SEMICLASSICAL APPROACH TO NUCLEAR SURFACE PROPERTIES: RADIAL SHAPES AND ENERGIES

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Abstract

Energy Density Formalism calculations in semi-infinite nuclear matter are performed. Analytical solution of the Euler equation is given. Geometrical properties of the density are studied. Surface and surface symmetry energies are calculated and simple compact formulae are given.

It is known that the surface symmetry energy ε_i^s plays an important role in the determination of fissions barriers heights, dipole resonance [1] strength and formation of the neutron skin. However experimental uncertainties do not allow even a rough estimate of this quantity. From experimental masses, one can only extract a correlation between volume and surface symmetry energies, so that the values of ε_i^s found in the literature lie in the range (-20, -160). On the other hand the theoretical calculation of ε_i^s is not accurate : with the same interaction, the results can vary by 50 % [2]. Besides the Droplet Model [2] two methods have been exploited i) a fitting procedure on calculated masses using an Extended Thomas Fermi (E.T.F.) calculation [4], ii) a direct H.F. calculation in the semi-infinite nuclear matter (SINM) [2,5]. The method proposed here combines both advantages : it gives directly ε_s^s through a self-consistent ETF calculation in SINM.

In the first part we study the SINM (N = Z). Exact integration of the Euler equation allows a detailed investigation of the nuclear surface shape which is shown to be poorly represented by the usual Fermi shape [6]. We mention some consequences of this departure in the analysis of actual nuclei. We then calculate the surface energy ε_s. Finally we generalize the method to the asymmetric case N ≠ Z. Analytical formulae are proposed for ε_s and ε_s^s .

1. On the shape of the surface

a) Case of SINM

When using Skyrme forces and an ETF approximation for the kinetic energy density τ , the total hamiltonian density $\mathcal{H}$ has the form

$$\mathcal{H}(\rho, \vec{\nabla}\rho) = h(\rho) + \frac{\hbar^2}{2m}\beta\frac{|\vec{\nabla}\rho|^2}{\rho} + d\,|\vec{\nabla}\rho|^2 \qquad (1)$$

where β is the coefficient of the Weiszäcker term in τ and d is a constant. The corresponding Euler equation can be integrated once and gives :

$$h(\rho) - \frac{\hbar^2}{2m}\beta\frac{\rho''}{\rho} - d\rho'' = \lambda_{nm} \qquad (2)$$

where λ_{nm} is the separation energy at saturation density ρ_{nm}.

A cubic expansion of h(ρ) around ρ_{nm} is a good approximation for all commonly used interactions :

$$h(\rho) = \lambda_{nm}\left[\rho + \frac{K}{18}\left(\frac{\rho-\rho_{nm}}{\rho_{nm}}\right)^2 + \frac{Kc}{18}\left(\frac{\rho-\rho_{nm}}{\rho_{nm}}\right)^3 + \cdots\right] \qquad (3)$$

where K is the nuclear incompressibility modulus and |c| is found smaller than 0.2.

Inserting (3) into (2), another quadrature can be performed analytically [8], giving x as a function of ρ . This function can be inverted in the two asymptotic regions, namely :

$$x \longrightarrow -\infty \qquad \rho \sim \rho_{nm}\left(1 - B_1 e^{\frac{x}{a_{in}}}\right) \qquad (4.a)$$

$$x \longrightarrow +\infty \qquad \rho \sim B_2 e^{-\vartheta\frac{x}{a_{in}}} \qquad (4.b)$$

B_1, B_2, ϑ and a are determined by the interaction. The coefficient a_{in} is given by :

$$a_{in} = \sqrt{\frac{18}{K}\left(\frac{\hbar^2}{2m}\beta + d\rho_{nm}\right)} \qquad (5)$$

and ϑ is found in the range $(2 \sim 4)$, according to the interaction and the value of β . We can then define an internal diffuseness a_{in} given by Eq.(5) and an "external" diffuseness $a_{out} = a_{in}/\vartheta$. The first quantity is mainly governed by K whereas the second one by λ_{nm}. There is no physical reason why they should be equal, and indeed they are not. However one assumes $a_{in} = a_{out}$ (i.e. $\vartheta = 1$) when parametrizing the density with a Fermi distribution. In order to preserve the simplicity of the latter while keeping somehow the asymptotic behaviour as given by Eqs.(4), we strongly favor the use of a ϑ -power of a Fermi distribution, hereafter labelled (F-ϑ) when geometrical properties of the density are involved. In Ref.[9] are derived analytical expressions for the various momenta of (F-ϑ) in powers of a/R.

b) Case of finite nuclei

In this case one cannot integrate analytically the Euler equation. Nevertheless the above considerations suggest the use of F-ϑ distributions as

$$\rho(r) = \frac{\rho_0}{\left(1 + e^{\frac{r-R}{a}}\right)^{\vartheta}} \qquad (6)$$

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where ρ_0, R, a and ν are mass-dependent. For actual nuclei ($N \neq Z$ and Coulomb force) the landscape is more intricated, but two remarks are in order i) people using a folding model for the real part of the optical potential have already introduced (F- ν) distributions with $\nu = 2.65$ in order to fit the data [10] ii) when fitting ETF or H.F. densities with F- ν distributions, one gets a better χ^2 with $\nu = 2$ or 3.

Let us briefly discuss two examples where the dissymmetry of the surface shape around inflexion point is significant. i) When fitting H.F. or ETF densities (N = Z, no Coulomb) with F-1 distribution for A going from 16 to 208, one obtains a 10-15 % variation of the surface thickness. But the same effect is obtained when fitting (F-2) distributions with constant 10-90 % distance (and increasing normalization) with (F-1) distributions. The conclusion is that a fitting procedure with (F-1) distributions can lead to spurious effect in the determination of the surface thickness.

ii) The D.M. predicts a larger value of $\rho(o)$ in finite nucleus as compared to ρ_{nm}. Self-consistent ETF calculations confirm the D.M. predictions.*. However in a recent paper [11], Pearson argues that from H.F. calculations one has $\rho(o) < \rho_{nm}$. We think that part of the discrepancy between the D.M. and Ref.[11] is due to the fact that Pearson uses (F-1) distributions to get ride of the shell oscillations in the interior. Fig.1 indicates what happens when (F-2.5) distribution are

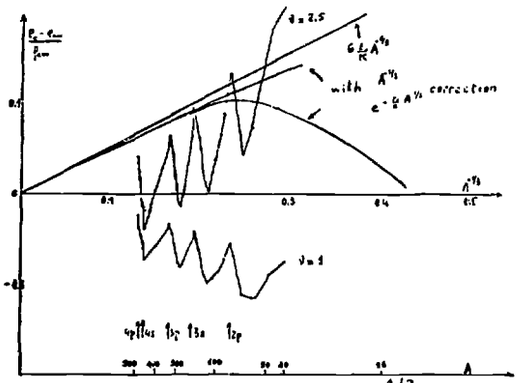

FIG 1 : Plot of $\frac{\rho(o)-\rho_{nm}}{\rho_{nm}}$ as a function of $A^{-1/3}$ (N=Z, no Coulomb)

*In fact, for A < 100, the constant density approximation of the Droplet Model breaks down, and an exponential term $\sim \exp(-\frac{r_0}{a} A^{1/3})$ can be shown to reduce significantly the compression.

used, instead of (F-1). For $\nu = 1$ one recovers the Pearson results, but for $\nu = 2.5$ one recovers on the average the central compression. Smooth curves show respectively D.M. and various corrections, broken curves show the fit to HF density using F- ν distributions. The importance of the filling of s and p shells is striking as can be seen in Fig.1.

Although the experimental densities do not oscillate as much as H.F. ones, the above discussion proves that great care must be taken when extracting a central density to be compared to the DM one.

2. Surface energy of SINM

a) N = Z

The surface energy ε_s and the surface tension σ_{nm} are defined as follows :

$$\varepsilon_s = 4\pi r_{nm}^2 \sigma_{nm} = \int [\mathcal{H}(\rho, \vec{\nabla}\rho) - \lambda_{nm}\rho]\, d\vec{r} \qquad (9)$$

Use of Eq.(2) proves that the contributions of the volume and gradient terms are equal. So one can write

$$\sigma_{nm} = 2\int_{-\infty}^{+\infty} [h(\rho) - \lambda_{nm}\rho]\, dx = 2\int_{o}^{\rho_{nm}} \left(\frac{\hbar^2}{2m}\beta + d\rho\right)^{1/2} \left(\frac{h(\rho)}{\rho} - \lambda_{nm}\right)^{1/2} d\rho \qquad (10)$$

where the last integral does not require the knowledge of $\rho(r)$ [7]. Using the cubic expansion (3) one obtains an explicit formula for σ_{nm}.

An alternative procedure is to perform a restricted variational calculation using a (F- ν) parametrization of the density. One then obtains

$$\sigma_{nm} = \frac{2\rho_{nm}}{a}\left[\frac{\hbar^2}{2m}\beta\frac{\nu}{\nu+1} + d\rho_{nm}\frac{\nu}{2(2\nu+1)}\right] \qquad (11)$$

which agrees very closely to the results of Eq.(10). With the choice $\beta = 1/18$ we reproduce for all Skyrme forces the H.F. results within 4 %. We will now generalize the method to the case $N \neq Z$.

b) N ≠ Z

ε_s, which now depends on the asymmetry $I = \frac{N-Z}{A}$, is defined as in Eq.(9)

$$\varepsilon_s = 4\pi r_o^2 \sigma = \int [\mathcal{H}(\rho_n, \rho_p, \vec{\nabla}\rho_n, \vec{\nabla}\rho_p) - \lambda_n\rho_n - \lambda_p\rho_p]\, d\vec{r} \qquad (12)$$

where $\delta = \frac{\rho_n - \rho_p}{\rho_n + \rho_p}$ and λ_n and λ_p are the chemical potentials for neutrons and protons. In Ref.[15] is presented a restricted variational calculation of $\sigma(I)$ using F- ν distri-

butions for neutrons and protons. We shall derive here a simple yet accurate expression for the surface symmetry energy.

As in the symmetrical case one can integrate once the two coupled Euler equations for ρ_n and ρ_p. One gets :

$$\mathcal{H} - (\lambda_n \rho_n + \lambda_p \rho_p) = 2\left[h(\rho,\delta) - (\lambda_n \rho_n + \lambda_p \rho_p)\right] \quad (13)$$

where $h(\rho, \delta)$ is the volume term of $\mathcal{H}$, which we write :

$$h(\rho,\delta) = h(\rho) + \rho\,\varepsilon_\delta(\rho)\,\delta^2 + \cdots \quad (14)$$

In Eq.(14) $\varepsilon_\delta(\rho)$ is the volume part of symmetry potential. It can be expanded as

$$\varepsilon_\delta(\rho) = \varepsilon_\delta^{nm} + \frac{L}{3}\,\frac{\rho-\rho_{nm}}{\rho_{nm}} + \frac{K_{sym}}{18}\left(\frac{\rho-\rho_{nm}}{\rho_{nm}}\right)^2 \quad (15)$$

ε_δ^{nm} is the symmetry energy of nuclear matter, $L = 3\rho_{nm}\frac{\partial \varepsilon_\delta}{\partial \rho}\Big|_{\rho_{nm}}$ and $K_{sym} = 9\rho_{nm}^2\frac{\partial^2 \varepsilon_\delta}{\partial \rho^2}\Big|_{\rho_{nm}}$

On the other hand, from the mass formula one has :

$$\lambda_n = \lambda_{nm} + \varepsilon_\delta^{nm} I\,(2-I) \quad (16.a)$$

$$\lambda_p = \lambda_{nm} - \varepsilon_\delta^{nm} I\,(2+I) \quad (16.b)$$

Using Eqs.(13), (14) and (16) in Eq.(12) one gets :

$$\sigma = 2\int_{-\infty}^{+\infty}\left[h(\rho) - \lambda_{nm}\rho\right]dx + 2\int_{-\infty}^{+\infty}\rho\left\{\delta^2\varepsilon_\delta(\rho) - \varepsilon_\delta^{nm}(2\delta I - I^2)\right\}dx \quad (17)$$

The first integral is equal to $\sigma_{nm} + o(I^4)$ despite the fact that $\rho(-\infty)$ is no longer equal to ρ_{nm} : it is known that σ_{nm} is stationary around ρ_{nm} [3].

If we define the surface symmetry tension σ_δ as :

$$\sigma = \sigma_{nm} + I^2\sigma_\delta$$

one has

$$\sigma_\delta = 2\int_{-\infty}^{+\infty}\rho\left\{\frac{\delta^2}{I^2}\varepsilon_\delta(\rho) - \varepsilon_\delta^{nm}\right\}dx \quad (18)$$

Formula (18) is exact within the Energy Density Formalism (EDF). (It will probably give reasonable results when using H.F. densities, but we did not check it). However it requires the knowledge of the function $\delta(r)$. We shall see that the approximation $\delta = I$ in Eq.(18) leads to a rapid and fair estimate of . Notice that this approximation should not be made directly in Eq.(12), because one would loose the contributions of the terms in $\nabla\delta$, i.e. $\sim$ half of σ_δ .

With this approximation Eq.(18) becomes :

$$\sigma_\delta = \int_{-\infty}^{+\infty}\rho\left[\varepsilon_\delta(\rho) - \varepsilon_\delta^{nm}\right]dx \quad (19)$$

which nicely exhibits the origin of σ_δ : the surface symmetry tension appears as the average of the defect of the symmetry potential with respect to its nuclear matter value. This defect is plot in Fig.2 and one understands why σ_δ of S-V is three times greater than of S-III.

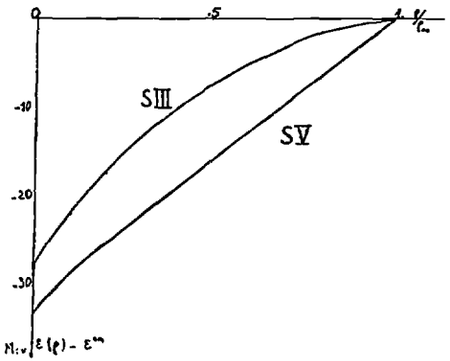

FIG 2 : $\varepsilon_\delta(\rho) - \varepsilon_\delta^{nm}$ is plotted as function of ρ/ρ_{nm} for S-III and S-V forces.

One can further simplify Eq.(19) by i) taking the expansion (15) for $\varepsilon_s(\rho)$ ii) using a F-1 parametrization for ρ. If one writes

$$\varepsilon_s = e_s^{nm} + I^2 \varepsilon_s^s$$

One gets finally

$$\varepsilon_s^s = -\frac{2a}{r_{nm}}\left(L - \frac{K_{sym}}{12}\right) + 2\varepsilon_s^{nm}\frac{L}{K} \qquad (20)$$

Table (I) compares results given by Eqs.(18), (20) and other calculations available.

TABLE I : Values of $-\varepsilon_s^s$ for various Skyrme and finite range forces

	SII	SIII	SIV	SV	SVI	SkM	D_1[12]	B_1[13]
Eq.(20)	54	31	57	77	22	52	39	133
Ref.[15]	56	30	66	99	20	56		
Refs.[2, (5)]	60	34	57	84	26		(38)	
Refs.[14, (4)]	85	47 (35)	105		38	(46)		

If one excepts the values of Ref.[14], which are obtained through a fitting procedure to calculated masses and therefore probably less accurate, an overall agreement between the different approaches ($\sim$20 %) is obtained.

Concluding remarks

The major interest of the method sketched here (see Refs.[15,16] for a more systematic development) when comparing to the others is that it gives rise to analytical formulae for macroscopic properties of interactions to be used in microscopic calculations. The method may facilitate the process of improving the existing effective interactions, incorporating more experimental information on static and dynamic properties.

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