The present work fills this gap, and we provide a spin-dependent density functional for the exchange and correlation energy suitable for DFT calculations of these systems. Indeed, the DFT framework has been applied quite successfully in 1D [10–12, 14], mainly on short-range 1D problems where the homogeneous reference was known via Bethe ansatz.

This paper is organized as follows. In section 2 we show the results for the ground-state energy and give a parametrization for the exchange–correlation part, while in section 3 we present conclusions. In the appendix we derive the polarization-dependent random phase approximation (RPA) expression for the correlation energy, which is used to set the high density limit of our parametrization.

2. Exchange–correlation energy and construction of an LSDA functional

We study the ground-state energy of the 1DEG as a function of density and spin polarization, and find a parametrization for the exchange–correlation energy based on theoretically known properties of the electron gas in various limits. The best parameters for the exchange–correlation functional will be determined via a χ^2 minimization of our LRDMC values for the total energy.

Following the usual notation, we separate the total energy ϵ into three parts

$$\epsilon(r_s, \zeta) = \epsilon_t(r_s, \zeta) + \epsilon_x(r_s, \zeta) + \epsilon_c(r_s, \zeta), \quad (2)$$

where ϵ_t is the kinetic energy of the noninteracting system, ϵ_x is the exchange energy calculated for the noninteracting wavefunction and ϵ_c is the correlation energy which includes corrections to both the potential energy and also the kinetic energy due to the interactions. The first two terms are known analytically, while the third one is fully determined by our numerical results for the total energy ϵ . The kinetic energy reads

$$\epsilon_t(r_s, \zeta) = \frac{\pi^2(1 + 3\zeta^2)}{48r_s^2}, \quad (3)$$

while the exchange energy is

$$\begin{aligned} \epsilon_x(r_s, \zeta) &= \frac{1+\zeta}{2b} F\left(\frac{4r_s}{(1+\zeta)\pi b}\right) + \frac{1-\zeta}{2b} F\left(\frac{4r_s}{(1-\zeta)\pi b}\right) \\ F(x) &= -\int_0^{2/x} dy \tilde{v}(y) \frac{1-xy/2}{2\pi}, \end{aligned} \quad (4)$$

with $\tilde{v}(x) = 2E_1(x^2) \exp(x^2)$, where $\tilde{v}(bx)$ is the Fourier transform of the potential in (1), and E_1 is the exponential integral function.

To derive an accurate parametrization for the exchange–correlation energy, it is useful to study both the high and low density limits in order to include them in the actual functional. The high density limit is estimated with the random phase approximation (RPA), while the low density physics is obtained through a mapping onto an effective one-dimensional Heisenberg model.

The RPA is very successful in describing the energy of the homogeneous electron gas at high density [1, 5]. Here we present the main result valid for $r_s \ll 1$ with the effective interaction in (1), while a detailed derivation is given in the appendix. It is worth stressing that in the high density limit (small r_s) the 1D model with effective pair interactions given by (1) does not accurately describe electrons confined in a transverse harmonic potential, since the condition $r_s \gg \frac{\pi b}{4}$ is in general manifestly violated, and the single subband approximation breaks down. The correlation energy evaluated within the RPA is

$$\epsilon_c^{RPA}(r_s, \zeta) = \begin{cases} -C \left(1 + \frac{1}{1-\zeta^2}\right) r_s^2 & \text{if } r_s \ll (1-\zeta)\pi b/2 \\ -\frac{C}{4} r_s^2 & \text{if } \zeta = 1, \end{cases} \quad (5)$$

where $C = \int_0^\infty z \tilde{v}^2(z) dz / (2\pi^4 b^2) \approx 4.9348 / (2\pi^4 b^2)$. Though from (5) the correlation energy may at first appear discontinuous at $\zeta = 1$, $\epsilon_c^{RPA}(r_s, \zeta)$ is in fact a continuous function of its variables as the two limiting behaviours in (5) clearly belong to different regions in the ζ, r_s plane.

The low density dependence of the correlation energy is difficult to determine since the effective coupling is very strong. This causes the electrons to repel each other and form a quasi-Wigner crystal [3]. As the exchange between the particles drops off very rapidly with the reduction in the density, different spin configurations become almost degenerate. However, the Lieb–Mattis theorem [14] proves that in one dimension the ground-state energy of a system of fermions corresponds to zero total spin. This theorem precludes the existence of a Bloch instability such as that predicted by an STLS-like theory [5, 6]. The low density spin dependence of the correlation energy can be determined approximately by noting that the spin sector of the 1DEG can be mapped to that of a Heisenberg spin chain [15] with coupling J . In fact at these densities the electron gas is a quasi-Wigner crystal with local antiferromagnetic correlations [1, 3, 16]. The Heisenberg coupling can be determined by an evaluation of the tunnelling (exchange) rate between electrons via the WKB approximation, which gives an exponential suppression of J at low density as stated by the relation [17]:

$$J(r_s) = \frac{J^*}{(2r_s)^{1.25}} e^{-\nu\sqrt{2r_s}}, \quad (6)$$

where J^* and ν are interaction dependent constants. The energy dependence as a function of J of the antiferromagnetic Heisenberg spin chain is known exactly from the Bethe ansatz [18]. The difference in energies between the polarized and unpolarized spin chains turns out to be $J \ln 2$ [19]. These relations define the spin dependence of the total energy of the electron gas

at low density. Note that in order to provide the exponentially small spin dependence given by (6), the correlation energy must cancel the power law and logarithmic terms of both the exchange and kinetic terms.

Our spin dependent exchange–correlation functional is built upon the parametrization of the exchange and correlation energy for the unpolarized ($\zeta = 0$) and polarized ($\zeta = 1$) wires, which reads

$$\epsilon_{xc}(r_s, \zeta) = \frac{a_\zeta + b_\zeta r_s + c_\zeta r_s^2}{1 + d_\zeta r_s + e_\zeta r_s^2 + f_\zeta r_s^3} + \frac{g_\zeta r_s \ln[r_s + \alpha_\zeta r_s^{\beta_\zeta}]}{1 + h_\zeta r_s^2}, \quad (7)$$

where the parameters are constrained to fulfil the high density limits of both exchange and correlation terms. Those limits imply the following conditions on the parameters:

$$a_0 = -\frac{\sqrt{\pi}}{2b}, \quad (8)$$

$$a_1 = -\frac{\sqrt{\pi}}{2b}, \quad (9)$$

$$b_0 = \frac{2 + \gamma + 2 \ln(\pi b/2)}{\pi^2 b^2} + a_0 d_0, \quad (10)$$

$$b_1 = \frac{2 + \gamma + 2 \ln(\pi b)}{2\pi^2 b^2} + a_1 d_1, \quad (11)$$

$$c_0 = -2C + \frac{2 + \gamma + 2 \ln(\pi b/2)}{\pi^2 b^2} d_0 + a_0 e_0, \quad (12)$$

$$c_1 = -C/4 + \frac{2 + \gamma + 2 \ln(\pi b)}{2\pi^2 b^2} d_1 + a_1 e_1, \quad (13)$$

$$g_0 = -\frac{2}{\pi^2 b^2} \quad \text{with } \beta_0 > 1, \quad (14)$$

$$g_1 = -\frac{1}{\pi^2 b^2} \quad \text{with } \beta_1 > 1, \quad (15)$$

where $\gamma = 0.577\,215\,6649$ is the Euler’s constant. On the other hand, the large r_s expansion of the expression in (7) goes as $\ln r_s/r_s$. Indeed, in previous work [1, 5] it was found that both the correlation and the exchange energies go as $\ln r_s/r_s$ at large r_s , with their ratio approaching a constant in that limit, a condition which is fulfilled by our parametrization.

It is useful also to define a constrained exchange–correlation functional for the unpolarized case in a way that is accurate for low densities. Since the QMC calculations have lower variance for the fully polarized system, we define $\epsilon_{xc}^{\text{con}}(r_s, 0)$ to be equal to the difference between the fully polarized and unpolarized energies of the antiferromagnetic spin chain with the coupling constant $J(r_s)$, determined using the WKB approximation. Thus we rewrite the exchange–correlation functional for $\zeta = 0$ as

$$\epsilon_{xc}^{\text{con}}(r_s, 0) = \frac{\epsilon_{xc}(r_s, 0)}{1 + e^{-\frac{r_s^2 - O^2}{r_s R}}} + \left(1 - \frac{1}{1 + e^{-\frac{r_s^2 - O^2}{r_s R}}}\right) \left(\epsilon_{xc}(r_s, 1) - J(r_s) \ln 2 + \frac{\pi^2}{16r_s^2}\right), \quad (16)$$

where O and R are additional fitting parameters, and $J(r_s)$ is the same as in (6) with $J^* = 184.53$ and $\nu = 2.849\,68$ determined via the WKB approach for our potential in (1). In this way both the high and the low density limits are fulfilled.

Finally, the fully spin-dependent density functional reads

$$\begin{aligned} \epsilon_{xc}(r_s, \zeta) = & \epsilon_{xc}^{\text{con}}(r_s, 0) + h_z(r_s, \zeta) + c_z(r_s, \zeta) + \frac{1}{1 + e^{t(r_s)(1-|\zeta|)^{\delta}}} \\ & \times \left[2((1 - w(r_s))\zeta^2 + w(r_s)\zeta^4) (\epsilon_{xc}(r_s, 1) - \epsilon_{xc}^{\text{con}}(r_s, 0)) \right. \\ & \left. - 2(h_z(r_s, \zeta) + c_z(r_s, \zeta)) \right], \end{aligned} \quad (17)$$

where the additional functions are

$$t(r_s) = \frac{t_1 e^{-t_2 r_s}}{r_s}, \quad (18)$$

$$w(r_s) = e^{-w_1 r_s}, \quad (19)$$

$$c_z(r_s, \zeta) = -C r_s^2 \zeta^2, \quad (20)$$

$$h_z(r_s, \zeta) = \frac{r_s \ln(1 - (|\zeta| - h_{\text{corr}}(r_s, \zeta))^2)}{\pi^2 b^2}, \quad (21)$$

$$h_{\text{corr}}(r_s, \zeta) = H_1 r_s^{H_2} \exp(-H_3 r_s) \zeta^4. \quad (22)$$

$c_z(r_s, \zeta)$ is the small ζ expansion of the correlation energy around $\zeta = 0$, while $h_z(r_s, \zeta)$ is the variation of the exchange energy with respect to $\zeta = 0$ at fixed r_s . Both expressions are taken in the high density limit. $h_z(r_s, \zeta)$ includes another parametric function ($h_{\text{corr}}(r_s, \zeta)$) which accounts for the non-analytic behaviour of the exchange energy around $\zeta = 1$ at $r_s = 0$. The form of (17) was chosen to constrain the parametrization to attain energies determined by (16) and (7). This allows the parametrization to, in principle, satisfy the non-analytic behaviour of the correlation energy at high density and $\zeta = 1$, while the low density behaviour is fulfilled by the mapping onto the Heisenberg model. Even if the parametrization looks complex at the first glance, there are only 21 independent parameters.

We have carried out extensive LRDMC simulations to find the best fitting parameters for our parametrization. We note that there is another ‘external’ parameter b , which sets the effective thickness of the wire and therefore defines the interparticle potential. It is of course possible to derive the parametrization for different widths, but here we chose to work with $b = 1$, which is close to the usual thickness of wires realized in semiconductor nanodevices [20]. The calculations for $b = 1$ yield a series of total energies as a function of density and spin polarization.

Great care is taken to remove all biases in the LRDMC calculations of the energy. The lattice space error is removed by calculating the energy for different lattice spacings and extrapolating the results with a quadratic fit in the lattice space. Finite size effects are removed by calculating the energy for several numbers of electrons and extrapolating the result to the thermodynamic limit by fitting the data to the form

$$E(N) = E + \frac{c_2 \sqrt{\ln N}}{N^2} + \frac{c_1}{N^2}, \quad (23)$$

where E is the energy extrapolated to the thermodynamic limit, N is the number of electrons in the calculation, and the constants c_1 and c_2 are fitting parameters determining the size of the one-body and two-body finite size corrections. Additionally, the number of electrons N is chosen in each calculation so that the number of electrons in each spin species is odd, thus avoiding degeneracy effects. The form in (23) is obtained by following the finite size analysis described in [21].

Our results are plotted in figures 1 and 2 which show the behaviour of the correlation energy as a function of the density and the polarization, respectively. The correlation energy at

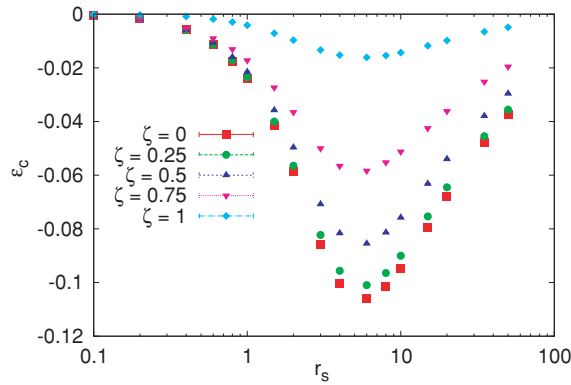


Figure 1. The correlation energy of the electron gas as a function of the density r_s is plotted for $b = 1$ at five values of the polarization, ζ .

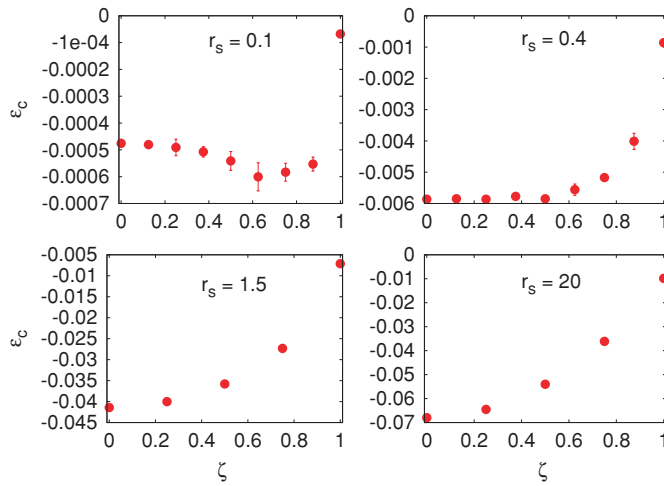


Figure 2. The correlation energy of the electron gas as a function of the polarization ζ is plotted for $b = 1$ at four values of the density, r_s . The upper right panel shows evidence of the RPA behaviour, quadratically as a function of ζ near $\zeta = 0$ and then assuming an abrupt change around $\zeta = 1$. The upper right and lower left panels plot the intermediate case, while the lower right panel shows the ζ dependence at low density.

high density ($r_s = 0.1$) as a function of the polarization shows vestiges of the non-analyticity in the correlation energy at $\zeta = 1$ for $r_s \rightarrow 0$ (see (5)).

Tables 1 and 2 present the various parameters that are obtained by a least-square minimization fitting of the LRDMC values for the exchange–correlation energy computed at 17 different densities ranging from $r_s = 0.1$ to $r_s = 50$. From $r_s = 0.1$ to $r_s = 1.5$ nine values of the polarization were used equally spaced from $\zeta = 0$ to $\zeta = 1$. For $r_s > 1.5$, five polarizations $\zeta = 0, \frac{1}{4}, \frac{1}{2}, \frac{3}{4}$ and 1 were used. These parameters produce a fit that has a reduced χ^2 of 5.3 and an overall accuracy on the order of $10^{-5} Ryd^*$. The exchange–correlation energy is plotted at several values of the density in figure 3. As one can see, it is in a good agreement with the parametrization at all densities.

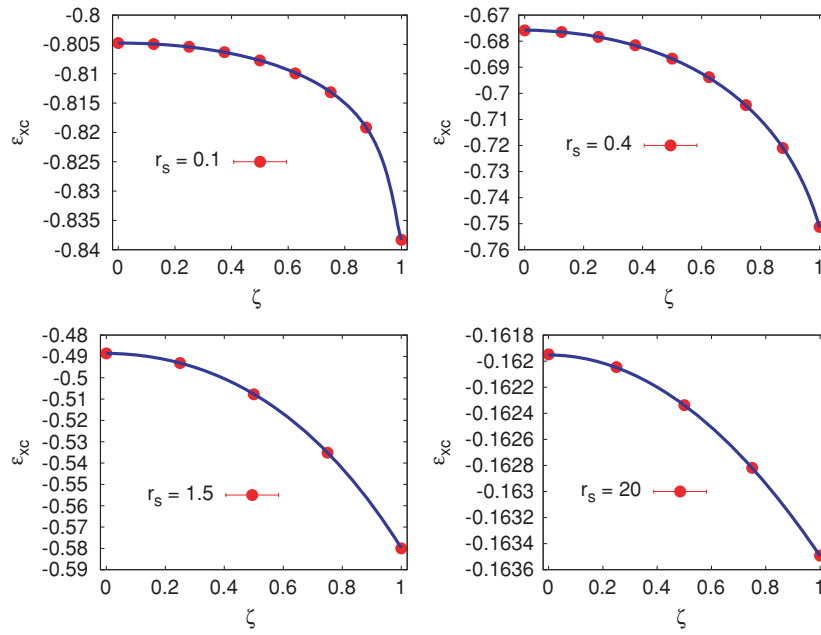


Figure 3. Exchange–correlation energy ϵ_{xc} versus the polarization ζ at various densities. The solid line comes from the parametrization while the points come from QMC calculations. Their error bars are smaller than the point size.

Table 1. Parameter values for the fit of $\epsilon_{xc}^{con}(r_s, 0)$ and $\epsilon_{xc}(r_s, 1)$.

a_0	-0.886 2269	a_1	-0.886 2269
b_0	-2.141 4101	b_1	-0.332 6405
c_0	0.472 1355	c_1	-0.177 1497
d_0	2.814 23	d_1	0.653 545
e_0	0.529 891	e_1	0.374 563
f_0	0.458 513	f_1	0.171 205
g_0	-0.202 642	g_1	-0.101 321
h_0	0.470 876	h_1	0.281 659
α_0	0.104 435	α_1	0.097 434
β_0	4.116 13	β_1	2.868 85
R	1.257 64		
O	3.118 28		

Table 2. Other parameters of the parametrization.

t_1	2.315 55	H_1	5.904 07
t_2	1.834 81	H_2	2.442 23
w_1	0.838 62	H_3	2.934 55
δ	0.705 84		

3. Conclusions

In this paper we have presented results for properties of a quasi-one-dimensional electron gas, with harmonic transverse confinement and long-range $1/r$ interactions, which is a model for confined semiconductor structures. By carrying out extensive lattice regularized diffusion Monte Carlo calculations, we have determined the ground-state energy as a function of spin and density, and we have presented a parameterized fit to the Monte Carlo data that can be used as a local density functional for exchange and correlation in spin density functional calculations. The form is given in (17)–(22). It fulfils the high density limits of both exchange and correlation energies around $\zeta = 0$ and at $\zeta = 1$. At low density a mapping to an Heisenberg spin chain has been used to work out the ζ dependence, while the determination of J comes from WKB calculations. The parameters are given in tables 1 and 2 for a typical wire width $b = 1$. The overall accuracy of the fit is on the order of $10^{-5} Ryd^*$.

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Appendix. RPA calculation of the spin-dependent correlation energy

In this appendix we compute the correlation energy of a spin polarized 1DEG in the high density limit, using the random phase approximation (RPA). We start from the general expression of the RPA correlation energy [22]:

$$\begin{aligned} \epsilon_c^{RPA} &= \frac{L}{2\pi} \int_{-\infty}^{+\infty} dk \epsilon(k), \\ \epsilon(k) &= \frac{1}{4\pi} \frac{|k|}{N} \int_{-\infty}^{+\infty} d\lambda \ln(1 - \tilde{v}(kb)\chi^0(k, ik\lambda)) + \tilde{v}(kb)\chi^0(k, ik\lambda), \end{aligned} \quad (\text{A.1})$$

where $\tilde{v}(kb)$ is the Fourier transform of the potential, and $\chi^0 = \chi_{\downarrow}^0 + \chi_{\uparrow}^0$ is the real part of the density–density response function for the free 1D electron gas

$$\chi_{\sigma}^0(k, \omega) = \frac{1}{4\pi k} \ln \left(\frac{\omega^2 - (k^2 - v_F^{\sigma}k)^2}{\omega^2 - (k^2 + v_F^{\sigma}k)^2} \right), \quad (\text{A.2})$$

with v_F^{σ} the Fermi velocity of the σ ($=\uparrow, \downarrow$) component. After some algebra, and a change of variables ($k = k_F q$, $\omega = ik_F q v_F u$), (A.1) can be rewritten at the leading r_s order as follows:

$$\epsilon_c^{RPA} \simeq -\frac{1}{8(2\pi)^3} \int_0^{+\infty} dq q \tilde{v}^2 \left(\frac{qb}{\alpha r_s} \right) \int_0^{+\infty} du (Q_q^{\uparrow}(u) + Q_q^{\downarrow}(u))^2, \quad (\text{A.3})$$

with $\alpha = 4/\pi$ in 1D. The derivation follows the work of Gell-Mann and Brueckner [23] in 3D, and Rajagopal and Kimball [24] in 2D. The ‘propagator’ $Q_q^{\sigma}(u)$ depends now on the spin polarization, and reads

$$Q_q^{\sigma}(u) = \int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dt f_{\sigma}(k)(1 - f_{\sigma}(k+q)) e^{-ituk} \exp \left(-|t| \left(\frac{1}{2}q^2 + kq \right) \right), \quad (\text{A.4})$$

where $f_{\uparrow}(x) = \theta(|x| - (1 + \zeta))$, $f_{\downarrow}(x) = \theta(|x| - (1 - \zeta))$ are the zero-temperature Fermi distributions for the two spin components, θ being the step function

$$\theta(x) = \begin{cases} 1 & \text{if } x < 0 \\ 0 & \text{if } x \geq 0. \end{cases} \quad (\text{A.5})$$

In order to factor out explicitly the r_s order dependence in (A.3), we apply another change of variables, by rescaling q ($q \rightarrow \frac{\alpha r_s}{b} q$), and we integrate over u . After these steps, the RPA correlation energy reads

$$\epsilon_c^{RPA}(r_s, \zeta) \simeq -\frac{1}{8(2\pi)^3} \left(\frac{\alpha r_s}{b}\right)^2 \int_0^{+\infty} dz z \tilde{v}^2(z) \sum_{\sigma, \sigma'} F_{\sigma, \sigma'}\left(\frac{\alpha r_s}{b} z, \zeta\right), \quad (\text{A.6})$$

where we have defined the set of functions

$$F_{\sigma, \sigma'}(q, \zeta) = \frac{2\pi}{q} \int_{-\infty}^{+\infty} dk_1 f_{\sigma}(k_1)(1 - f_{\sigma}(k_1 + q)) \int_{-\infty}^{+\infty} dk_2 f_{\sigma'}(k_2)(1 - f_{\sigma'}(k_2 + q)) \\ \times \frac{1}{q^2 + q(k_1 + k_2)}, \quad (\text{A.7})$$

where the ζ dependence is included in the zero-temperature Fermi distributions $f_{\sigma}(k)$. From the above equation it is apparent that $F_{\downarrow, \uparrow} = F_{\uparrow, \downarrow}$.

For $\zeta = 1$, $F_{\uparrow, \uparrow}(q, 1) \neq 0$, while $F_{\downarrow, \downarrow}(q, 1) = F_{\uparrow, \downarrow}(q, 1) = 0 \forall q$. Since $F_{\uparrow, \uparrow}(0, 1) = \pi/2$, for the fully polarized 1DEG we obtain

$$\epsilon_c^{RPA}(r_s, \zeta = 1) = -\frac{A}{8\pi^4 b^2} r_s^2, \quad (\text{A.8})$$

a result which is in agreement with the mean spherical approximation [5].

To evaluate $E_c^{RPA}(r_s, \zeta)$ at intermediate polarizations, we need to compute the limits

$$\lim_{x \rightarrow 0} F_{\sigma, \sigma'}(x, \zeta) \quad \text{with} \quad \zeta < 1. \quad (\text{A.9})$$

It turns out that $F_{\uparrow, \uparrow}(0, \zeta) = \pi/(1 + \zeta)$, $F_{\uparrow, \downarrow}(0, \zeta) = \pi$ and $F_{\downarrow, \downarrow}(0, \zeta) = \pi/(1 - \zeta)$. Thus, our final result for the spin-dependent RPA correlation energy is the following:

$$\epsilon_c^{RPA}(r_s, \zeta) = \begin{cases} -\frac{A}{2\pi^4 b^2} \left(1 + \frac{1}{1 - \zeta^2}\right) r_s^2 & \text{if } r_s \ll 2(1 - \zeta)b/\alpha \\ -\frac{A}{8\pi^4 b^2} r_s^2 & \text{if } \zeta = 1. \end{cases} \quad (\text{A.10})$$

Note that when $\zeta = 0$ we recover the RPA correlation energy for the unpolarized 1DEG derived in [1].

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