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Extending the Hedin-Lundqvist approximation, originally developed for the three-dimensional electron gas, we derive the correlation energy E_c for the two-dimensional electron gas as a function of electron density ρ. A simple two-parameter function $E_c(\rho)$ reproduces very well the first-principles numerical results in the whole density range. We also present a simple and accurate form of the correlation part of the chemical potential, which can be used, e.g., as a correlation part of the effective potential in the local-density approximation for two-dimensional electron systems.

I. INTRODUCTION

The ground-state energy E_g of interacting electrons in three (3D) and two (2D) dimensions represents one of the most extensively studied many-body problems.[1,2] This system, usually referred to as the electron gas, in spite of its innumerable applications, still has not been solved in a way to give a satisfactory functional dependence E_g on the electron density ρ in the whole electron density range.

In the standard theoretical approaches the ground-state energy (per one electron) of the n-dimensional electron gas ($n = 2,3$) is written in the form[1,2]

$$E_g^{(n)}(r_s) = E_k^{(n)}(r_s) + E_x^{(n)}(r_s) + E_c^{(n)}(r_s) . \qquad (1)$$

The density parameter r_s is defined as the average distance between electrons in units of the Bohr radius a_0

$$r_s = \frac{1}{a_0} \left[\frac{1}{\pi\rho} \right]^{1/2} (n=2), \quad r_s = \frac{1}{a_0} \left[\frac{3}{4\pi\rho} \right]^{1/3} (n=3) . \qquad (2)$$

The energies will be given in Ry. The first term in Eq. (1) is the kinetic energy[1,2]

$$E_k^{(n)} = \frac{a_n}{r_s^2}, \quad a_2 = 1, \quad a_3 = 2.21 , \qquad (3)$$

while the second term is the Hartree-Fock (or unscreened) exchange energy.

$$E_x^{(n)} = -\frac{b_n}{r_s}, \quad b_2 = 1.2004, \quad b_3 = 0.916 . \qquad (4)$$

The Hartree term, i.e., average electron-electron interaction, is exactly cancelled by the positive background, making the system neutral.

The third term in Eq. (1) is the correlation energy and all the relevant theories try to calculate this term. In the diagrammatic expansion, E_c contains contributions from all diagrams with two or more Coulomb lines,[1] while

from the density-functional approach[3] follows that E_g and, therefore, E_c can be obtained in principle as a solution of the one-particle Schrödinger equation with the (unknown) effective exchange-correlation potential. In both approaches even an approximate derivation of E_c for a certain density range becomes a very complicated task.

On the other hand, one can easily determine E_g from the chemical potential μ (Ref. 1)

$$\mu = E_g + \rho \left[\frac{dE_g}{d\rho} \right] . \qquad (5)$$

Let us decompose μ in the same way as E_g in Eq. (1)

$$\mu = \mu_k + \mu_x + \mu_c . \qquad (6)$$

Knowing E_k and E_x we can determine E_c from Eq. (5) when μ_c is known. We shall do this in Sec. II, using the Hedin-Lundqvist (HL) approach,[4] based on the density-functional theory.[3] The discussion of the results and the concluding remarks are given in Sec. III.

II. CORRELATION ENERGY

From Eq. (2) we find $\rho \sim r_s^{-n}$, so Eq. (5) can be rewritten in terms of r_s as

$$\mu(r_s) = E_g(r_s) - \frac{r_s}{n} \left[\frac{dE_g}{dr_s} \right] . \qquad (7)$$

The exchange part of the chemical potential follows from Eqs. (4) and (7)

$$\mu_x^{(n)}(r_s) = -\frac{c_n}{r_s}, \quad c_n = \left[1 + \frac{1}{n} \right] b_n . \qquad (8)$$

Notice that E_x and μ_x depend upon r_s in the same way for both $n = 3$ and $n = 2$. Therefore, we shall apply the HL approach,[4] originally developed for a 3D electron gas, to find E_c for 2D electrons.

We shall first determine μ_c, starting with the definition

$$\mu_c(r'_s) = \alpha(r'_s)\mu_x(r'_s) \ . \tag{9}$$

Here $r'_s = r_s + \varepsilon'$, and the shift $\varepsilon' \ll 1$ is introduced in order to ensure the correct $r_s \rightarrow 0$ behavior of $\mu_c(r_s)$, as will be discussed later. Equation (9) together with Eq. (8) leads to

$$\frac{d}{dr'_s}(\mu_x + \mu_c) = \gamma(r'_s)\left[\frac{d\mu_x}{dr'_s}\right] \ , \tag{10}$$

$$\gamma(r'_s) = 1 + \alpha(r'_s) - r'_s\left[\frac{d\alpha}{dr'_s}\right] \ . \tag{11}$$

From Eq. (10) we expect γ to be a smooth function of r_s. Following HL, who made this approximation for $n = 3$, we take for $n = 2$

$$\gamma(r'_s) = 1 + B\frac{y}{(1+y)} \ ,$$

$$y = \frac{1}{A}r'_s = x + \varepsilon, \quad x = \frac{1}{A}r_s, \quad \varepsilon = \frac{\varepsilon'}{A} \ . \tag{12}$$

Here A and B are two parameters to be determined later, and we assume that γ takes this form for all electron densities. Now we can integrate Eq. (11) to find $\alpha(r'_s)$, which together with Eqs. (8) and (9) gives

$$\mu_c(r_s) = -C\ln\left[1 + \frac{1}{y}\right], \quad C = c_n\frac{B}{A} \ . \tag{13}$$

Of course, the coefficients (A,B,C) depend upon n.

Now we can use Eq. (7) to connect μ_c and E_c. After integration, we obtain the correlation energy for $n = (2,3)$

$$E_c^{(n)} = -C\,n\,x^n\int_x^\infty dt\frac{1}{t^{n+1}}\ln\left[1 + \frac{1}{t+\varepsilon}\right] \ . \tag{14}$$

III. RESULTS AND DISCUSSION

Let us first discuss the asymptotic behavior of the correlation energy (14)

(a) In the low-density limit $(x \gg 1)$

$$E_c^{(n)} = -C\left[\frac{n}{n+1}\right]\frac{1}{x}\left[1 + O\left[\frac{1}{x}\right]\right] \ , \tag{15}$$

which has the expected $1/r_s$ behavior in the $r_s \rightarrow \infty$ limit, and the leading term does not contain the "shifting parameter" ε.

(b) In the high-density limit $(x \ll 1)$,

$$E_c^{(n)} = -C\begin{cases}\ln\left[\dfrac{1}{x}\right] - \dfrac{1}{n} + O(x), & \varepsilon = 0 \\[3mm] \ln\left[1 + \dfrac{1}{\varepsilon}\right] + O(x), & \varepsilon > 0 \ . \end{cases} \tag{16}$$

For $\varepsilon = 0$, $E_c^{(n)}$ diverges as $\ln r_s$ in the $r_s \rightarrow 0$ limit. This ln divergence is expected for a 3D electron gas, so one should take $\varepsilon = 0$ for $n = 3$. An explicit form of Eq. (14) for a 3D electron gas was given by HL. Here we are particularly interested in the 2D electron gas, in which case $E_c^{(2)}(r_s \rightarrow 0)$ is expected to be finite, i.e., to behave like: $\alpha + O(r_s\ln r_s)$. The constant α then depends upon the theoretical model, and is estimated to be roughly about -0.4.

This argument leads us, therefore, to take $\varepsilon > 0$ for $n = 2$. However, we shall first discuss the $\varepsilon = 0$ limit, in which case Eq. (14) takes a simple form

$$E_c^{(2)} = -C\left[(1-x^2)\ln\left[1 + \frac{1}{x}\right] + x - \frac{1}{2}\right] \ . \tag{17}$$

We shall test the validity of Eq. (17) by comparing it with the relevant numerical data obtained from the first-principles calculations by Tanatar and Ceperley (TC), Ref. 5. These data are very representative, because they cover a large scale of 2D electron densities, from $r_s = 1$ to $r_s = 75$, and also take into account the spin polarization of 2D electrons, defined by the polarization parameter $\xi = (N_\uparrow - N_\downarrow)/N$. We can similarly incorporate spin dependence in our result (17) for E_c, i.e., we only need to redefine the parameter b_n, given by Eq. (4)

$$b_n \rightarrow b_n\frac{1}{2}\left[(1+\xi)^2 + (1-\xi)^2\right] \ . \tag{18}$$

From Eq. (13) we see that this substitution will only change the relation between the coefficients A, B, and C. The TC data for $E_c(r_s)$ for unpolarized ($\xi = 0$) and fully polarized ($\xi = \pm 1$) electron gas, were originally approximated by the four-parameter Padé function.[5] Fitting the TC numerical results to our function (17) by using the least-square procedure, we find the coefficients

$$\begin{aligned}\xi = 0: \quad & A = 13.48, \quad C = 0.096\,73 \ , \\ \xi = \pm 1: \quad & A = 46.87, \quad C = 0.013\,53 \ . \end{aligned} \tag{19}$$

All the results for $E_c(r_s)$ are presented in Table I. The coefficients for the Padé approximation are taken from TC.

From Table I we can conclude that our simple result (17), given as an analytic function with only two parameters, gives at least as good a fit to E_c as the four-parameter Padé approximation. Moreover, we obtain better results in the high-density region ($1 \leq r_s \leq 10$) than in the Padé approximation. This certainly comes as a surprise because one expects that our approximation should fail in this limit. In fact, Eq. (17) gives reasonable values of $E_c(r_s)$ even for $r_s \gtrsim 0.5$.

Let us now take $\varepsilon > 0$. In that case, Eq. (14) can also be analytically integrated, but the result is rather cumbersome. Following Eq. (17) we can obviously obtain the same analytical behavior as from Eq. (14), if we simply interchange $x \rightarrow y = x + \varepsilon$ in Eq. (17)

$$E_c^{(2)} = -C\left[(1-y^2)\ln\left[1 + \frac{1}{y}\right] + y - \frac{1}{2}\right] \ . \tag{20}$$

It has the correct $\varepsilon = 0$ limit, correct behavior for $r_s \gg 1$, given by Eq. (15), and a finite value $E_c(y = \varepsilon)$ at $r_s = 0$. In order to determine the parameter ε, we first notice that

fitting the numerical data for E_c, obtained for $r_s \geq 1$, with some fitting curve (e.g., Padé or ours) and then making an analytic extrapolation to $r_s \rightarrow 0$, is a questionable procedure, because the result can strongly depend on the curve used. Specifically, the two curves that agree very well for $r_s \geq 1$ could give different results for $E_c(r_s=0)$ which vary between a small constant [Padé[5]: $E_c(0) = -0.357$] and a logarithmic divergency (our result for $\varepsilon = 0$). Therefore, we shall determine the parameter ε by fitting $E_c(r_s=0)$ in Eq. (20) to the correct $E_c(0)$ value. For an unpolarized electron gas ($\xi=0$) we take $E_c(0) = -0.39$. In that case the least-square procedure gives the following coefficients:

$$\xi=0: \quad A=11.75, \quad C=0.1094 . \quad (21)$$

The corresponding results for $E_c(r_s)$, which are also given in Table I, are roughly the same as in the case of the Padé approximation. Notice that, although the "shift" ε (here $\varepsilon=0.0178$) gives the correct $E_c(0)$ value, with $\varepsilon=0$ we still obtain a slightly better fit to the

TABLE I. Correlation energy E_c for a 2D electron gas. The data from Tanatar-Ceperley (TC) numerical calculation (Ref. 5) are fitted by the Padé approximation and by our (LS) [Eq. (17)] and LS$_\varepsilon$ [Eq. (20)] expressions. Some relevant theoretical data are also given for comparison.

Unpolarized electron gas ($\xi=0$)				
r_s	TC	Padé	LS	LS$_\varepsilon$
0.0		−0.356 8	∞	−0.390 0
1.0	−0.217	−0.220 2	−0.215 9	−0.213 4
5.0	−0.095 5	−0.099 01	−0.096 57	−0.097 56
10.0	−0.060 85	−0.060 90	−0.060 52	−0.060 89
20.0	−0.035 16	−0.035 17	−0.035 28	−0.035 28
30.0	−0.025 02	−0.024 96	−0.025 01	−0.024 93
50.0	−0.015 90	−0.015 92	−0.015 84	−0.015 74

Fully polarized electron gas ($\xi=\pm1$)			
r_s	TC	Padé	LS
5.0	−0.026 3	−0.025 30	−0.025 97
10.0	−0.018 3	−0.018 50	−0.018 57
20.0	−0.012 3	−0.012 38	−0.012 37
30.0	−0.009 42	−0.009 418	−0.009 410
40.0	−0.007 653	−0.007 639	−0.007 632
75.0	−0.004 652	−0.004 656	−0.004 635

Theoretical values ($\xi=0$)				
r_s	Ref. 6	Ref. 10	Ref. 11	Ref. 12
0.0			−0.39	−0.39
0.5	−0.250		−0.29	−0.28
1.0	−0.211	−0.218	−0.25	−0.22
2.0	−0.155	−0.165	−0.18	−0.16
4.0	−0.108			−0.11
5.0		−0.0998		
8.0	−0.066			−0.064
10.0		−0.0618		
16.0	−0.038			−0.037
20.0		−0.0354		
30.0		−0.0187		
50.0		−0.0151		

$E_c(r_s \geq 1)$ TC values.

The chemical potential μ_c should now be computed from Eqs. (7) and (20)

$$\mu_c = -C\left[(1-\varepsilon y)\ln\left|1+\frac{1}{y}\right| + \varepsilon\left|1-\frac{1}{2y}\right|\right] . \quad (22)$$

In the $r_s \rightarrow 0$ limit it has a finite value $\mu_c(0)=E_c(0)$ and it exhibits a correct $1/r_s$ behavior at $r_s \gg 1$.

All this allows us to draw the following conclusions:

(1) The correlation energy E_c, Eq. (17), agrees very well with the TC data, calculated numerically from the first principles, so one can take Eq. (17) with confidence to describe E_c in the region $1 \leq r_s \leq 75$.

In that sense we also propose our simple form of $\mu_{xc}=\mu_x+\mu_c$ [Eqs. (8) and (13)], as the effective exchange-correlation potential,[4] for the Kohn-Sham equation[3] in the case of 2D electrons. Notice that, for $\varepsilon=0$, Eqs. (13) and (22) give the same result for μ_c, with the coefficients (19). For $\varepsilon>0$, one can use Eq. (22) for μ_c, with coefficients (21). However, if one prefers to take for $\varepsilon>0$ the simpler expression (13) for μ_c, one has to optimize E_c given by Eq. (14) to the TC data and to $E_c(0)$. In that case, one finds (for $\xi=0$) $A=11.48$, $C=0.1119$, $\varepsilon=0.0316$. The corresponding data for $E_c(r_s)$ are practically the same as the LS$_\varepsilon$ data in Table I.

(2) A 2D electron gas provides an excellent testing ground for many-body theory and many authors have treated this problem.[6-13] Standard techniques such as random-phase approximation or Hubbard approximation are not particularly successful and even for high electron densities they are less satisfactory for 2D than for a 3D electron gas.[6] Some simple approaches, based, e.g., on the ring approximation[7] or on the analytical continuation to the low-density regime,[8] give a correct $r_s \rightarrow 0$ limit, but rather poor results for $E_c(r_s)$ at finite densities. As we have noticed, the benchmark against which other results are valued is the numerical, fixed-node Green's function Monte Carlo calculation of $E_c(r_s)$.[5] A similar calculation, based on the variational Monte Carlo method, was performed earlier by Ceperley.[9] The authors of Ref. 5 claimed that the new calculation is more rigorous and in fact it gives only slightly lower E_c than Ref. 9.

In Table I, we also show relevant theoretical results for $E_c(r_s)$ for unpolarized 2D electrons, obtained by Jonson,[6] with the self-consistent STLS approximation, by Takada[10] who used the method of effective-potential expansion in the two-body approximation, by Nagano, Singwi, and Ohniski[11] who summed exactly ladder diagrams, and by Freeman[12] who performed coupled-cluster and ladder approximations. Although the results differ by only a few percent, more precise knowledge of $E_c(r_s)$ is necessary if one wishes to derive unambiguously the ground state of a 2D electron gas. Namely, the unpolarized (paramagnetic) state, the fully polarized (ferromagnetic) state and the Wigner (crystal) state are very close in energy. In some earlier works, the paramagnetic to ferromagnetic transition was predicted,[7,9] but a more precise calculation of Ref. 5 or the ground-state calculation performed by Sim, Tao, and Wu,[13] who used a correlated-basis-function ap-

proach, assumes a paramagnetic ground state for all electron densities below the Wigner transition. The Wigner crystal is expected to have lower energy for $r_s > 37 \pm 5$,[5,9] but as pointed out in Ref. 5, all phases have approximately equal energies at $r_s = 40$.

In conclusion, we have derived a simple analytic result for the correlation energy of a 2D electron gas, which is in excellent agreement with other existing calculations in a wide region of densities between $r_s = 1$ and the onset of the Wigner lattice. The great precision in the determination of $E_c(r_s)$ is needed in order to obtain correct ground-state energy of the 2D electron gas, so we expect that our simple but accurate form can be successfully used in further applications.

[1]See e.g., G. D. Mahan, *Many Particle Physics*, 3rd ed. (Plenum, New York, 1986).

[2]For a 2D electron gas, see e.g., J. T. Devreese and F. M. Peeters, *The Physics of the 2D electron Gas* (Plenum, New York, 1988); A. Isihara, *Solid State Physics* (Academic, New York, 1989), Vol. 42, p. 271.

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