Accurate and simple analytic representation of the electron-gas correlation energy

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We propose a simple analytic representation of the correlation energy ε_c for a uniform electron gas, as a function of density parameter r_s and relative spin polarization ζ. Within the random-phase approximation (RPA), this representation allows for the $r_s^{-3/4}$ behavior as $r_s \to \infty$. Close agreement with numerical RPA values for $\varepsilon_c(r_s,0)$, $\varepsilon_c(r_s,1)$, and the spin stiffness $\alpha_c(r_s) = \partial^2 \varepsilon_c(r_s, \zeta=0)/\delta\zeta^2$, and recovery of the correct $r_s \ln r_s$ term for $r_s \to 0$, indicate the appropriateness of the chosen analytic form. Beyond RPA, different parameters for the same analytic form are found by fitting to the Green's-function Monte Carlo data of Ceperley and Alder [Phys. Rev. Lett. **45**, 566 (1980)], taking into account data uncertainties that have been ignored in earlier fits by Vosko, Wilk, and Nusair (VWN) [Can. J. Phys. **58**, 1200 (1980)] or by Perdew and Zunger (PZ) [Phys. Rev. B **23**, 5048 (1981)]. While we confirm the practical accuracy of the VWN and PZ representations, we eliminate some minor problems with these forms. We study the ζ-dependent coefficients in the high- and low-density expansions, and the r_s-dependent spin susceptibility. We also present a conjecture for the exact low-density limit. The correlation potential $\mu_c^\sigma(r_s,\zeta)$ is evaluated for use in self-consistent density-functional calculations.

I. INTRODUCTION

An analytic representation of the uniform electron-gas correlation energy $\varepsilon_c(r_s,\zeta)$ is an essential ingredient of most local[1,2] and nonlocal[3] density functionals. An *accurate* representation is needed, especially for the description of delicate magnetic effects.[4] Here ε_c is the correlation energy per electron; the density parameter r_s and relative spin polarization ζ are

$$r_s = [3/4\pi(n_\uparrow + n_\downarrow)]^{1/3} , \tag{1}$$

$$\zeta = (n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow) , \tag{2}$$

where $n_\uparrow$ and $n_\downarrow$ are the up- and down-spin electron densities. (All equations are expressed in atomic units: $e^2 = \hbar = m = 1$.) The correlation energy ε_c has the small-ζ expansion[5]

$$\varepsilon_c(r_s,\zeta) = \varepsilon_c(r_s,0) + \tfrac{1}{2}\alpha_c(r_s)\zeta^2 + \cdots , \tag{3}$$

the small-r_s or high-density expansion[5-8]

$$\varepsilon_c(r_s,\zeta) = c_0(\zeta)\ln r_s - c_1(\zeta) + c_2(\zeta)r_s \ln r_s$$
$$- c_3(\zeta)r_s + \cdots , \tag{4}$$

and the large-r_s or low-density expansion[5,7,9]

$$\varepsilon_c(r_s,\zeta) = \frac{-d_0(\zeta)}{r_s^p} + \frac{d_1(\zeta)}{r_s^{2p-1/2}} + \cdots . \tag{5}$$

The exact correlation energy has $p = 1$. The same exponent has been assumed[2,5,10] to hold within the random-phase approximation (RPA), but we have recently found[11] that the correct RPA exponent is $p = \tfrac{3}{4}$.

This discovery has led us to reconsider the analytic representation of $\varepsilon_c(r_s,\zeta)$. Within the RPA, our repre-

sentation is definitely more accurate than the Vosko-Wilk-Nusair[5] (VWN-RPA) and Cole-Perdew[10] (CP) forms, which assume $p = 1$. Beyond RPA, we fit to the Green's-function Monte Carlo results of Ceperley and Alder,[9] as in the earlier parametrizations of Vosko, Wilk, and Nusair[5] (VWN) or Perdew and Zunger[7] (PZ). While we confirm the practical accuracy of the VWN and PZ forms, we also avoid some of the minor problems of those parametrizations.

The PZ and CP forms for $\varepsilon_c(r_s,\zeta)$ display an artificial discontinuity of second and higher derivatives with respect to r_s at $r_s = 1$. In the high-density limit ($r_s \to 0$), these forms do not recover the exact[5] spin stiffness $\alpha_c(r_s)$. Furthermore, we note the exact relations

$$c_0(\zeta) = c_0^{RPA}(\zeta) , \tag{6}$$

$$c_1(\zeta) = c_1^{RPA}(\zeta) - x_2 , \tag{7}$$

where $x_2 = 0.024\,179$ hartree is the second-order exchange constant.[12] The PZ form relies upon an older and less precise constant ($x_2 = 0.023$ hartree).[6]

The VWN and VWN-RPA forms[5] are analytically complicated and nontransparent. In the high-density limit, they are not constrained to reproduce the exact $c_1(0)$ and $c_1(1)$ (although these constants are fitted in a least-squares sense). Furthermore, they artificially make $c_2(0) = c_2(1) = 0$. For low electron densities, the VWN form produces an unphysical maximum of the spin susceptibility enhancement χ/χ_0 at $r_s = 50$ (Sec. III). Finally, we note that the VWN fit does not employ all of the Ceperley-Alder data ($\zeta = 0$ and 1; $r_s = 1,2,5,10,20,50,100$), but only the data for $r_s \geq 10$. Although the data set for $r_s < 10$ is less precise, its known uncertainty can be taken into account.

Our parametrization avoids these problems, and pro-

vides estimates of the ζ-dependent coefficients in the high-density expansion of Eq. (4). Previous estimates of these coefficients by Perdew and Zunger[7] and by Aguilera-Navarro, Baker, and de Llano[8] have been restricted to $\zeta=0$ and 1, and have not taken into account the uncertainties of the Monte Carlo data. We also discuss the ζ-dependent coefficients of the low-density expansion (5). Finally, we report results for the spin susceptibility enhancement χ/χ_0 as a function of r_s, where $\chi_0=2.589\times10^{-6}/r_s$ is the spin susceptibility for noninteracting electrons.

II. PARAMETRIZED CORRELATION ENERGY

Vosko, Wilk, and Nusair[5] made a careful study of the ζ dependence of $\varepsilon_c^{RPA}(r_s,\zeta)$, which they evaluated numerically from RPA integrals.[2] On the basis of this study, they proposed the spin-interpolation formula we will use:

$$\varepsilon_c(r_s,\zeta)=\varepsilon_c(r_s,0)+\alpha_c(r_s)\frac{f(\zeta)}{f''(0)}(1-\zeta^4)$$
$$+[\varepsilon_c(r_s,1)-\varepsilon_c(r_s,0)]f(\zeta)\zeta^4 , \qquad (8)$$

$$f(\zeta)=\frac{[(1+\zeta)^{4/3}+(1-\zeta)^{4/3}-2]}{(2^{4/3}-2)} . \qquad (9)$$

Note that $f(0)=0$, $f(1)=1$, and $f''(0)=1.709\,921$. (The PZ spin interpolation,[7] taken from Ref. 2, amounts to $\alpha_c(r_s)=f''(0)[\varepsilon_c(r_s,1)-\varepsilon_c(r_s,0)]$.) Instead of the rather complicated analytic VWN form for $\varepsilon_c(r_s,0)$, $\varepsilon_c(r_s,1)$, and $-\alpha_c(r_s)$, we use the simpler form

$$G(r_s,A,\alpha_1,\beta_1,\beta_2,\beta_3,\beta_4,p)=-2A(1+\alpha_1 r_s)\ln\left[1+\frac{1}{2A(\beta_1 r_s^{1/2}+\beta_2 r_s+\beta_3 r_s^{3/2}+\beta_4 r_s^{P+1})}\right] . \qquad (10)$$

The parameters A, β_1, and β_2 are chosen to match the exact high-density expansion (4), for which c_0 and c_1 are known:[5]

$$A=c_0 , \qquad (11)$$

$$\beta_1=\frac{1}{2c_0}\exp(-c_1/2c_0) , \qquad (12)$$

$$\beta_2=2A\beta_1^2 . \qquad (13)$$

We easily find

$$c_2=A\alpha_1 , \qquad (14)$$

$$c_3=-2A\left[\alpha_1\ln(2A\beta_1)-\left[\frac{\beta_2}{\beta_1}\right]^2+\frac{\beta_3}{\beta_1}\right] . \qquad (15)$$

The parameter $p=\frac{3}{4}$ (RPA, Ref. 11) or 1 (beyond RPA) fixes the low-density expansion (5), for which

$$d_0=\alpha_1/\beta_4 , \qquad (16)$$

$$d_1=\alpha_1\beta_3/\beta_4^2 . \qquad (17)$$

Since the exact RPA $d_0(\zeta)$ is independent[11] of ζ, $p=1$ for the RPA $\alpha_c(r_s)$. The parameters α_1, β_3, and β_4 are adjusted to give a "best fit" to numerical data for $r_s=2$, 5, 10, 20, 50, and 100.

Within RPA, we known $\varepsilon_c(r_s,0)$, $\varepsilon_c(r_s,1)$, and $-\alpha_c(r_s)$ exactly from the VWN numerical calculation.[5] So we simply adjust α_1, β_3, and β_4 to minimize the sum of the squared errors

$$\sum_{r_s}|G(r_s,\dots)-a(r_s)|^2 . \qquad (18)$$

The resulting fit is remarkably accurate, with a maximum error over the range $0.5<r_s<100$ of only 0.2 mRy, compared to 1.6 mRy for VWN-RPA. (2000 mRy=1 hartree.) This level of accuracy gives us confidence in the analytic form (10).

Beyond RPA, we know the Ceperley-Adler[9] Monte Carlo $\varepsilon_c(r_s,0)$ and $\varepsilon_c(r_s,1)$, and the uncertainties $\Delta\varepsilon_c$. Thus we perform a "chi-square fit " by minimizing

$$\sum_{r_s}\left|\frac{G(r_s,\dots)-a(r_s)}{\Delta a(r_s)}\right|^2 , \qquad (19)$$

i.e., we fit within the uncertainty for each r_s. By using more information than VWN, we hope to obtain a more accurate representation of the correlation energy. The resulting $\varepsilon_c(r_s,1)$ is very close (within 0.2 mRy) to that of VWN, but $\varepsilon_c(r_s,0)$ and $\alpha_c(r_s)$ show differences over the range $0.5<r_s<100$ as great as 1.0 and 2.2 mRy, respectively.

The beyond-RPA spin stiffness $\alpha_c(r_s)$ requires special treatment because of the lack of exact or Monte Carlo values to fit. We follow a proposal of VWN,[5] fitting $\alpha_c(r_s)$ to

$$\frac{\varepsilon_c(r_s,1)-\varepsilon_c(r_s,0)}{\varepsilon_c^{RPA}(r_s,1)-\varepsilon_c^{RPA}(r_s,0)}\alpha_c^{RPA}(r_s) \qquad (20)$$

at $r_s=2$, 5, 10, and 20. However, we note that the spin susceptibility depends sensitively upon r_s at large values of r_s. To fix the low-density behavior, we also fit $\alpha_c(r_s)$ at $r_s=75$ to a value which makes the spin susceptibility enhancement

$$\frac{\chi}{\chi_0}=\left[1-\left[\frac{4}{9\pi}\right]^{1/3}\frac{r_s}{\pi}+3\left[\frac{4}{9\pi}\right]^{2/3}r_s^2\alpha_c(r_s)\right]^{-1} \qquad (21)$$

diverge at a density $(r_s=77.5)$ slightly lower than the density $(r_s=73)$ at which the electronic spins spontaneously polarize (from $\zeta=0$ to $\zeta=1$). This susceptibility behavior, which is consistent with the approximate validity of assumption (20), is very similar to that found in RPA, where χ/χ_0 diverges at $r_s=19$, and the ferromagnetic transition occurs at $r_s=17$. It is also similar to the behavior in the Hartree-Fock approximation $(\alpha_c=0)$, where χ/χ_0 diverges at $r_s=6.03$ and the ferromagnetic

TABLE I. Parameters of the fit to Eq. (10), and of the resulting high-density [Eq. (4)] and low-density [Eq. (5)] expansions. Asterisks indicate parameters that are constrained to exact values from Ref. 5. (Energies are in hartree.)

	$\varepsilon_c^{RPA}(r_s,0)$	$\varepsilon_c^{RPA}(r_s,1)$	$-\alpha_c^{RPA}(r_s)$	$\varepsilon_c(r_s,0)$	$\varepsilon_c(r_s,1)$	$-\alpha_c(r_s)$
*p	0.75	0.75	1.00	1.00	1.00	1.00
*$A=c_0$	0.031 091	0.015 545	0.016 887	0.031 091	0.015 545	0.016 887
α_1	0.082 477	0.035 374	0.028 829	0.213 70	0.205 48	0.111 25
β_1	5.148 6	6.486 9	10.357	7.595 7	14.118 9	10.357
β_2	1.648 3	1.308 3	3.623 1	3.587 6	6.197 7	3.623 1
β_3	0.236 47	0.151 80	0.479 90	1.638 2	3.366 2	0.880 26
β_4	0.206 14	0.082 349	0.122 79	0.492 94	0.625 17	0.496 71
*c_1	0.070 823	0.049 778	0.035 475	0.046 644	0.025 599	0.035 475
c_2	0.002 56	0.000 55	0.000 49	0.006 64	0.003 19	0.001 88
c_3	0.009 36	0.002 30	0.003 59	0.010 43	0.003 84	0.005 21
d_o	0.400 1	0.429 6	0.234 8	0.433 5	0.328 7	0.224 0
d_1	0.459 0	0.791 8	0.917 7	1.440 8	1.769 7	0.396 9

transition is found at $r_s = 5.45$.

Table I shows the parameters of the fit. The asterisk indicates parameters which have been constrained to exact values. Numerical results for $\varepsilon_c(r_s,\zeta)$ from the present Perdew-Wang (PW) parametrization within RPA are compared to VWN-RPA (Ref. 5) and exact-RPA (Ref. 5) values in Table II of Ref. 11, while beyond-RPA PW results are compared to VWN (Ref. 5) and PZ (Ref. 7) values in Table III of the same reference.

Our numerical RPA calculations for r_s up to 10^6 show that the low-density limit of $\varepsilon_c^{RPA}(r_s,0)$ is $-0.40/r_s^{3/4}+0.46/r_s$, as the parameters of Table I suggest. An alternative and preferred set of parameters for $\varepsilon_c^{RPA}(r_s,1)$ may be constructed from those for $\varepsilon_c^{RPA}(r_s,0)$ via the Misawa spin-scaling relation[13]

$$\varepsilon_c^{RPA}(r_s,1)=\tfrac{1}{2}\varepsilon_c^{RPA}(2^{-4/3}r_s,0) \ . \tag{22}$$

The result is $\alpha_1=0.032\,731$, $\beta_1=6.4868$, $\beta_2=1.3083$, $\beta_3=0.118\,24$, $\beta_4=0.081\,81$; $c_2=0.000\,51$, $c_3=0.002\,33$, $d_0=0.4001$, $d_1=0.5782$.

The *exact* ζ dependence in the high-density limit could be recovered by replacing Eq. (9) by

$$f(\zeta)=[I(\zeta)-1]/[I(1)-1] \ ,$$

where $I(\zeta)$ is the analytic function of Eq. (32) of Ref. 14, making $f''(0)=1.086\,28$. However, this change would not necessarily improve the fit for $r_s \geq 0.5$, where Eq. (9) actually gives a better description of the RPA correlation energy. For the sake of the low-density limit (discussed at the end of Sec. III), we retain Eq. (9).

III. DISCUSSION OF RESULTS BEYOND RPA

Equations (8)–(10) and Table I generate what may be the most accurate available representation of the correlation energy $\varepsilon_c(r_s,\zeta)$. The corresponding correlation potential $\mu_c^\sigma(r_s,\zeta)$ is presented in Appendix A. We recommend the use of these formulas in density-functional and other calculations, although they may show little practi-

cal difference from the VWN (Ref. 5) and PZ (Ref. 7) formulas.

From these equations, we estimate the ζ-dependent coefficients of the high-density expansion:

$$c_0(\zeta)=0.031\,09-0.009\,88f(\zeta)(1-\zeta^4)$$
$$-0.015\,55f(\zeta)\zeta^4 \ , \tag{23}$$

$$c_1(\zeta)=0.046\,64-0.020\,75f(\zeta)(1-\zeta^4)$$
$$-0.021\,05f(\zeta)\zeta^4 \ , \tag{24}$$

etc. Table II compares $c_0(\zeta)$ from Eq. (23) to the exact $c_0(\zeta)$, which we have recently evaluated,[14] and also displays $c_1(\zeta)$ from Eq. (24).

In Table III, we compare the coefficients $c_2(0)$, $c_3(0)$, $c_2(1)$, and $c_3(1)$ obtained here (PW) with those from PZ (Ref. 7) and from Aguilera-Navarro, Baker, and de Llano,[8] and with exact values.[5,15,16] The close agreement between the PZ and Aguilera-Navarro values may be a consequence of the fact that neither of those fits takes into account the uncertainties in the Monte Carlo data, which are largest at small r_s.[17] The PW coefficients are significantly closer to the exact values for c_2; exact values

TABLE II. The ζ-dependent coefficients $c_0(\zeta)$ and $c_1(\zeta)$ of the high-density expansion (4). (Energies are in hartree.) The percent error of Eq. (23), relative to exact values from Ref. 11, is also shown, as is the percent error of Eq. (24), relative to exact values from Ref. 19.

ζ	$c_0(\zeta)$ [Eq. (23)]		$c_1(\zeta)$ [Eq. (24)]	
0.0	0.0311	(0.0%)	0.0466	(−0.6%)
0.2	0.0308	(−0.0%)	0.0459	(−0.6%)
0.4	0.0297	(−0.0%)	0.0438	(−0.6%)
0.6	0.0277	(−0.1%)	0.0400	(−0.3%)
0.8	0.0239	(−2.0%)	0.0343	(+0.8%)
0.9	0.0206	(−5.0%)	0.0305	(+2.6%)
0.999	0.0156	(−2.1%)	0.0257	(+2.6%)
1.0	0.0155	(0.0%)	0.0256	(−0.5%)

TABLE III. More coefficients of the high-density expansion (4). Note that $c_2^{RPA}=c_2=0$ for the VWN form of Ref. 5. (Energies are in hartree.)

| | $\zeta=0$ | | | $\zeta=1$ | | |
	c_2^{RPA}	c_2	c_3	c_2^{RPA}	c_2	c_3
PZ[a]	0.0021	0.0020	0.0116	0.0005	0.0007	0.0048
Aguilera-Navarro, Baker, and de Llano[b]		0.0036	0.0118		0.0014	0.0049
PW[c]	0.0026	0.0066	0.0104	0.0006	0.0032	0.0038
Exact	0.0027[d]	0.0092[d]		0.0005[e]	0.0031[e]	

[a] Reference 7 (RPA: Ref. 10).
[b] Reference 8.
[c] Present work.
[d] Reference 15.
[e] Appendix B.

for c_3 are unknown.

We turn now to lower densities. Besides the correlation energy $\varepsilon_c(r_s,\zeta)$, the total energy per electron includes noninteracting kinetic

$$t_s(r_s,\zeta)=\frac{3}{10r_s^2}\left[\frac{9\pi}{4}\right]^{2/3}[(1+\zeta)^{5/3}+(1-\zeta)^{5/3}]/2 \tag{25}$$

and exchange

$$\varepsilon_x(r_s,\zeta)=-\frac{3}{4\pi r_s}\left[\frac{9\pi}{4}\right]^{1/3}[(1+\zeta)^{4/3}+(1-\zeta)^{4/3}]/2 \tag{26}$$

contributions. The total energy $\varepsilon(r_s,0)$ minimizes at $r_s=4.19$, close to the density of metallic sodium. The ferromagnetic transition (from $\zeta=0$ to $\zeta=1$) in our parametrization occurs at $r_s=73$, close to the transition density estimated by Ceperley and Alder[9] ($r_s=75\pm5$). Using the expression[17]

$$-\frac{0.895\,93}{r_s}+\frac{1.325}{r_s^{3/2}}-\frac{0.365}{r_s^2} \tag{27}$$

for the energy of the body-centered-cubic Wigner crystal, we find a second transition to the crystalline state at $r_s=98$, close to the density estimated by Ceperley and Alder ($r_s=100\pm20$).

In the low-density limit ($r_s\to\infty$), the energy of the fluid phase in our parametrization is $-d_{xc}(\zeta)/r_s$, where

$$d_{xc}(\zeta)=0.4582[(1+\zeta)^{4/3}+(1-\zeta)^{4/3}]/2$$
$$+0.4335-0.1310f(\zeta)+0.0262f(\zeta)\zeta^4 , \tag{28}$$

which depends very weakly upon ζ (Table IV). The exact $d_{xc}(\zeta)$ is probably[11] independent of ζ.

Table V shows the spin susceptibility enhancement of Eq. (21). Note the peculiar maximum of the VWN χ/χ_0 (as pointed out to us by Clougherty) at $r_s=50$, well below the ferromagnetic transition (at $r_s=80$ in VWN), and also

the more physical behavior of the PW χ/χ_0. The PZ, VWN, and PW values are all consistent with measured spin susceptibilities for the alkali metals[18] ($3\lesssim r_s\lesssim6$).

In summary, we have presented a simple and useful analytic form for the correlation energy $\varepsilon_c(r_s,\zeta)$. Tests within the random-phase approximation show errors less than 0.2 mRy for $\varepsilon_c(r_s,0)$, $\varepsilon_c(r_s,1)$, and $\alpha_c(r_s)$ over the range $0.5<r_s<100$. Another positive indicator is the correct value found for c_2^{RPA} (Table III). Beyond RPA, our representation also seems highly accurate, and may be improved through parameter reoptimization when more precise Monte Carlo data (including correlation energies for $0<\zeta<1$) become available. An appealing avenue is to demand that Eq. (10) reproduce the exact d_0, leaving only two adjustable-fit parameters (α_1 and β_3). The exact $d_{xc}(\zeta)$ is presumably 0.895 93 from Eq. (27) (see Table IV). We can achieve this low-density limit with $d_0(\zeta=0)=0.437\,76$, $d_0(\zeta=1)=0.318\,67$, and $d_0(-\alpha_c)=0.203\,63$. In fact, with further development of the high- and low-density limits, it may be possible to construct $\varepsilon_c(r_s,\zeta)$ accurately with no Monte Carlo input.

Recently, Hoffman[19] has made an "exact" numerical evaluation of $c_1(\zeta)$ of Eq. (4), with results that are rather similar to those of our analytic representation (Table II). However, his values for $\zeta=0$ and 1 [$c_1(0)=0.046\,921$, $c_1(1)=0.025\,738$ hartree], are slightly (0.5%) larger than the values from Ref. 5 that we have used in our Table I.

TABLE IV. Spin dependence of the exchange-correlation energy $\varepsilon_{xc}(r_s,\zeta)\to-d_{xc}(\zeta)/r_s$ in the low-density limit $r_s\to\infty$, from Eq. (28). The exact $d_{xc}(\zeta)$ is probably independent of ζ. (Energies are in hartree.)

ζ	$d_{xc}(\zeta)$
0.0	0.892
0.2	0.891
0.4	0.890
0.6	0.889
0.8	0.891
0.9	0.896
1.0	0.906

TABLE V. Spin susceptibility enhancement of Eq. (21). The RPA values (from our present parametrization) agree with the numerical RPA values from Ref. 5.

r_s	RPA	χ/χ_0 PZ[a]	VWN[b]	PW[c]
0.5	1.08	1.08	1.08	1.08
1	1.16	1.15	1.15	1.15
2	1.31	1.27	1.31	1.30
3	1.48	1.39	1.46	1.44
4	1.66	1.51	1.62	1.58
5	1.86	1.62	1.79	1.72
6	2.08	1.73	1.97	1.86
10	3.44	2.15	2.83	2.43
20	−26.77	3.12	6.71	4.16
30	−3.64	3.93	17.87	6.95
50	−1.60	5.69	282.41	24.52
60	−1.31	6.72	83.29	63.01
75	−1.07	13.00	20.15	930.61

[a] Reference 7.
[b] Reference 5.
[c] Present work.

We have checked and confirmed the numerical part of Hoffman's calculation, i.e., the integral $\langle \ln(R) \rangle$.[20]

ACKNOWLEDGMENTS

APPENDIX A: CORRELATION POTENTIAL AND INTERACTING KINETIC ENERGY

The correlation potential for electrons of spin σ is

$$\mu_c^\sigma(r_s,\zeta) = \partial[n\varepsilon_c(r_s,\zeta)]/\partial n_\sigma$$

$$= \varepsilon_c(r_s,\zeta) - \frac{r_s}{3}\frac{\partial\varepsilon_c(r_s,\zeta)}{\partial r_s}$$

$$-(\zeta - \text{sgn}\sigma)\frac{\partial\varepsilon_c(r_s,\zeta)}{\partial\zeta} , \qquad \text{(A1)}$$

where sgnσ is $+1$ for $\sigma=\uparrow$ and -1 for $\sigma=\downarrow$. From Eq. (8),

$$\frac{\partial\varepsilon_c(r_s,\zeta)}{\partial r_s} = \frac{\partial\varepsilon_c(r_s,0)}{\partial r_s}[1-f(\zeta)\zeta^4] + \frac{\partial\varepsilon_c(r_s,1)}{\partial r_s}f(\zeta)\zeta^4$$

$$+ \frac{d\alpha_c(r_s)}{dr_s}\frac{f(\zeta)}{f''(0)}(1-\zeta^4) \qquad \text{(A2)}$$

and

$$\frac{\partial\varepsilon_c(r_s,\zeta)}{\partial\zeta} = 4\zeta^3 f(\zeta)\left[\varepsilon_c(r_s,1)-\varepsilon_c(r_s,0)-\frac{\alpha_c(r_s)}{f''(0)}\right]$$

$$+ f'(\zeta)\left[\zeta^4\varepsilon_c(r_s,1)-\zeta^4\varepsilon_c(r_s,0)\right.$$

$$\left. + (1-\zeta^4)\frac{\alpha_c(r_s)}{f''(0)}\right] , \qquad \text{(A3)}$$

where

$$f'(\zeta) = \frac{4}{3}\frac{[(1+\zeta)^{1/3}-(1-\zeta)^{1/3}]}{(2^{4/3}-2)} . \qquad \text{(A4)}$$

Finally, we obtain $\partial\varepsilon_c(r_s,0)/\partial r_s$, $\partial\varepsilon_c(r_s,1)/\partial r_s$, and $-d\alpha_c(r_s)/dr_s$ from Eq. (10):

$$\frac{\partial G}{\partial r_s} = -2A\alpha_1\ln(1+1/Q_1) - \frac{Q_0 Q_1'}{Q_1^2+Q_1} , \qquad \text{(A5)}$$

where

$$Q_0 = -2A(1+\alpha_1 r_s) , \qquad \text{(A6)}$$

$$Q_1 = 2A(\beta_1 r_s^{1/2}+\beta_2 r_s+\beta_3 r_s^{3/2}+\beta_4 r_s^{p+1}) , \qquad \text{(A7)}$$

$$Q_1' = A[\beta_1 r_s^{-1/2}+2\beta_2+3\beta_3 r_s^{1/2}+2(p+1)\beta_4 r_s^p] . \qquad \text{(A8)}$$

By generalizing the derivation of Ref. 21 to $\zeta\neq0$, or by combining Eq. (34) of Ref. 22 with Eq. (A1), we find the interacting or correlation contribution to the kinetic energy per electron:

$$t_c(r_s,\zeta) = -4\varepsilon_c(r_s,\zeta) + 3\left[\frac{(1+\zeta)}{2}\mu_c^\uparrow(r_s,\zeta)\right.$$

$$\left. + \frac{(1-\zeta)}{2}\mu_c^\downarrow(r_s,\zeta)\right] . \qquad \text{(A9)}$$

The simplest version of the virial theorem,

$$t_s + \varepsilon_x + \varepsilon_c = -(t_s+t_c) ,$$

is obeyed at the equilibrium density ($r_s=4.19$ and $\zeta=0$).

APPENDIX B: EXACT COEFFICIENT OF $r_s \ln r_s$ IN EQ. (4)

Carr and Maradudin[15] found $c_2^{\text{RPA}}(0)=0.0027$ hartree and $c_2(0)-c_2^{\text{RPA}}(0)=0.0065$ hartree. We have evaluated the numerical integral of their Eq. (15) to higher precision, with the result

$$c_2^{\text{RPA}}(0) = 0.002\,709\,5 \text{ hartree} , \qquad \text{(B1)}$$

and the numerical integral of their Eq. (22), with the result

$$c_2(0)-c_2^{\text{RPA}}(0) = 0.006\,519\,7 \text{ hartree} . \qquad \text{(B2)}$$

The latter integral is greatly simplified by our analytic expression for $R^{(1)}(iu)$, which Carr and Maradudin left in the form of a two-dimensional integral [Eq. (A5) of Du-Bois[23]]:

$$R^{(1)}(iu) = 4[(1+3u^2)-(2+3u^2)u \tan^{-1}(u)]/(1+u^2) .$$

(B3)

To find the RPA coefficient for $\zeta = 1$, we use Eq. (22) with the result

$$c_2^{RPA}(1) = c_2^{RPA}(0)/2^{7/3} .$$

(B4)

A different spin-scaling relation[13] for the second-order ex-

change contribution

$$\varepsilon_{1x}(r_s,1) = \varepsilon_{1x}(2^{-4/3}r_s,0) ,$$

gives

$$c_2(1) - c_2^{RPA}(1) = [c_2(0) - c_2^{RPA}(0)]/2^{4/3} ,$$

(B5)

as in Ref. 5.

We hope to generalize these results to arbitrary ζ in future work.

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