

Spin Polarization of the Uniform Three-Dimensional Electron Gas

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Abstract

A simple-and-analytic form for total energy (or ground-state energy) in the uniform three-dimensional electron gas, expressed as a function of any Wigner-Seitz radius r_s and relative spin polarization ζ is obtained with a very good accuracy of 0.036% from the Stoner model and our interpolation between high-and-low density limits with use of a two-point approach for the correlation energy and spin stiffness at $r_s = 1$ and 70. This suggests a satisfactory description of some physical properties such as: paramagnetic-ferromagnetic phase transition and thermodynamic-and-optical phenomena.

Keywords: Electron Gas, Correlation Energy; Spin Stiffness, Total Energy, Spin Susceptibility, Paramagnetic-and-Ferromagnetic Phase Transitions, Wigner States

1. Introduction

First of all, in the uniform three-dimensional electron gas (U3DEG) at zero temperature, it should be noted that the state of this system is entirely specified by the Wigner-Seitz radius r_s being related to the total electron density n by: $n(r_s) \equiv 3/(4\pi r_s^3 a_B^3)$, where $a_B = 0.53 \times 10^{-8}$ cm is the Bohr radius, and the relative spin polarization ζ defined by: $-1 \leq \zeta \equiv (n^\uparrow - n^\downarrow)/n \leq 1$. Here, $n \equiv n^\uparrow + n^\downarrow$, and n^\uparrow and n^\downarrow mean the up-and down-spin electron densities, respectively, noting that the two particular values of ζ ($= 0$ and ± 1) denote the paramagnetic (P) and ferromagnetic, (F) states, respectively. Furthermore, all the energies given in the following are calculated in Rydbergs (Ry). Such an U3DEG is one of the basic models of many-body physics, and has been investigated for over 73 years [1-14]. In particular, for $\zeta = 0$, some physical properties at any r_s such as: Ferrell's condition for the stability of the total energy [7], electronic pressure and compressibility [7], virial theorem [12], asymptotic forms for plasmon-dispersion. Coefficients obtained in low-and-high plasmon-energy limits [10], and spin susceptibility [8,9,11], were expressed in terms of the total energy and correlation energy, and their respective derivatives, being denoted in general forms for a presentation simplicity as:

$$\frac{\partial^n}{\partial x^n} f(x, y) \equiv [f(x, y)]_x^{(n)}$$

$$\frac{\partial^n}{\partial y^n} f(x, y) \equiv [f(x, y)]_y^{(n)}, \text{ for } n = 1, 2, \dots$$

The aim of the present paper is to investigate a simple-and-analytic form for $E(r_s, \zeta)$ in the U3DEG, obtained with a very good accuracy of 0.036% from the Stoner model, an interpolation between high-and-low density limits (HLDL), and a two-point approach for correlation energy $E_c(r_s, \zeta)$ and spin stiffness $\alpha_c(r_s)$ at $r_s = 1$ and 70, giving rise to a satisfactory description of some physical properties such as: PF-phase transition and thermodynamic-and-optical phenomena.

2. Accurate and Simple Analytic Form for $E(r_s, \zeta)$ at Any r_s and ζ

Accounting for a neutralizing positive background and denoting $\alpha(4/9\pi)^{1/3}$, the total energy per particle is given by:

$$E(r_s, \zeta) = E_{HE}^{stoner}(r_s, \zeta) + E_C(r_s, \zeta),$$

$$E_{HE}^{stoner}(r_s, \zeta) \equiv [K_0(r_s, \zeta) + \Delta K_0(\zeta; g)] + E_x(r_s, \zeta), \quad (1)$$

where $E_x(r_s, \zeta) = 3h(\zeta)/(2\pi\alpha r_s^2)$ is the exchange energy, $K_0(r_s, \zeta) = 3k(\zeta)/5(\alpha r_s)^2$ is the kinetic energy at Fermi surface, $\Delta K_0(\zeta, g) = 3g(1-\zeta^2)/10\alpha^2$

is the kinetic energy correction calculated within the mean-field Hartree-Fock approximation using the non-interacting wave function (*i.e.*, a Stoner model [10]), and g is an empirical parameter chosen so that the relative errors of $E(r_s, \zeta)$ for any r_s and are minimized (its value is given in **Table 1**). Moreover, we use in this work a general spin-interpolation formula for $E_c(r_s, \zeta)$ proposed by Vosko *et al.* [5]

$$E_c(r_s, \zeta) = E_c(r_s, 0) + \alpha_c(r_s) \left[\frac{f(\zeta)}{[f(\zeta)]_{\zeta=0}^{(2)}} \right] (2) \\ (1 - \zeta^4) + [E_c(r_s, 1) - E_c(r_s, 0)] f(\zeta) \zeta^4.$$

In Equations (1) and (2), the three functions $k(\zeta)$, $h(\zeta)$ and $f(\zeta)$ are defined by:

$$2k(\zeta) \equiv (1 + \zeta)^{5/3} + (1 - \zeta)^{5/3}, \\ 2h(\zeta) \equiv (1 + \zeta)^{4/3} + (1 - \zeta)^{4/3}, \\ [2^{1/3} - 1] f(\zeta) \equiv h(\zeta) - 1,$$

that gives: $[f(\zeta)]_{\zeta=0}^{(2)} \equiv 2 \left[(1 + \zeta)^{-2/3} + (1 - \zeta)^{-2/3} \right] / 9 (2^{1/3} - 1) = 1.709921$ for $\zeta = 0$.

From Equations (1) and (2) one notes that: $E(r_s, \zeta) = E_c(r_s, -\zeta)$ and $E_c(r_s, \zeta) = E_c(r_s, -\zeta)$, reducing to the interval: $0 \leq \zeta \leq 1$, and that if the three functions: $E_c(r_s, 0)$, $E_c(r_s, 1)$ and $\alpha_c(r_s)$, represented by $X(r_s; a)$, are known, then $E_c(r_s, \zeta)$ and $E(r_s, \zeta)$ are therefore determined. Here, the function $X(r_s; a)$ can be expressed in terms of its two exact asymptotic results given in HLDL, $G(r_s)$ and $W(r_s, a)$,

$$X(r_s; a) \equiv W(r_s; a) + [G(r_s) - W(r_s; a)] / [1 + \lambda r_s^\gamma], \quad (3)$$

reducing in the HDL to: $\lim X(r_s; a) = G(r_s)$ and in the LDL to: $\lim_{\zeta \rightarrow \infty} X(r_s; a) \equiv \bar{W}^0(r_s; a)$. Thus, the present method used to obtain our result (3) for $X(r_s; a)$ is the interpolation between HLDL, being similar to those also used in [8,9,11]. It should be noted that this is the unique method used to obtain the analytic expression for $X(r_s; a)$ at any r_s .

In the HDL, in which the random-phase approxima

Table 1. Parameters of the best fit to Equations (4) and (7). Energies in mRy.

For	$E_p(r_s)$	$E_c(r_s)$	$\alpha_c(r_s)$
X_1 [9]	- 119.571	- 63.185	80.64
X_{70}	- 8.68307 [10]	- 5.533 [10]	5.3205 [9]
x [9]	875.53	637.356	- 407.26
y [9]	62.18	31.09	- 33.77
Z [9]	93.288	51.198	- 70.95
a	0.0908	0.085	0
	$g = 7.7 \times 10^{-3}$ from Stoner model		
λ	0.03848	0.02287	0.02968
γ	1.67379	1.63995	2.01735

tion (RPA) may be used, the function $G(r_s)$ can be written under a condensed Gell-Mann-and-Bruecker's as [2,9]:

$$G(r_s) = y \ln(r_s) - z, \quad (4)$$

where the values of y and z [13] are given in **Table 1**.

In the LDL (or beyond RPA), the function $W(r_s)$ can be written under a condensed Wigner's form [1,9] as:

$$W(r_s) = -x/(a + r_s), \quad (5)$$

where the values of the empirical parameter a are chosen so that the relative errors of $E(r_s, \zeta)$ for any r_s and ζ are minimized. The values of a and x [9] are reported in **Table 1**.

Going back to Equation (3), in order to determine the constants λ and γ , we now use a two-point approach by denoting: $X(r_s = 1) \equiv X_1$ [9] and $X(r_s = 70) \equiv X_{70}$ [9,10], being reported in **Table 1**. Thus, those constants λ and γ are determined by:

$$\lambda = [G(r_s) - X_1] / [X_1 - W(r_s)] \text{ for } r_s = 1, \quad (6)$$

and

$$\gamma = [1/\ln(r_s)] \times \ln \left(\frac{[G(r_s) - X_{70}]}{\lambda [X_{70} - W(r_s)]} \right) \text{ for } r_s = 70 \quad (7)$$

In summary, from Equations (3)-(7) and **Table 1**, the correlation energy $E_c(r_s, \zeta)$ given in Equation (2) and total energy $E(r_s, \zeta)$ in Equation (1) are thus determined. Then, in order to calculate the relative errors (RE) of $E(r_s, \zeta)$ from the present result (1) and those from other approximate results evaluated from [4,8,9,11], neglecting the Stoner model, we will use the accurate results obtained from their diffusion Monte Carlo (DMC) method [4] by using backflow wave functions and twist averaged boundary conditions to obtain the accurate values of $E(r_s, \zeta)$ at low densities $40 \leq r_s \leq 100$ and for $0 \leq \zeta \leq 1$ with standard errors in units of 10^{-8} Ry. This formula of RE is defined by: $1 - (\text{Approximate results} / \text{ZLC's results})$. So, it is found that our present results of $E(r_s, \zeta)$ are accurate to within 0.036% while other approximate ones [4, 8,9,11] only give: 0.24%, 0.29%, 0.42% and 0.471%, respectively. In **Table 2**, for a comparison, we only report our results of RE and those obtained from [4,11].

Furthermore, if neglecting the Stoner model [*i.e.*, $g = 0$], then the maximal RE in absolute value of the present results is now found to be equal to 0.0625% ($>0.036\%$), suggesting that such a Stoner model used is needed to obtain a better accuracy.

Now, it is interesting to extend our numerical results of $E(r_s, \zeta)$ for $0 \leq \zeta \leq 1$ at higher density range: $0.1 \leq r_s \leq 30$, being reported in **Table 3**, in which for a comparison we also include some CA's results [4].

Some physical properties derived from our accurate-and-simple forms for $E(r_s, \zeta)$ and $E_c(r_s, \zeta)$ given in Equa-

Table 2. REs (%) of the present results of $E(r_s, \zeta)$ (Present) are compared with those of CA [4] and SPS [11].

r_s	ζ	0	0.185	0.333	0.519	0.667	0.852	1
40	Present	-0.036		-0.006		0.036		-0.032
50	CA	0.200						0.240
	Present	-0.004	0.002	0.017	0.024	0.029	0.027	-0.035
60	Present	-0.004	-0.008	0.001	0.024	0.002	-0.001	-0.019
70	Present	0.001	-0.002	0.006	0.004	-0.006	-0.011	-0.015
75	SPS	0.456	0.459	0.468		0.471		0.444
	Present	0.001	0.001	0.005		-0.011		-0.006
85	Present	0.008		0.003		-0.021		0.004
100	CA	0.210						0.110
	Present	0.008		-0.010		-0.035		0.015

Table 3. Present results of total energy for $0 \leq \zeta \leq 1$ and in $0.1 \leq r_s \leq 30$ compared with CA [4].

r_s/ζ	0	0.185	0.333	0.519	0.667	0.852	1
0.1							
Present	211.587	215.727	225.039	224.470	266.323	302.237	339.130
1 CA	1.17401						
Present	1.17401	1.21047	1.29243	1.46323	1.65502	1.92929	2.29031
2 CA	0.00410						0.25170
Present	0.00383	0.01196	0.03021	0.06820	0.11082	0.18078	0.25174
3							
Present	-0.13519	-0.13189	-0.12449	-0.10909	-0.09184	-0.06359	-0.03517
4							
Present	-0.15628	-0.15455	-0.15067	-0.14260	-0.13359	-0.11891	-0.10436
5 CA	-0.15120						-0.12140
Present	-0.15291	-0.15187	-0.14950	-0.14462	-0.13918	-0.13040	-0.12186
6							
Present	-0.14373	-0.14303	-0.14146	-0.13822	-0.13463	-0.12888	-0.12341
10 CA	-0.10675						-0.10130
Present	-0.10775	-0.10753	-0.10704	-0.10603	-0.10492	-0.10321	-0.10173
15							
Present	-0.08020	-0.08012	-0.07993	-0.07955	-0.07913	-0.07851	-0.07804
20 CA	-0.06329						
Present	-0.06379	-0.06371	-0.06362	-0.06344	-0.06325	-0.06296	-0.06276
30							
Present	-0.04531	-0.04527	-0.04527	-0.04522	-0.04516	-0.04507	-0.04503

tions (1,2) are investigated as follows.

3. Phase Transition

3.1. First-Order Phase Transition from the Total Energy

From the three states such as: the P-state represented by $E_P(r_s)$, the F-state by $E_F(r_s)$, and the Fermi Wigner crystal (W) state by [13]:

$$E_w(r_s) = -\frac{1.79186}{r_s} + \frac{2.65279}{r_s^{3/2}} - \frac{0.73}{r_s^2} + 0(r_s^{-5/2})$$

being obtained at low electron densities and beyond RPA, we can evaluate the total-energy differences: $D_{FP}(r_s) \equiv [E_P(r_s) - E_F(r_s)]$ and $D_{WF}(r_s) \equiv [E_F(r_s) - E_W(r_s)]$.

1) The $D_{FP}(r_s)$ is negative for $r_s < 78.147$ (the P-phase) and positive for $r_s > 78.147$, giving rise to a first-order PE-phase transition which occurs at a critical value: $r_{sC} = 78.147$, in accordance with CA's data [4]: $r_{sC} = 75 \pm 5$ and with ZLC's data [10]: $75 < r_{sC} < 85$. One notes that this critical value: $r_{sC} = 78.147$ corresponds to a critical density: $n_C = 3.37 \times 10^{18} \text{ cm}^3$ being found to be equivalent to the metal-insulator transition in the n-type excited intrinsic Si occurring at $2.71 \times 10^{18} \text{ cm}^3$ [13] and in the P-Si at $3.52 \times 10^{18} \text{ cm}^3$ [14].

2) The $D_{WF}(r_s)$ is negative for $r_s < 115.49$ (the F-phase) and positive for $r_s \geq 115.49$, giving rise to the WF-phase transition which occurs at a critical value: $r_{sC} = 115.49$, in good agreement with CA's data [4]: $r_{sC} = 100 \pm 20$.

We further evaluate the total-energy difference times as: $[E(r_s, \zeta) - E(r_s, 0)] \times r_s^{3/2}$ (Ry) and plot versus spin polarization ζ for different values of r_s in the following **Figure 1**.

Some concluding remarks are given below.

1) At $r_s \leq 63$, the system is P, with the unpolarized phase stable.

2) As the electron density decreases, at $r_s \approx 64.4$, the system becomes unstable with respect to spin fluctuations while ZLC [10] obtained the corresponding instable point at $r_s \approx 50$.

3) The partially polarized states become stable at $r_s \approx 65.6$.

4) As the electron density continues to decrease, the fully polarized state has a lower energy with respect to unpolarized state at $r_s \geq 78.147$ while a corresponding ZLC's estimation [10] is $r_s \geq 80$. We also find that the partially polarized state has an even lower energy.

3.2. Second-Order Phase Transition from the Spin Susceptibility

First of all, if denoting the unit vector, Bohr magneton, magnetic field and spin susceptibility, respectively, by: $u \equiv M/M$, $\mu_B = 9.274096 \times 10^{-21}$ (erg/G), B(G) and χ (erg/cm³·G²) the magnetization vector is given by: $\vec{M} \equiv (n^\uparrow - n^\downarrow) \mu_B \vec{u} = (n \mu_B) (\zeta \vec{u}) = x (B \vec{u})$, leading to: B

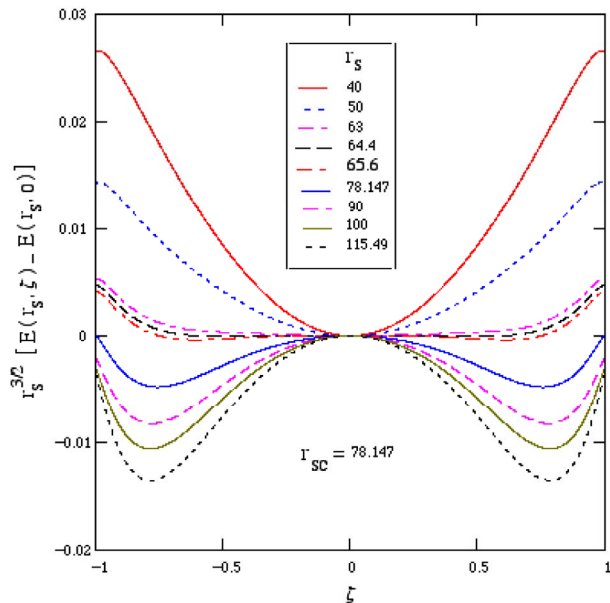


Figure 1. $r_s^{3/2} [E(r_s, \zeta) - E(r_s, 0)]$ vs ζ for different r_s .

$= \zeta n \mu_B / \chi$. Then, the interaction-energy density U required to build up this magnetization is given by

$$U = \int_0^M B dM' = \int_0^M (M'/\chi) dM' = (1/2\chi) M^2 = (1/2\chi) (\zeta n \mu_B)^2 \tag{8}$$

Now, from Equation (1), by a variable change: $x = c\zeta$, c being a length unit, x thus varies from $-c$ to c and the U3DEG induces from the Hook's law an elastic (or conservative) force for $|\zeta| \ll 1$: $\vec{F}(x) = -dE(r_s, x/c)/dx \vec{u} = -k_1(r_s) x \vec{u}$, where the spring constant (or force constant) is defined by: $k_1(r_s) \equiv (d^2 E(r_s, x/c)/dx^2)_{x=0} \equiv (d^2 E(r_s, \zeta)/c^2 d\zeta^2)_{\zeta=0} \equiv [k(r_s)/c^2]$, that gives:

$$k(r_s) = (2/3 r_s^2 \alpha^2) - (3g/5 \alpha^2) - (2/3 \pi r_s \alpha) + \alpha_c(r_s),$$

being a simple-and-analytic form and used to compute following physical quantities.

Then, in such an elastic-force model, the work required to build up the magnetization is

$$\Delta E \left(r_s, \frac{x}{c} = \zeta \right) \equiv E \left(r_s, \frac{x}{c} = \zeta \right) - E(r_s, 0) = \int_0^x k_1 x' dx' = (1/2) k_1 x^2 = (1/2) k \zeta^2,$$

being used to define the interaction-energy density by: $U = n \Delta E(r_s, \zeta)$, identical to the result (8), that leads to a simple form for the spin susceptibility χ (erg/cm³·G²) as:

$$\chi(r_s) \equiv N(r_s) \mu_B^2 / k(r_s) \tag{9}$$

We now evaluate our present result (9) and plot versus r_s in the following **Figure 2**, in which we also report other results from [8,9], indicating that our present result of χ shows a singularity at a critical value: 65.6, defining thus the second-order PF-phase transition, which can be compared with ZLC's result [10]: 50.

4. Some Thermodynamic-Optical Phenomena

1) We first investigate the Ferrell's condition for the stability of the total energy $E(r_s, \zeta)$ defined by [7]:

$$\left[r_s^2 E(r_s, \zeta) \right]_{r_s}^{(2)} = 2E(r_s, \zeta) + 4r_s \left[E(r_s, \zeta) \right]_{r_s}^{(1)} + r_s^2 \left[E(r_s, \zeta) \right]_{r_s}^{(2)} \leq 0 \tag{10}$$

Our numerical calculation indicates that it is valid up to a superior value of r_s found to be given by: $r_{sS} = 1200, 1400, 2200, 2300, 2600, 2700, 16000$ and $+\infty$ for $\zeta = 0, 0.5, 0.78, 0.79, 0.83, 0.84, 0.99$ and 1, respectively, suggesting that r_{sS} increases with increasing ζ .

2) The electronic pressure is defined [7] and related to the generalized virial theorem given in Equation (A4) of

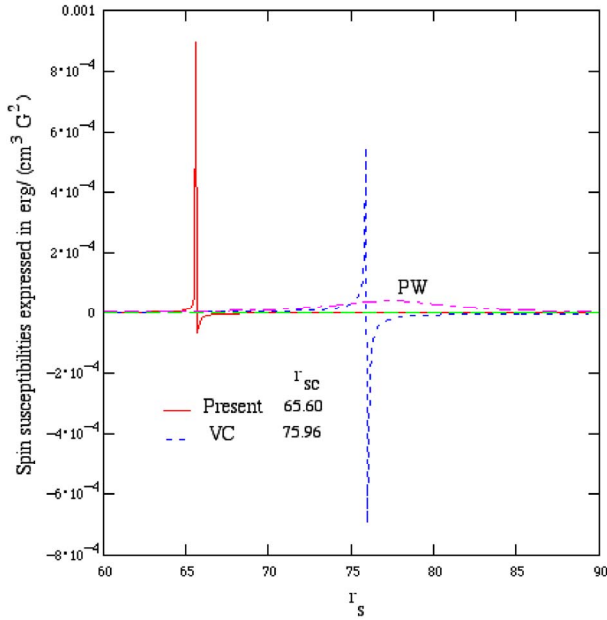


Figure 2. Spin susceptibilities vs r_s .

the Appendix A by:

$$P(r_s, \zeta) = -nr_s \times [E(r_s, \zeta)]_{r_s}^{(1)} / 3 \quad (11)$$

$$= (n/3) [2T(r_s, \zeta) + V(r_s, \zeta)],$$

which becomes negative for $r_s \geq 4.1908$ at $\zeta = 0$ (in good accordance with the Ichimaru's result [7], $r_s > 4.2$), for $r_s \geq 4.569$ at $\zeta = 0.5$, and for $r_s \geq 5.653$ at $\zeta = 1$. This means that the equilibrium densities of the total energy $E(r_s, \zeta)$ occur at 4.1908, 4.569 and 5.653 for $\zeta = 0, 0.5$ and 1, respectively, suggesting that those values increase with increasing ζ .

3) The compressibility of the non-interacting U3DEG is defined by: $\kappa_o(r_s, \zeta) = 3/[2nE_F(r_s, \zeta)]$, where $E_F(r_s, \zeta)$ is the Fermi energy, and via the compressibility sum rule, the inverse reduced compressibility can thus be evaluated by:

$$\kappa_o(r_s, \zeta) / \kappa(r_s, \zeta) = 1 - [4\alpha r_s \gamma_o(r_s, \zeta)] / \pi, \quad (12)$$

where $\gamma_o(r_s, \zeta)$ is determined in Equation (B3) of the the Appendix B.

Our numerical calculation indicates that it becomes negative for $r_s \geq 5.2597$ at $\zeta = 0$ (in good accordance with the Ichimaru's result [7]: $r_s > 5.3$), for $r_s \geq 5.08$ at $\zeta = 0.5$, and for $r_s \geq 4.55$ at $\zeta = 1$, noting also that this negative compressibility does not imply an instability of the system when a rigid background of compensating charge is assumed.

4) Finally, in order to compare the two functions γ_∞ and γ_o determined in Equations (B2) and (B3) of the Appendix B, we can study the asymptotic forms for plas-

mon dispersion coefficient β as follows.

For sufficiently low plasmon energies ($\hbar\omega_p$) and if one disregards the relaxation effect in the short-time domain, β is thus reduced to [7]: $\beta_o(r_s, \zeta) \approx \beta_{RPA}(r_s, \zeta) - (\omega_p/4\omega_F)\gamma_o(r_s, \zeta)$, where $\omega_F \equiv E_F/\hbar$ and in the RPA: $\beta_{RPA} = 3\omega_F/5\omega_p$, and for a sufficiently high plasmon energies, one obtains [7]: $\beta_\infty(r_s, \zeta) \approx \beta_{RPA}(r_s, \zeta) - (\omega_p/4\omega_F)\gamma_\infty(r_s, \zeta)$. Therefore, one gets:

$$R(r_s, \zeta) \approx \frac{\beta_o(r_s, \zeta) - \beta_{RPA}(r_s, \zeta)}{\beta_\infty(r_s, \zeta) - \beta_{RPA}(r_s, \zeta)} = \frac{\gamma_o(r_s, \zeta)}{\gamma_\infty(r_s, \zeta)}. \quad (13)$$

giving for any r_s and ζ : $1.3 \leq R(r_s, \zeta) \leq 1.7$, meaning that $(r_s, \zeta) > 1$ or $\beta_o(r_s, \zeta) > \beta_\infty(r_s, \zeta)$.

5. Concluding Remarks

In summary, we have developed simple analytic forms for $E(r_s, \zeta)$ and $E_c(r_s, \zeta)$, by basing on the Stoner model and interpolation between correct HLDL with the use of a two-point approach for correlation energy and spin stiffness at $r_s = 1$ and 70, giving rise to:

1) A best precision of the order of 0.036% for our present form for total energy, being found to be more accurate compared with other works [4,8,9,11], as given in **Table 2**, and

2) A satisfactory description of some physical properties such as: PF-phase transition and thermodynamic and optical phenomena, as given in above Sections 3 and 4.

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Appendix A. Generalized Virial Theorem

If denoting the average kinetic and potential energies by $T(r_s, \zeta)$ and $V(r_s, \zeta)$, respectively, the conjunction taken here is then given in the form:

$$T(r_s, \zeta) + V(r_s, \zeta) = E(r_s, \zeta). \quad (\text{A1})$$

From [8], from which we replace the correlation energy by the total energy, the chemical potential for electrons of spin σ is defined by:

$$\begin{aligned} \mu_E^s(r_s, \zeta) &\equiv [nE(r_s, \zeta)]_{n_s}^{(1)} = E(r_s, \zeta) \\ &- \frac{r_s}{3} [E(r_s, \zeta)]_{r_s}^{(1)} - (\zeta - \text{sgn } \sigma) [E(r_s, \zeta)]_{\zeta}^{(1)}, \end{aligned} \quad (\text{A2})$$

where $\text{sgn } \sigma$ is +1 for $s = \uparrow$ and -1 for $s = \downarrow$. Taking into account Equation (A2), we define the average kinetic energy, expressed in terms of chemical potentials: $\mu_E^\uparrow(r_s, \zeta)$ and $\mu_E^\downarrow(r_s, \zeta)$, by [8]:

$$\begin{aligned} T(r_s, \zeta) &\equiv -4E(r_s, \zeta) + (3/2) \\ &\left\{ \left[\mu_E^\uparrow(r_s, \zeta) + \mu_E^\downarrow(r_s, \zeta) \right] + \zeta \left[\mu_E^\uparrow(r_s, \zeta) - \mu_E^\downarrow(r_s, \zeta) \right] \right\}, \end{aligned}$$

which reduces to:

$$\begin{aligned} T(r_s, \zeta) &= -E(r_s, \zeta) - r_s [E(r_s, \zeta)]_{r_s}^{(1)} \\ &= -[r_s E(r_s, \zeta)]_{r_s}^{(1)} \end{aligned} \quad (\text{A3})$$

Then, replacing the conjunction (A1) in Equation (A3), the virial theorem generalized to the case of $0 \leq \zeta \leq 1$ is proved:

$$2T(r_s, \zeta) + V(r_s, \zeta) = -r_s \times [E(r_s, \zeta)]_{r_s}^{(1)}, \quad (\text{A4})$$

reducing to that given in [12] for $\zeta = 0$. Our numerical calculation indicates that this result (A4) becomes negative for $r_s \geq 4.1908$ at $\zeta = 0$, for $r_s \geq 4.569$ at $\zeta = 0.5$, and for $r_s \geq 5.653$ at $\zeta = 1$, meaning that the equilibrium densities of the total energy $E(r_s, \zeta)$ occur at $r_{sEq} = 4.1908$, 4.569 and 5.653 for $\zeta = 0$, 0.5 and 1, respectively, suggesting that those values of r_{sEq} increase with increasing ζ .

Appendix B. Useful Expressions $\gamma_{o(\infty)}(r_s, \zeta)$

The analytic forms for $\gamma_o(r_s, \zeta)$ and $\gamma_\infty(r_s, \zeta)$ as $\zeta = 0$ de-

veloped in [7] are now generalized to the case of any ζ . The function $\gamma_o(r_s, \zeta)$ may be related to $\gamma_\infty(r_s, \zeta)$ by [7]:

$$\gamma_o(r_s, \zeta) = -\frac{5\gamma_\infty(r_s, \zeta)}{2} + \frac{5r_s}{12} \times [\gamma_\infty(r_s, \zeta)]_{r_s}^{(1)} + \frac{25}{6} \times \left[\frac{3}{20} - \frac{\pi\alpha r_s E_c(r_s, \zeta)}{10} \right], \quad (\text{B1})$$

where the function $\gamma_\infty(r_s, \zeta)$ used to calculate the total energy can be defined by [7]:

$$\gamma_\infty(r_s, \zeta) \equiv \frac{3h(\zeta)}{20} - \frac{\pi\alpha}{10} \times \left\{ r_s^2 [E_c(r_s, \zeta)]_{r_s}^{(1)} + 2r_s E_c(r_s, \zeta) \right\}, \quad (\text{B2})$$

being replaced in Equation (B1) one finally gets:

$$\gamma_o(r_s, \zeta) = \frac{h(\zeta)}{4} - \frac{\pi\alpha}{24} \times \left\{ r_s^3 [E_c(r_s, \zeta)]_{r_s}^{(2)} - 2r_s^2 [E_c(r_s, \zeta)]_{r_s}^{(1)} \right\}, \quad (\text{B2})$$

noting that Equations (B1,B2) for $\zeta = 0$ are well identical to Ichimaru's results [7].