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 $\zeta$ 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:

$$n\left( r_s \right) = \frac{3}{4\pi a_B^3} \left( 4\pi r_s^3 a_B^3 \right),$$

where $a_B = 0.53 \times 10^{-8}$ cm is the Bohr radius, and the relative spin polarization $\zeta$ defined by:

$$\zeta \equiv \frac{n^\uparrow - n^\downarrow}{n^\uparrow + n^\downarrow},$$

and $n^\uparrow$ and $n^\downarrow$ mean the up-and down-spin electron densities, respectively, noting that the two particular values of $\zeta$ ($= 0$ and $\pm 1$) 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:

$$\frac{\partial^n}{\partial \zeta^n} f(x, y) \equiv \left[ f(x, y) \right]^{(n)}_\zeta,$$

for $n = 1, 2, \cdots$

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 $\zeta$

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

$$E(r_s, \zeta) = E_C^{\text{Stoner}}(r_s, \zeta) + E_C(r_s, \zeta),$$

$$E_C^{\text{Stoner}}(r_s, \zeta) = \left[ K_0 (r_s, \zeta) + \Delta K_0 (\zeta; g) \right] + E_C(r_s, \zeta),$$

for $n = 1, 2, \cdots$

where $E_C(r_s, \zeta) = 3h (\zeta)/(2\pi a_B r_s)$ is the exchange energy, $K_0 (r_s, \zeta) = 3k (\zeta)/S (a_B r_s)$ is the kinetic energy at Fermi surface, $\Delta K_0 (\zeta; g) = 3g (1 - \zeta^2)/10a^2$.
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 $\zeta$ are minimized (its value is given in Table 1). Moreover, we use in this work a general spin-interpolation formula for $E_s(r_s, \zeta)$ proposed by Vosko et al. [5]

$$E_s(r_s, \zeta) = E_s(r_s, 0) + \alpha(r_s)[f(\zeta)/f(\zeta)^{2}]$$

(2)

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

$$2k(\zeta) = (1+\zeta)^{3/2} + (1-\zeta)^{3/2},$$

$$2h(\zeta) = (1+\zeta)^{3/2} + (1-\zeta)^{3/2},$$

$$[2^{3/2} - 1]f(\zeta) = h(\zeta) - 1,$$

that gives:

$$[f(\zeta)^2] = 2[(1+\zeta)^{20} + (1-\zeta)^{20}] / 9[2^{20} - 1] = 1.70992$$

for $\zeta = 0$.

From Equations (1) and (2) one notes that: $E(r_s, \zeta) \equiv E_s(r_s, \zeta)$ and $E(r_s, -\zeta) = E_s(r_s, -\zeta)$, reducing to the interval: $0 \leq \zeta \leq 1$, and that if the three functions: $E_s(r_s, 0), E_s(r_s, 1)$ and $\alpha(r_s)$, represented by $X(r_s; a)$, are known, then $E_s(r_s, \zeta)$ and $E_s(r_s, -\zeta)$ 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 $W(r_s, a)$.

$$X(r_s; a) = W(r_s; a) + [G(r_s) - W(r_s; a)] / [1 + \lambda r_s^a],$$

(3)

reducing in the HDL to: $\operatorname{Lim} X(r_s; a) = G(r_s)$ and in the LDL to: $\operatorname{Lim} X(r_s; a) = W(r_s; a)$. 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.

<table>
<thead>
<tr>
<th>$r_s$</th>
<th>$E_s(r_s)$</th>
<th>$E_s(r_s)$</th>
<th>$\alpha(r_s)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$X_1$ [9]</td>
<td>-119.517</td>
<td>-63.185</td>
<td>80.64</td>
</tr>
<tr>
<td>$Y$ [9]</td>
<td>62.18</td>
<td>31.09</td>
<td>-33.77</td>
</tr>
<tr>
<td>$Z$ [9]</td>
<td>93.288</td>
<td>51.198</td>
<td>-70.95</td>
</tr>
<tr>
<td>$a$</td>
<td>0.0908</td>
<td>0.085</td>
<td>33.77</td>
</tr>
<tr>
<td>$g = 7.7 \times 10^{-3}$ from Stoner model</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>( r_s )</th>
<th>( \zeta )</th>
<th>0</th>
<th>0.185</th>
<th>0.333</th>
<th>0.519</th>
<th>0.667</th>
<th>0.852</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>Present</td>
<td>0.036</td>
<td>0.185</td>
<td>0.333</td>
<td>0.519</td>
<td>0.667</td>
<td>0.852</td>
<td>1</td>
</tr>
<tr>
<td>50</td>
<td>CA</td>
<td>0.200</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>0.004</td>
<td>0.002</td>
<td>0.017</td>
<td>0.024</td>
<td>0.029</td>
<td>0.027</td>
<td>0.035</td>
</tr>
<tr>
<td>60</td>
<td>Present</td>
<td>0.004</td>
<td>-0.008</td>
<td>0.001</td>
<td>0.024</td>
<td>0.002</td>
<td>-0.001</td>
<td>-0.019</td>
</tr>
<tr>
<td>70</td>
<td>Present</td>
<td>0.001</td>
<td>-0.002</td>
<td>0.006</td>
<td>0.004</td>
<td>-0.006</td>
<td>-0.011</td>
<td>-0.015</td>
</tr>
<tr>
<td>75</td>
<td>SPS</td>
<td>0.456</td>
<td>0.459</td>
<td>0.468</td>
<td>0.471</td>
<td>0.444</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>0.001</td>
<td>0.001</td>
<td>0.005</td>
<td>-0.011</td>
<td>-0.006</td>
<td></td>
<td></td>
</tr>
<tr>
<td>85</td>
<td>Present</td>
<td>0.008</td>
<td>0.003</td>
<td>-0.021</td>
<td>0.004</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>100</td>
<td>CA</td>
<td>0.210</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>Present</td>
<td>0.008</td>
<td>-0.010</td>
<td>-0.035</td>
<td>0.015</td>
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</tr>
</tbody>
</table>

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].

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

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]:

\[
E_w(r_s) = -\frac{1.79186}{r_s^2} + \frac{2.65279}{r_s^{3/2}} - \frac{0.73}{r_s} + 0\left(r_s^{-3/2}\right)
\]

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

1) The \( D_{\text{FP}}(r_s) \) 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 $D_{nn}(r_s)$ 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: $r_{cc} = 115.49$, in good agreement with CA’s data [4]: $r_{cc} = 100 \pm 20$.

We further evaluate the total-energy difference times as:

$$E(r_s,\zeta) - E(r_s,0) \times \hat{r}^{1/2}$$

and plot versus spin polarization $\zeta$ 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 partially polarized states continue to decrease, the fully polarized state is then a lower energy with respect to unpolarized states 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: $u = M/M$, $\mu_B = 9.274096 \times 10^{-21}$ (erg/G), $B(G)$ and $\chi$ (erg/cm$^3$·G$^2$) the magnetization vector is given by:

$$M = (n^+ - n^-) \mu_B u = (n\mu_B)(\hat{\zeta} \hat{u}) = x(B\hat{u})$$

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

$$U = \int_0^M B dM' = \int_0^M (M'/\chi) dM' = (1/2\chi)M^2$$

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 $\zeta < 115.49$ (the F-phase)

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

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

$$\Delta E = \int_0^r \frac{k(x)}{c^2} dx = \int_0^r \frac{k(x)}{c^2} dx = (1/2)kx^2 = (1/2)k\zeta^2,$$

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 $\chi(\text{erg/cm}^3\cdot\text{G}^2)$ as:

$$\chi(r_s) = N(r_s)\mu_B^2/k(r_s)$$

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 $\chi$ 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]:

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

Our numerical calculation indicates that it is valid up to a superior value of $r_s$ 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 $\zeta$.

2) The electronic pressure is defined [7] and related to the generalized virial theorem given in Equation (A4) of
the Appendix A by:
\[
P(r_s, \zeta) = -n_r \times \left[ E(r_s, \zeta) \right]_{\text{Rs}}^{(l)} / 3
\]
\[
= \left( n/3 \right) \left[ 2T(r_s, \zeta) + V(r_s, \zeta) \right],
\]
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 \( \zeta \).

3) The compressibility of the non-interacting U3DEG is defined by: \( \kappa_s(r_s, \zeta) = 3 \left[ 2n_r E^2_s(r_s, \zeta) \right] \), where \( E_s(r_s, \zeta) \) is the Fermi energy, and via the compressibility sum rule, the inverse reduced compressibility can thus be evaluated by:
\[
\kappa_s(r_s, \zeta) / \kappa(r_s, \zeta) = 1 - \left[ 4a_r \gamma_s(r_s, \zeta) \right] / \pi,
\]
where \( \gamma_s(r_s, \zeta) \) is determined in Equation (B3) of 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 \( \gamma_c \) and \( \gamma_s \) determined in Equations (B2) and (B3) of the Appendix B, we can study the asymptotic forms for plasmon dispersion coefficient \( \beta \) as follows.

For sufficiently low plasmon energies (\( \hbar \omega_p \)) and if one disregards the relaxation effect in the short-time domain, \( \beta \) is thus reduced to [7]:
\[
\beta_s(r_s, \zeta) \approx \beta_{\text{RPA}}(r_s, \zeta) - (\omega_p/4a_r) \gamma_s(r_s, \zeta),
\]
where \( \omega_p = E_F / h \) and in the RPA:
\[
\beta_{\text{RPA}} = 3 \omega_p / 5 a_r,
\]
and for a sufficiently high plasmon energies, one obtains [7]:
\[
\beta_s(r_s, \zeta) \approx \beta_{\text{RPA}}(r_s, \zeta) - (\omega_p/4a_r) \gamma_s(r_s, \zeta). \tag{13}
\]

Figure 2. Spin susceptibilities vs \( r_s \)

5. Concluding Remarks

In summary, we have developed simple analytic forms for \( E(r_s, \zeta) \) and \( E_s(r_s, \zeta) \), 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 [4,9,11], as given in Table 2.

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.

6. Acknowledgements

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7. References


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:

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

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

$$\mu_{r_s}^\sigma (r_s, \zeta) = \left[ nE(r_s, \zeta) \right]_{rs}^{(0)} = E(r_s, \zeta)$$

$$-\frac{r_s}{3} \left[ E(r_s, \zeta) \right]_{rs}^{(1)} - (\zeta - \text{sgn} \sigma) \left[ E(r_s, \zeta) \right]_{rs}^{(1)}, \tag{A2}$$

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: $\mu_{r_s}^\delta (r_s, \zeta)$ and $\mu_{r_s}^\gamma (r_s, \zeta)$, by [8]:

$$T(r_s, \zeta) = -4E(r_s, \zeta) + (3/2)$$

$$\left[ \mu_{r_s}^\delta (r_s, \zeta) + \mu_{r_s}^\gamma (r_s, \zeta) \right] + \zeta \left[ \mu_{r_s}^\delta (r_s, \zeta) - \mu_{r_s}^\gamma (r_s, \zeta) \right],$$

which reduces to:

$$T(r_s, \zeta) = -E(r_s, \zeta) - \frac{r_s}{3} \left[ E(r_s, \zeta) \right]_{rs}^{(1)}$$

$$- (\zeta - \text{sgn} \sigma) \left[ E(r_s, \zeta) \right]_{rs}^{(1)} \tag{A3}$$

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

$$2T(r_s, \zeta) + V(r_s, \zeta) = -r_s \times \left[ E(r_s, \zeta) \right]_{rs}^{(1)}, \tag{A4}$$

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 $r_{\text{eq}} = 4.1908$, 4.569 and 5.653 for $\zeta = 0, 0.5$ and 1, respectively, suggesting that those values of $r_{\text{eq}}$ increase with increasing $\zeta$.

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

The analytic forms for $\gamma_o(r_s, \zeta)$ and $\gamma_\omega(r_s, \zeta)$ as $\zeta = 0$ de-
The function $y_o(r, \zeta)$ may be related to $y_\infty(r, \zeta)$ by [7]:

$$y_o(r, \zeta) = -\frac{5y_\infty(r, \zeta)}{2} + \frac{5r_r}{12} \times \left[ y_\infty(r, \zeta) \right]_o^{(l)}$$

$$+ \frac{25}{6} \times \left[ \frac{3}{20} \pi \alpha r_r E_i(r, \zeta) \right]_o^{(l)},$$

(B1)

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

$$y_\infty(r, \zeta) = \frac{3h(\zeta)}{20} - \frac{\pi \alpha}{10}$$

$$\times \left\{ r_r^3 \left[ E_i(r, \zeta) \right]_o^{(l)} + 2r_r E_i(r, \zeta) \right\},$$

(B2)

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