Turk J Phys
27 (2003) , 107 – 119.

Semi-Infinite Polarized Nuclear Matter with a Seyler-Blanchard Interaction

Hesham Mohamed Mohamed MANSOUR, Khaled Abd El Aziz RAMADAN
Physics Department, Faculty of Science, Cairo University, Giza-EGYPT

Received 11.03.1999

Abstract

The surface and curvature properties of semi-infinite polarized nuclear matter (SPNM) are calculated using a modified form of the Seyler-Blanchard potential. The level density parameter is extracted from the free energy using T^2-approximation. Good agreement is obtained between our calculations for the level density and other parameters which characterize the surface and curvature properties of SPNM and previous theoretical estimates.

PACS number(s): *21.65.+f, 21.30.Fe*

Key Words: Nuclear matter, Free energy, Level density parameters, Seyler-Blanchard interaction.

1. Introduction

An important aspect of finite nuclei and SPNM is their surfaces. This is simply because it affects the binding energy, reactions and level spectra.

One approach to study such systems is by using the liquid drop model (LDM). In the LDM the energy of the nucleus is written as a sum of volume, surface, curvature and Coulomb terms. The surface and curvature properties are very interesting and have several applications in heavy ion collisions and astrophysics, e.g., in studying supernovas and neutron stars. It is of interest to determine equilibrium sizes of nuclei; electron capture rates [1] and level densities [2]. Also, the phase transition [3] between nuclei and bubbles has astrophysical applications. Similarly, liquid-gas phase transition may occur in heavy-ion collisions. Surface and curvature energies are important in calculating fission barriers, heights and shapes of the saddle point configuration [4]. Studying the temperature effects on the bulk properties of semi-infinite nuclear matter (SNM) leads to a sensitive quantity, namely, the level density parameter, which is a good parameter for testing theoretical calculations.

In this work an attempt is made to test a modified Seyler-Blanchard potential [5], to study the effect of symmetry excess parameters on the surface and curvature properties of SNM, and to estimate their dependence by studying the effect of those parameters on the level density parameters. We start with a two-body extended Seyler-Blanchard [5] potential to calculate the energy of SPNM; then the density matrix is expanded in the relative coordinates up to second order to account for the gradient term of the potential. An expansion up to T^2 to obtain the free energy is then used. In addition, we use a Woods-Saxon form for the density and expanded the free energy in powers of $A^{1/3}$. Analytical expansions are obtained for the surface and curvature properties in terms of the potential parameters up to second order in the temperature and symmetry excess parameters.

In the present work, we use the set, of parameters given in Ref [6]. In section II we present the theory and section III is devoted to the results and discussion.

2. Theory

The direct two-body matrix element between two nucleons in the states i and j is given by

$$< ij|V|ij >= \int \rho_i(\mathbf{r}_1)\rho_j(\mathbf{r}_2)V(\mathbf{r},\mathbf{s})d\mathbf{r}d\mathbf{s} \tag{1}$$

where $\mathbf{r} = \frac{1}{2}(\mathbf{r}_1+\mathbf{r}_2)$ is the center of mass coordinates and $\mathbf{S} = (\mathbf{r}_1-\mathbf{r}_2)$ is the relative coordinate. Expanding ρ in powers of s, we obtain

$$\rho_i(\mathbf{r}_1) = \rho_i(\mathbf{r}) + \frac{1}{2}\mathbf{s}\cdot\nabla\rho_i(\mathbf{r}) + \frac{1}{8}\,\mathbf{s}\cdot\nabla\Big(\mathbf{s}\cdot\nabla\rho_i(\bar{\mathbf{r}})\Big). \tag{2}$$

From Equations (1) and (2) we get

$$\begin{aligned} < ij|V|ij > \quad = \quad & \int \rho_i(\mathbf{r}_1)\rho_j(\mathbf{r}_2)V(r,s)d\mathbf{r}d\mathbf{s} \\ & -\frac{1}{6}\iint \nabla\rho_i(\mathbf{r})\cdot\nabla\rho_i(\mathbf{r})V(\mathbf{r},\mathbf{s})d\mathbf{r}s^2d\mathbf{s} \end{aligned} \tag{3}$$

The potential used here is the Seyler-Blanchard potential [5,7] which is given in the form

$$V(\mathbf{r},\mathbf{s}) = -C_L, u\frac{e^{-s/a}}{s/a}(1-\frac{P^2}{b^2}) = V(\mathbf{r})V(\mathbf{s}) \tag{4}$$

The potential energy E_p of polarized NM is given in Appendix A. The kinetic energy term in the extended TF approximation is given by

$$K.E. = \frac{\hbar^2}{2m}\int [\alpha\rho_{\tau,s}^{5/3} + \beta\frac{(\nabla\rho_{\tau,s})^2}{\rho_{\tau,s}} + \gamma\nabla^2\rho_{\tau,s}]d\mathbf{r} \tag{5}$$

where τ = neutron (n) or proton (p), and s = spin up (↑) or spin down(↓), and

$$\alpha = \frac{3}{5}(3\pi^2/2)^{2/3}$$

$$\beta = \frac{1}{36}\left[1 - \frac{21\pi^2}{12\times 8}\left(\frac{3\pi^2}{2}\right)^{4/3}T^2\rho^{4/3} + \frac{3\times 31\pi^4}{(12)^2\times 8}\left(\frac{3\pi^2}{2}\right)^{8/3}T^2\rho^{8/3}\right] \tag{6}$$

At T = 0, the values of β and γ are taken as

$$\beta = \frac{1}{36} \quad \text{and} \quad \gamma = 1/3.$$

Using a Woods- Saxon form for the densities in SPNM one can calculate the total energy E and the free energy F = E − TS, where S is the entropy.

In the low temperature limit, the entropy per nucleon becomes

$$S = \frac{\pi^2}{4}\sum_{\tau,s}\rho_{\tau,s}[\frac{2m}{\hbar^2 b_{\tau,s}K_f^2}]T + O(T^3). \tag{7}$$

This equation can be written as

$$S = S_V + S_x X^2 + S_y Y^2 + S_z Z^2, \tag{8}$$

where

$$S_V = \pi^2 mT/\hbar^2 b_{\tau,s} K_f^2, \tag{9}$$

$$S_x = S_y = S_z = -\pi^2 mT/9\hbar^2 b_{\tau,s} K_f^2 \tag{10}$$

and X, Y and Z are the neutron excess parameter, spin up nucleon excess parameter and the spin-down neutron excess parameter, respectively. The total free energy of the SPNM can be written as the sum of volume, surface and curvature terms (see Appendix A):

$$F = F_v A + F_s A^{2/3} + F_c A^{1/3} \tag{11}$$

where

$$F_v = F_{vo} + F_{vx} X^2 + F_{vy} Y^2 + F_{vz} Z^2 \tag{12}$$

$$F_s = F_{so} + F_{sx} X^2 + F_{sy} Y^2 + F_{sz} Z^2, \tag{13}$$

and

$$F_c = F_{co} + F_{cx} X^2 + F_{cy} Y^2 + F_{cz} Z^2 \tag{14}$$

The surface diffuseness parameter d is defined as a function of the temperature and symmetry parameters by minimization of F_v with respect to d, i.e., $\partial F/\partial d = \partial F_s/\partial d = 0$. By writing

$$F_s = P(\rho_o) d + N(\rho_o)/d \tag{15}$$

then

$$d = [N(\rho_o)/P(\rho_o)]^{1/2} \tag{16}$$

where

$$N(\rho_o) = N_o + N_x X^2 + N_y Y^2 + N_z Z^2 \tag{17}$$

and

$$P(\rho_o) = P_o + P_x X^2 + P_y Y^2 + P_z Z^2, \tag{18}$$

The functions N_o, N_i, ρ_o and ρ_i are given in Appendix (B). The density in the above equations is the equilibrium density for zero temperature symmetric NM. In SPNM, we obtain the equilibrium density by minimizing the free energy with respect to ρ_o, i.e.,

$$\frac{\partial F}{\partial \rho_o} = \frac{\partial F_v}{\partial \rho_o} = 0 \tag{19}$$

Hence, ρ_o may take the form

$$\begin{aligned}\rho_o &= \rho_{on}[1 - \frac{9\rho_{on}}{K}\frac{\partial F_x}{\partial \rho_o}|_{\rho_{on}} X^2 + \frac{\partial F_y}{\partial \rho_o}|_{\rho_{on}} Y^2 + \frac{\partial F_z}{\partial \rho_o}|_{\rho_{on}} Z^2 \\ &\quad + \frac{\pi^2 m T^2}{3\rho_{on}^{5/3}}(\frac{2}{3\pi^2})^{2/3}]\end{aligned} \tag{20}$$

and we get

$$\rho_o = \rho_{on}[1 - \rho_T T^2 - (\rho_x - \rho' T^2)X^2 - (\rho_y - \rho' T^2)Y^2 - (\rho_z - \rho' T^2)Z^2], \tag{21}$$

where

$$\rho_i = \frac{-9\pi a^3}{2K} C_i \rho_{on} + \frac{10\pi a^3}{Kb^2}(\frac{3\pi^2}{8})^{2/3} C_i' \rho_{on}^{5/3} + \frac{h^2}{km}(\frac{3\pi^2}{2})^{2/3}\rho_{on}^{2/3} \tag{22}$$

$$\rho' = \frac{\pi^2 m}{3h^2 K \rho_{on}^{2/3}}(\frac{2}{3\pi^2})^{2/3} \tag{23}$$

$$\rho_T = 9\rho\prime \tag{24}$$

and i runs over X, Y and Z.

The surface and curvature properties as well as the diffuseness parameter are calculated at the equilibrium density of symmetric NM up to second order in T, X, Y, and Z and the results are given in Appendix C, viz.,

$$d = d_o + \alpha_o T^2 + (d_x + \alpha_x T^2)X^2 + (d_y + \alpha_y T^2)Y^2 + (d_z + \alpha_z T^2)Z^2 \tag{25}$$

$$F_s = F_{so} + a_{so}T^2 + (F_{sx} + a_{sx}T^2)X^2 + (F_{sy} + a_{sy}T^2)Y^2 + (F_{sz} + a_{sz}T^2)Z^2 \tag{26}$$

$$F_c = F_{co} + a_{co}T^2 + (F_{cx} + a_{cx}T^2)X^2 + (F_{cy} + a_{cy}T^2)Y^2 + (F_{cz} + a_{cz}T^2)Z^2 \tag{27}$$

Also, the level density parameter can be expressed as

$$a_i = a_{io} + a_{ix}X^2 + a_{iy}Y^2 + a_{iz}Z^2 \tag{28}$$

where

$$a_{vo} = \frac{\pi^2 m}{2\hbar^2}(\frac{2}{3\pi^2})^{2/3}\rho_o^{-2/3} \tag{29}$$

and

$$a_{vx} = a_{vy} = a_{vz} = -\frac{1}{9}a_{vo} \tag{30}$$

3. Results and Discussion

In our previous work [6], the EOS was used to study the bulk properties of PNM using different versions of the Seyler- Blanchard interaction. Here, we study the surface and curvature properties of SPNM using the set of parameters for the Seyler-Blanchard interaction as discussed previously in Ref [6].

The results below are given for different forms of ρ_o, viz.,

$$\rho_o = \rho_{on} \tag{31}$$

$$\rho_o = \rho_{on}(1 - \rho_T T^2) \tag{32}$$

and the full expression given by Equation (21). Equations (21), (31) and (32) are here referred to as PW1, PW2 and PW3, respectively.

Table 1 gives the coefficients of the density expansion, Equation (21), in comparison with previous works. We notice that there is fair agreement between the values of the coefficient ρ_z with that of Ref. [8], but there is a difference in the values of ρ_x and ρ_y Table 2 gives the coefficients of the diffuseness parameter d, Eq. (25). The values of d_o is less than the empirical value ($d_o = 0.5$ fm [19]) by a small factor. This result can be modified by using the Fermi distribution for the density [15]. The parameter α_o has different values corresponding to the application of different forms of ρ_o. It is also sensitive to the two body interaction used. The effect of d_i is to decrease the diffuseness parameter in the case PW3 and increase it in the case PW1 and PW2, which is in agreement with the other calculations [9]. The effect of α_i is to decrease (increase) the diffuseness parameter in case of PW2 (PW1 and PW3). The parameters of the surface energy, Eq. (26), are listed in Table 3. The values obtained are in agreement with the previous theoretical estimates [20]. The values of a_{so} is very sensitive to the form of density used (PW1, PW2 and PW3) and it varies largely with the type of the force used. We notice from Table 3 that the values found in the literature for the surface symmetry energy F_{sx} lies between: – 22 and 97 MeV [19], and our values of F_{sx} lies in the same range. The coefficients of the expansion of the curvature free energy, Eq. (27), are listed in Table 4. F_{co} agrees with the known theoretical values, which lies between 6 and 13 MeV. Here again the results are comparable with previous works.

Table 1. Coefficients of the density expansion [Eq. (21)]. The units of these coefficients are fm^{-3}. (PW: present work)

ρ_{on}	ρ_X	ρ_Y	ρ_Z	ρ_t	$\rho\prime$	Ref.
0.1533	0	0	0	0	0	PW1
0.1533	0	0	0	0.0013	0.0015	PW2
0.1533	0.742	0.609	0.958	0.0013	0.00015	PW3
0.1440	0.09	1.62	0.84	0.012		[8]
0.2250	0.49					[9]
0.1850	0.45					[10]

The volume level density parameter, Eq. (28), is given in Table 5 for PW3. The results for PW1 and PW2 are the same as those of PW3 for a_{vo} but differ slightly for a_{vi}. The values of a_{vo} is in agreement with the values in the literature ([11,13,17]). The agreement between the calculated level density parameter and the experimental values reflects the fact that our formulas for the temperature of the surface and curvature properties are reasonable.

The present approximation of using $T = 0$, ETF functional and adding the lowest T^2 correlation has been shown to fail for the level density parameter a, giving an overestimation of about 30%. Also several new values for the parameters a_{vi}, a_{si} and a_{ci} are calculated in this work.

Table 2. Coefficients of the diffuseness parameter expansion equation (25). The units of d_i are fm and the units of α_i are fm Mev^{-2}.

Parameter / Force	d_o	d_X	d_Y	d_Z	α_o $\times 10^3$	α_X $\times 10^3$	α_Y $\times 10^3$	α_Z $\times 10^3$
PW1	0.431	0.36	0.37	0.35	0.0038	0.040	0.40	0.041
PW2	0.31	0	0	0	0.007	0	0	0
PW3	0.31	-0.286	-0.209	-0.42	0.007	0.229	0.179	0.316
SII	0.421[a]				0.0035[a]			
SIII	0.398[a]				0.0033[a]			
SIV	0.445[a]				0.0037[a]			
SV	0.467[a]				0.0038[a]			
SVI	0.394[a]				0.003[a]			
SKT	0487				0.0043[a]			
SEI	0.469[a]				0.0041[a]			

[a]Reference [11].

Table 3. Coefficients of the surface free energy expansion [Eq. (26)]. The units of F_{si} are Mev and the units of a_{si} are Mev^{-1}.

Parameter / Force	$-F_{so}$	$-F_{sx}$	$-F_{sy}$	$-F_{sz}$	a_{so}	a_{sx}	a_{sy}	a_{sz}
PW1	60.85	-25.73	-17.91	-38.49	-0.141	0.0157	0.0157	0.0157
PW2	57.56	-17.43	-13.57	-23.72	-0.143	0.0159	0.0159	0.0159
PW3	57.19	-17.26	-13.43	-23.51	-0.144	0.016	0.016	0.016
SII	19.65[a]	52[b]			0.189[a]			
	20.08[c]				-0.199[c]	-0.917[c]		
	20.17[d]	60[d]						
SIII	18.9[a]	29[d]			0.183[e]			
	19.29[c]	47.9[c]			-0.194[c]	0.0171[c]		
	18.89[e]	33.2[e]						
	20.37[f]				0.233[g]			
	18.79[d]	35[d]						
	18.04[h]	88.11[h]						
SIV	20.28[a]	55[b]			-0.193[a]			
	18.75[c]	29.6[c]			-0.185[c]	0.0161[c]		
	20.12[d]	64[d]						
SKM (ITF)	61.61[h]	58.64[h]			-0.139[g]			

[a]Reference [11] [b]Reference [12] [c]Reference [13]
[d]Reference [14] [e]Reference [15] [f]Reference [16]
[g]Reference [17] [h]Reference [18]

Table 4. Same as Table 3 but for the curvature free energy expansion [Eq. (27)].

Parameter / Force	$-F_{co}$	$-F_{cx}$	$-F_{cy}$	$-F_{cz}$	a_{co}	a_{cx}	a_{cy}	a_{cz}
PW1	7.085	18.88	14.79	25.56	-0.269	0.029	0.029	0.029
PW2	7.84	24.01	16.54	36.18	-0.269	0.029	0.029	0.029
PW3	7.93	23.82	16.40	35.93	-0.269	0.029	0.029	0.029
SI	6.49[a]	27[a]						
SII	11.6[b]							
SIII	7.22[a]	26[a]						
	11.29[c]				0.103[d]			
	10.0[b]							
	8.66[e]	49.32[e]						
SV	13.8[b]				0.039[d]			
SVI	9.3[b]				0.166[d]			
SKM*	10.63[a]	52[a]						

[a]Reference [15] [b]Reference [14] [c]Reference [16]
[d]Reference [17] [e]Reference [18]

Table 5. Volume level density parameters [Eq. (28) and (29)] in units of Mev^{-1}

Force	a_{vo}	a_{vx}	a_{vy}	a_{vz}
PW3	0.0714	-0.008	-0.008	-0.008
SII	0.041[a]	-0.0035[b]		
SIII	0.054[b,c]	-0.0061[c]		
SIV	0.068[b]	-0.0082[b]		
SKM	0.053[b]	-0.005[b]		

[a]Reference [11], [b]Reference [13], [c]Reference [17]

APPENDIX A

The potential energy E_p of polarized NM (with exchange term neglected) is

$$\begin{aligned}
E_p = & - 2\pi a^3 C_{LL} \int (\rho_{n\uparrow}^2 + \rho_{n\downarrow}^2 + \rho_{p\uparrow}^2 + \rho_{p\downarrow}^2) d\mathbf{r} \\
& + \frac{12\pi a^3}{5b^2} C_{LL} (\frac{3\pi^2}{2})^{2/3} \int (\rho_{n\uparrow}^{8/3} + \rho_{n\downarrow}^{8/3} + \rho_{p\uparrow}^{8/3} + \rho_{p\downarrow}^{8/3}) d\mathbf{r} \\
& - \frac{12\pi a^5}{5b^2} C_{LL} (\frac{3\pi^2}{2})^{2/3} \int [(\nabla\rho_{n\uparrow})^2 \rho_{n\uparrow}^{2/3} + (\nabla\rho_{n\downarrow})^2 \rho_{n\downarrow}^{2/3} + (\nabla\rho_{p\uparrow})^2 \rho_{p\uparrow}^{2/3} + (\nabla\rho_{p\downarrow})^2 \rho_{p\downarrow}^{2/3}] d\mathbf{r} \\
& + 2\pi a^5 C_{LL} \int [(\nabla\rho_{n\uparrow})^2 + (\nabla\rho_{n\downarrow})^2 + (\nabla\rho_{p\uparrow})^2 + (\nabla\rho_{p\downarrow})^2] d\mathbf{r} \\
& - 4\pi a^3 C_{Lu} \int (\rho_{n\uparrow}\rho_{n\downarrow} + \rho_{p\uparrow}\rho_{p\downarrow}) d\mathbf{r} \\
& + \frac{12\pi a^3}{5b^2} C_{Lu} (\frac{3\pi^2}{2})^{2/3} \int [\rho_{n\uparrow}^{5/3}\rho_{n\downarrow} + \rho_{n\downarrow}^{5/3}\rho_{n\uparrow} + \rho_{p\uparrow}^{5/3}\rho_{p\downarrow} + \rho_{p\downarrow}^{5/3}\rho_{p\uparrow}] d\mathbf{r} \\
& + 4\pi a^5 C_{Lu} \int (\nabla\rho_{n\uparrow}\nabla\rho_{n\downarrow} + \nabla\rho_{p\uparrow}\nabla\rho_{p\downarrow}) d\mathbf{r} \\
& - \frac{12\pi a^5}{5b^2} C_{Lu} (\frac{3\pi^2}{2})^{2/3} \int [\nabla\rho_{n\uparrow}\nabla\rho_{n\downarrow}\rho_{n\uparrow}^{2/3} + \nabla\rho_{n\uparrow}\nabla\rho_{n\downarrow}\rho_{n\downarrow}^{2/3} \\
& + \nabla\rho_{p\uparrow}\nabla\rho_{p\downarrow}\rho_{p\uparrow}^{2/3} + \nabla\rho_{p\uparrow}\nabla\rho_{p\downarrow}\rho_{p\downarrow}^{2/3}] d\mathbf{r} \\
& + \frac{12\pi a^3}{5b^2} C_{uL} (\frac{3\pi^2}{2})^{2/3} \int [\rho_{n\uparrow}^{5/3}\rho_{p\uparrow} + \rho_{p\uparrow}^{5/3}\rho_{n\uparrow} + \rho_{n\downarrow}^{5/3}\rho_{p\downarrow} + \rho_{p\uparrow}^{5/3}\rho_{n\uparrow}] d\mathbf{r} \\
& - 4\pi a^3 C_{uL} \int (\rho_{n\uparrow}\rho_{p\uparrow} + \rho_{n\downarrow}\rho_{p\downarrow}) d\mathbf{r} \\
& + 4\pi a^5 C_{uL} \int (\nabla\rho_{n\uparrow}\rho_{p\uparrow} + \nabla\rho_{n\downarrow}\rho_{p\downarrow}) d\mathbf{r} \\
& - \frac{12\pi a^5}{5b^2} C_{uL} (\frac{3\pi^2}{2})^{2/3} \int [\nabla\rho_{n\uparrow}\nabla\rho_{p\uparrow}\rho_{n\uparrow}^{2/3} + \nabla\rho_{n\uparrow}\nabla\rho_{p\uparrow}\rho_{p\uparrow}^{2/3} \\
& + \nabla\rho_{n\downarrow}\nabla\rho_{p\downarrow}\rho_{n\downarrow}^{2/3} + \nabla\rho_{n\downarrow}\nabla\rho_{p\downarrow}\rho_{p\downarrow}^{2/3}] d\mathbf{r} \\
& - 4\pi a^3 C_{uu} \int (\rho_{n\downarrow}\rho_{p\uparrow} + \rho_{n\uparrow}\rho_{p\downarrow}) d\mathbf{r} \\
& + \frac{12\pi a^3}{5b^2} C_{uu} (\frac{3\pi^2}{2})^{2/3} \int [\rho_{n\downarrow}^{5/3}\rho_{p\uparrow} + \rho_{n\downarrow}\rho_{p\uparrow}^{5/3} + \rho_{n\uparrow}^{5/3}\rho_{p\downarrow} + \rho_{n\uparrow}\rho_{p\downarrow}^{5/3}] d\mathbf{r} \\
& + 4\pi a^5 C_{uu} \int (\nabla\rho_{n\downarrow}\nabla\rho_{p\uparrow} + \nabla\rho_{n\uparrow}\nabla\rho_{p\downarrow}) d\mathbf{r} \\
& - \frac{12\pi a^5}{5b^2} C_{uu} (\frac{3\pi^2}{2})^{2/3} \int [\nabla\rho_{n\uparrow}\nabla\rho_{p\downarrow}\rho_{n\uparrow}^{2/3} + \nabla\rho_{n\uparrow}\nabla\rho_{p\downarrow}\rho_{p\downarrow}^{2/3} \\
& + \nabla\rho_{n\downarrow}\nabla\rho_{p\uparrow}\rho_{n\downarrow}^{2/3} + \nabla\rho_{n\downarrow}\nabla\rho_{p\uparrow}\rho_{p\uparrow}^{2/3}] d\mathbf{r} \qquad \text{(A1)}
\end{aligned}$$

The total free energy is $F = F_v + F_s A^{2/3} + F_c A^{1/3}$ and

$$\begin{aligned}
F_{vo} = & \frac{-\pi a^3}{2} C\rho_o + \frac{3\pi a^3}{5b^2} (\frac{3\pi^2}{8})^{2/3} C\rho_o^{5/3} + \frac{3\hbar^2}{10m} (\frac{3\pi^2}{2})^{2/3} C\rho_o^{2/3} \\
& - \frac{\pi^2 m T^2}{2\hbar^2} (\frac{2}{3\pi^2})^{2/3} C\rho_o^{-2/3}; \qquad \text{(A2)}
\end{aligned}$$

$$F_{vi} = \frac{-\pi a^3}{2} C_i \rho_o + \frac{2\pi a^3}{3b^2} (\frac{3\pi^2}{8})^{2/3} C_i' \rho_o^{5/3} + \frac{\hbar^2}{6m} (\frac{3\pi^2}{2})^{2/3} \rho_o^{2/3}$$
$$+ \frac{\pi^2 m T^2}{18\hbar^2 \rho_o^{2/3}} (\frac{2}{3\pi^2})^{2/3}; \quad \text{(A3)}$$

$$F_{so} = 2\pi^2 a^3 d (\frac{3}{4\pi})^{2/3} C \rho_o^{4/3} - \frac{12\pi^2 a^3}{5b^2} (\frac{9\pi}{32})^{2/3} A_1(8/3) d C \rho_o^2$$
$$- \frac{2\pi^2 a^5}{d} (\frac{3}{4\pi})^{2/3} C \rho_o^{4/3} (A_1(2) + A_1(1) - 2A_1(3))$$
$$+ \frac{12\pi^2 a^5}{5b^2 d} (\frac{9\pi}{32})^{2/3} C \rho_o^2 (A_1(8/3) + A_1(14/3) - 2A_1(11/3))$$
$$- \frac{6\pi\hbar^2}{5m} d (\frac{9\pi}{8})^{2/3} \rho_o A_1(5/3)$$
$$- \frac{2\pi\hbar^2 \beta}{md} (\frac{3}{4\pi})^{2/3} \rho_o^{1/3} (A_1(3) - 2)$$
$$+ \frac{2\pi m T^2 d}{\hbar^2 \rho_o^{1/3}} (\frac{1}{2})^{2/3} A_1(1/3); \quad \text{(A4)}$$

$$F_{si} = 2\pi^2 a^3 d (\frac{3}{4\pi})^{2/3} C_i \rho_o^{4/3} - \frac{8\pi^2 a^3}{3b^2} d (\frac{9\pi}{32})^{2/3} A_1(8/3) C_i' \rho_o^2$$
$$- \frac{2\pi^2 a^5}{d} (\frac{3}{4\pi})^{2/3} C_i \rho_o^{4/3} (A_1(2) + A_1(1) - 2A_1(3))$$
$$+ \frac{8\pi^2 a^5}{3b^2 d} (\frac{9\pi}{32})^{2/3} C_i' \rho_o^2 (A_1(8/3) + A_1(14/3) - 2A_1(11/3))$$
$$- \frac{2\pi\hbar^2}{3m} d (\frac{9\pi}{8})^{2/3} \rho_o A_1(5/3)$$
$$- \frac{2\pi m T^2 d}{9\hbar^2 \rho_o^{1/3}} (\frac{1}{2})^{2/3} A_1(1/3); \quad \text{(A5)}$$

$$F_{co} = -4\pi^2 a^3 d^2 (\frac{3}{4\pi})^{1/3} A_2(2) C \rho_o^{5/3}$$
$$+ \frac{24\pi^2 a^3 d^2}{5b^2} (\frac{3\pi^2}{8})^{2/3} (\frac{3}{4\pi})^{1/3} A_2(8/3) C \rho_o^{7/3}$$
$$+ 4\pi^2 a^5 (\frac{3}{4\pi})^{1/3} C \rho_o^{5/3} (A_2(2) + A_2(1) - 2A_2(3))$$
$$- \frac{24\pi^2 a^5}{5b^2} (\frac{3\pi^2}{8})^{2/3} (\frac{3}{4\pi})^{1/3} C \rho_o^{7/3}$$
$$(A_2(8/3) + A_2(14/3) - 2A_2(11/3))$$
$$+ \frac{12\pi\hbar^2 d^2}{5m} (\frac{3\pi^2}{2})^{2/3} (\frac{3}{4\pi})^{1/3} \rho_o^{4/3} A_2(5/3)$$
$$+ \frac{4\pi\hbar^2 \beta}{m} (\frac{3}{4\pi})^{1/3} \rho_o^{2/3} (A_2(3) + A_2(1) - 2A_2(2))$$
$$- \frac{4\pi\hbar^2 \gamma}{m} (\frac{3}{4\pi})^{1/3} \rho_o^{2/3} (3A_2(2) - 2A_2(3) - A_2(1))$$
$$- \frac{4\pi^3 m T^2 d^2}{\hbar^2} (\frac{2}{3\pi^2})^{2/3} (\frac{3}{4\pi})^{1/3} A_2(1/3); \quad \text{(A6)}$$

$$
\begin{aligned}
F_{ci} = & -4\pi^2 a^3 d^2 (\frac{3}{4\pi})^{1/3} A_2(2) C_i \rho_o^{5/3} \\
& + \frac{16\pi^2 a^3 d^2}{3b^2} (\frac{3\pi^2}{8})^{2/3} (\frac{3}{4\pi})^{1/3} A_2(8/3) C'_i \rho_o^{7/3} \\
& + 4\pi^2 a^5 (\frac{3}{4\pi})^{1/3} C_i \rho_o^{5/3} (A_2(2) + A_2(1) - 2A_2(3)) \\
& - \frac{16\pi^2 a^5}{3b^2} (\frac{3\pi^2}{8})^{2/3} (\frac{3}{4\pi})^{1/3} C'_i \rho_o^{7/3} \\
& (A_2(8/3) + A_2(14/3) - 2A_2(11/3)) \\
& + \frac{4\pi\hbar^2 d^2}{3m} (\frac{3\pi^2}{2})^{2/3} (\frac{3}{4\pi})^{1/3} \rho_o^{4/3} A_2(5/3) \\
& + \frac{4\pi^3 m T^2 d^2}{9\hbar^2} (\frac{2}{3\pi^2})^{2/3} (\frac{3}{4\pi})^{1/3} A_2(1/3);
\end{aligned}
\tag{A7}
$$

where

$$
\begin{aligned}
& C = C_{LL} + C_{Lu} + C_{uL} + C_{uu}, \\
& C\prime_x = 2C_{LL} + 2C_{Lu} - C_{uL} - C_{uu}, \\
& C_x = C_{LL} + C_{Lu} - C_{uL} - C_{uu}, \\
& C\prime_y = 2C_{LL} - C_{Lu} + 2C_{uL} - C_{uu}, \\
& C_y = C_{LL} - C_{Lu} + C_{uL} - C_{uu}, \\
& C\prime_z = 2C_{LL} - C_{Lu} - C_{uL} + 2C_{uu}, \\
& C_z = C_{LL} - C_{Lu} - C_{uL} + C_{uu}
\end{aligned}
\tag{A8}
$$

and i runs over x, y and z.

APPENDIX B

The functions for $N(\rho_o)$ and $P(\rho_o)$ are given by

$$
N(\rho_o) = N_o + N_x X^2 + N_y Y^2 + N_z Z^2 \tag{B1}
$$

$$
P(\rho_o) = P_o + P_x X^2 + P_y Y^2 + P_z Z^2 \tag{B2}
$$

where

$$
\begin{aligned}
N_o \quad = \quad & -2\pi^2 a^5 (\frac{3}{4\pi})^{2/3} C \rho_o^{4/3} (A_1(2) + A_1(1) - 2A_1(3)) \\
& + \frac{12\pi^2 a^5}{5b^2} (\frac{9\pi}{32})^{2/3} C \rho_o^2 (A_1(8/3) + A_1(14/3) - 2A_1(11/3)) \\
& - \frac{2\pi\hbar^2 \beta}{m} (\frac{3}{4\pi})^{2/3} \rho_o^{1/3} (A_1(3) - 2);
\end{aligned}
$$

$$
\begin{aligned}
N_i \quad = \quad & -2\pi^2 a^5 (\frac{3}{4\pi})^{2/3} C_i \rho_o^{4/3} (A_1(2) + A_1(1) - 2A_1(3)) \\
& + \frac{8\pi^2 a^5}{3b^2} (\frac{9\pi}{32})^{2/3} C'_i \rho_o^2 (A_1(8/3) + A_1(14/3) - 2A_1(11/3));
\end{aligned}
$$

and

$$\begin{aligned} P_o &= 2\pi^2 a^3 (\frac{3}{4\pi})^{2/3} C \rho_o^{4/3} - \frac{12\pi^2 a^3}{5b^2}(\frac{9\pi}{32})^{2/3} C \rho_o^2 A_1(8/3) \\ & -\frac{6\pi\hbar^2}{5m}(\frac{9\pi}{8})^{2/3}\rho_o A_1(5/3) + \frac{2\pi m T^2}{\hbar^2 \rho_o^{1/3}}(\frac{1}{2})^{2/3} A_1(1/3); \end{aligned}$$

$$\begin{aligned} P_i &= -2\pi^2 a^3 (\frac{3}{4\pi})^{2/3} C_i \rho_o^{4/3} - \frac{8\pi^2 a^5}{3b^2}(\frac{9\pi}{32})^{2/3} C_i' \rho_o^2 A_1(8/3) \\ & -\frac{2\pi\hbar^2}{8m}(\frac{9\pi}{8})^{2/3}\rho_o A_1(5/3) - \frac{2\pi m T^2}{9\hbar^2 \rho_o^{1/3}}(\frac{1}{2})^{2/3} A_1(1/3). \end{aligned}$$

These functions are written at the equilibrium density. Using the denity expansion (Eqn. (21)) we get

$$N(\rho_{on}) = N^o(\rho_{on}) + N^1(\rho_{on})T^2 \tag{B3}$$

$$P(\rho_{on}) = P^o(\rho_{on}) + P^1(\rho_{on})T^2, \tag{B4}$$

where the functions $N(\rho_{on})$ and $P(\rho_{on})$ are expanded in x, y and z up to second order. Thus results

$$F^{0,1} = F_o^{0,1} + F_x^{0,1} X^2 + F_y^{0,1} Y^2 + F_z^{0,1} Z^2 \tag{B5}$$

where

$$\begin{aligned} N_o^0 = & -2\pi^2 a^5 (\frac{3}{4\pi})^{2/3} C \rho_{on}^{4/3} (A_1(2) + A_1(1) - 2A_1(3)) \\ & + \frac{12\pi^2 a^5}{5b^2}(\frac{9\pi}{32})^{2/3} C \rho_{on}^2 (A_1(8/3) + A_1(14/3) - 2A_1(11/3)) \\ & - \frac{2\pi\hbar^2\beta}{m}(\frac{3}{4\pi})^{2/3}\rho_{on}^{1/3}(A_1(3) - 2); \end{aligned} \tag{B6}$$

$$\begin{aligned} N_i^0 = & \frac{8\pi^2 a^5}{3}(\frac{3}{4\pi})^{2/3} C \rho_{on}^{4/3} \rho_i (A_1(2) + A_1(1) - 2A_1(3)) \\ & - \frac{24\pi^2 a^5}{5b^2}(\frac{9\pi}{32})^{2/3} C' \rho_{on}^2 \rho_i (A_1(8/3) + A_1(14/3) - 2A_1(11/3)) \\ & + \frac{2\pi\hbar^2\beta}{3m}(\frac{3}{4\pi})^{2/3}\rho_{on}^{1/3}\rho_i(A_1(3) - 2) \\ & - 2\pi^2 a^5 (\frac{3}{4\pi})^{2/3} C_i' \rho_{on}^{4/3}(A_1(2) + A_1(1) - 2A_1(3)) \\ & + \frac{8\pi^2 a^5}{3b^2}(\frac{9\pi}{32})^{2/3} C_i' \rho_{on}^2 (A_1(8/3) + A_1(14/3) - 2A_1(11/3)); \end{aligned} \tag{B7}$$

$$\begin{aligned} N_o^1 = & \frac{8\pi^2 a^5}{3}(\frac{3}{4\pi})^{2/3} C \rho_{on}^{4/3} \rho_t (A_1(2) + A_1(1) - 2A_1(3)) \\ & - \frac{24\pi^2 a^5}{5b^2}(\frac{9\pi}{32})^{2/3} C \rho_{on}^2 \rho_t (A_1(8/3) + A_1(14/3) - 2A_1(11/3)) \\ & + \frac{2\pi\hbar^2\beta}{3m}(\frac{3}{4\pi})^{2/3}\rho_{on}^{1/3}\rho_t(A_1(3) - 2); \end{aligned} \tag{B8}$$

$$N_i^1 = \frac{8\pi^2 a^5}{3}(\frac{3}{4\pi})^{2/3} C_i \rho_{on}^{4/3} \rho_t (A_1(2) + A_1(1) - 2A_1(3))$$
$$- \frac{16\pi^2 a^5}{3b^2}(\frac{9\pi}{32})^{2/3} C_i' \rho_{on}^2 \rho_t (A_1(8/3) + A_1(14/3) - 2A_1(11/3)); \quad \text{(B9)}$$

$$P_o^0 = 2\pi^2 a^5 (\frac{3}{4\pi})^{2/3} C \rho_{on}^{4/3} - \frac{12\pi^2 a^3}{5b^2}(\frac{9\pi}{32})^{2/3} C \rho_{on}^2 A_1(8/3)$$
$$- \frac{6\pi\hbar^2}{5m}(\frac{9\pi}{8})^{2/3} \rho_{on} A_1(5/3); \quad \text{(B10)}$$

$$P_i^0 = -\frac{8\pi^2 a^3}{3}(\frac{3}{4\pi})^{2/3} C_i \rho_{on}^{4/3} \rho_i + \frac{24\pi^2 a^3}{5b^2}(\frac{9\pi}{32})^{2/3} C_i' \rho_{on}^2 \rho_i A_1(8/3)$$
$$+ \frac{6\pi\hbar^2}{5m}(\frac{9\pi}{8})^{2/3} \rho_{on} \rho_i A_1(5/3); \quad \text{(B11)}$$

$$P_o^1 = -\frac{8\pi^2 a^3}{3}(\frac{3}{4\pi})^{2/3} C \rho_{on}^{4/3} \rho_t + \frac{24\pi^2 a^3}{5b^2}(\frac{9\pi}{32})^{2/3} C \rho_{on}^2 \rho_t A_1(8/3)$$
$$+ \frac{6\pi\hbar^2}{5m}(\frac{9\pi}{8})^{2/3} \rho_{on} \rho_t A_1(5/3) + \frac{2\pi m}{\hbar^2 \rho_{on}^{1/3}}(\frac{1}{2})^{2/3} A_1(1/3); \quad \text{(B12)}$$

$$P_i^1 = \frac{8\pi^2 a^3}{3}(\frac{3}{4\pi})^{2/3} C_i \rho_{on}^{4/3} \rho_t + \frac{24\pi^2 a^3}{5b^2}(\frac{9\pi}{32})^{2/3} C_i' \rho_{on}^2 \rho_t A_1(8/3)$$
$$+ \frac{6\pi\hbar^2}{5m}(\frac{9\pi}{8})^{2/3} \rho_{on} \rho_t A_1(5/3) - \frac{2\pi m}{9\hbar^2 \rho_{on}^{1/3}}(\frac{1}{2})^{2/3} A_1(1/3)(1 + 3\rho_t); \quad \text{(B13)}$$

APPENDIX C

We use Eqns. (B3) and (B4) to express the surface energy and the diffuseness parameter in terms of ρ_{on} The result up to second order in X, Y, Y and T can be written in the form

$$d = d_o + \alpha_o T^2 + (d_x + \alpha_x T^2) X^2 + (d_y + \alpha_y T^2) Y^2 + (d_z + \alpha_z T^2) Z^2 \quad \text{(C1)}$$

$$F_s = F_{so} + a_{so} T^2 + (F_{sx} + a_{sx} T^2) X^2 + (F_{sy} + a_{sy} T^2) Y^2 + (F_{sz} + a_{sz} T^2) Z^2 \quad \text{(C2)}$$

where

$$d_o = (N_o^0 / P_o^0)^{1/2} \quad \text{(C3)}$$

$$\alpha_o = \frac{1}{2} d_o (\frac{N_o^1}{N_o^0} - \frac{P_o^1}{P_o^0}) \quad \text{(C4)}$$

$$d_i = \frac{1}{2} d_o (\frac{N_i^0}{N_i^0} - \frac{P_i^0}{P_i^0}) \quad \text{(C5)}$$

and

$$\alpha_i = \frac{1}{2} d_o [\frac{1}{2}(\frac{N_i^0}{N_o^0} - \frac{P_i^0}{P_o^0})(\frac{N_o^1}{N_o^0} - \frac{P_o^1}{P_o^0}) - \frac{P_o^1}{P_o^0}(\frac{N_i^1}{N_o^1} - \frac{N_i^0}{N_o^0}) + \frac{N_o^1}{N_o^0}(\frac{P_i^1}{P_o^1} - \frac{P_i^0}{P_o^0}). \quad \text{(C6)}$$

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