A SIMPLE APPROXIMATION TO THE KINETIC ENERGY DENSITY

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Abstract :

A new functional of the density and its
derivative is proposed to the kinetic energy density and the
corresponding Euler equations are solved. Comparisonswith
Hartree-Fock results show a close agreement, particularly for
the shape of the density at the surface, for heavy as well as
for light nuclei. The dynamical properties of this functional
are tested in the case of the giant monopole resonance and are
satisfactory.

In recent years, an increasing interest has been devoted to approximate treatments of Hartree-Fock (HF) calculations. Although the use of schematic effective forces [1] simplifies the calculations, they still remain very involved and may be overdetailed, if one is interested in large systems, or in dynamical studies likes description of giant resonances, or heavy ions collisions. In the energy density formalism (EDF) [2] , one assumes that the energy density H is a functional of the diagonal part of the one-body densities of neutrons and protons, ρ_n and ρ_p and of their derivatives. Instead of dealing with as many functions as single particle occupied states, one deals with only two functions ρ_q, q = n,p. One then writes and solves [3] two Euler equations to determine these densities. The construction of the functional can be divided in two parts : the potential term and the kinetic term.

Concerning the first one, schematic effective interactions have been precisely introduced so that the potential part of the H.F. hamiltonian density is, for spherical nuclei, a functional of ρ_q and its derivatives. In this letter, we shall restrict ourselves to these cases.

The second one is the main object of this letter ; our starting point is the following simple remark : the kinetic energy density $\tau_q(r) = \frac{\hbar^2}{2m} \sum_{i_q} |\nabla \varphi_{i_q}|^2$, where i_q labels occupied states φ_{i_q}, is exactly a functional of ρ_q and its derivatives not only in infinite nuclear matter where, as it is well known,

$$\tau_q(r) = \frac{\hbar^2}{2m} \frac{3}{5}(3\pi^2)^{2/3} \rho_q^{5/3} \tag{1}$$

but also in ⁴He, where :

$$\tau_q(r) = \frac{\hbar^2}{2m} \, 2|\nabla\varphi_q|^2 = \frac{\hbar^2}{2m} \, \frac{1}{4} \, \frac{(\nabla\varphi_q)^2}{\rho_q} \tag{2}$$

In eq.(2), $\rho_q = 2|\varphi_q|^2$, and φ_q is the wave function of the single occupied state. This suggests to define a modified Thomas-Fermi approximation (MTF) to the kinetic energy density where the functional $\tau_q^{MTF}(r)$ is also a function of the number of particles A_q, of the following form :

$$\tau_q^{MTF}(r) = \frac{\hbar^2}{2m} \left(\alpha(A_q)\rho_q^{5/3} + \beta(A_q)\frac{(\nabla\rho_q)^2}{\rho_q} \right) \tag{3}$$

with the conditions $\alpha(2) = 0$, $\alpha_\infty = \frac{3}{5}(3\pi^2)^{2/3}$, $\beta(2) = \frac{1}{4}$ which assure that eqs.(1) and (2) are satisfied. Next, we determine the functions $\alpha(A_q)$ and $\beta(A_q)$ through the following procedure : for a set of nuclei with equal number of neutrons and protons and no Coulomb interaction, one looks for the couple of values $\alpha(A_q)$, $\beta(A_q)$ which leads, when solving the Euler equations,to the closest results to the HF ones calculated with the same interaction.

One can see in table 1 the quality of the fit : energies per particle, kinetic energies per particle, mean square radii are calculated for spherical nuclei and agree with the H.F. values to less than 1 % for the energies and to less than 0.2 % for the radii. This shows that expression (3) is a good approximation not only for large systems, but also throughout the periodic table.

In fig.1 are plotted the densities and the kinetic energy densities of protons calculated in ¹⁶O and ²⁰⁸Pb.

One can see that the surface shapes are correctly reproduced.
In order to make some quantitative comparisons, we have calculated
the surface thickness a of proton densities using the definition
proposed by Campi in ref.[4]: $a = [6R_k(dR_k/dk)]^{1/2}\pi^{-1}$ where
$R_k = [((k+3)/2)<r^k>]^{1/k}$ are the moments of the density . When
the density is exactly a Fermi distribution one recovers the usual
definition of surface thickness (the 10 % - 90 % variation in ρ
corresponds to 4.4 a). One can see in table (1) that the agreement
with the H.F. values is better than 5 %.

We have plotted in fig.2 the function $\dfrac{\alpha(A_q)}{\alpha_\infty}$.
It can be seen that although this function is very rapidly
increasing in the region $A_q \lesssim 10$, even in the lead region ($A_q \sim 100$)
it differs from the asymptotic value by an amount of $\sim$ 4 %. Thus
the contribution to the total kinetic energy of the $\rho_q^{5/3}$ term
is sensitively less than what gives the T.F. approximation,
in which $\alpha = \alpha_\infty$ and $\beta = 0$.

The function $\beta(A_q)$ is found to be rapidly
varying from the value $\frac{1}{4}$ for $A_q = 2$ to a value which is smaller,
independent of the nucleus as soon as $A_q \gtrsim 8$ and dependent on
the interaction. We shall briefly analyze these three points.
i) For a system consisting of one occupied state (^{4}He) or in the
asymptotic region ($r \to \infty$) of a larger nucleus where a shell model
density ρ_q^{SM} is also determined by only one wave function, namely
that of the last occupied state, the fall off of the density
is given by

$$\rho_q^{SM}(r) \underset{r\to\infty}{\sim} \frac{1}{r^2} e^{-2\sqrt{-\frac{2m}{\hbar^2}\lambda_q}\cdot r} \tag{4}$$

where λ_q is the one particle separation energy. On the other hand, it can be shown [3] that the Euler equations using a form like that of eq.3 for $\tau_q(r)$, lead to the following behaviour of the density in the asymptotic region :

$$\rho_q^{MTF}(r) \underset{r\to\infty}{\sim} \frac{1}{r^2} e^{-\sqrt{-\frac{2m}{\hbar^2}\frac{\lambda_q}{\beta}}\, r} \qquad (5)$$

Eq.(5) coïncides obviously with eq.(4) if one sets $\beta = 1/4$ (which is another way to state that eq.(2) is valid). But if β determines the asymptotic behaviour of the density, one can see numerically that it also governs the shape of the external part of the surface. In this region, the decreasing of $\rho_q^{SM}(r)$ is greater than what gives eq.(4), as all occupied states contribute to the density. Thus a good agreement between $\rho_q^{SM}(r)$ and $\rho_q^{MTF}(r)$ in the external part of the surface requires a smaller value for β than $\beta = 1/4$. Thus we rather prefer to abandon a theoretical asymptotic limit in a region where there is practically no matter in order to obtain a correct surface shape.

ii) That we find a constant value for $\beta(A_q)$ $(A_q \gtrsim 8)$ is related to the well-known fact that the surface thickness is roughly the same in all nuclei.

iii) The shape of $\rho_q^{SM}(r)$ in the outer part of the surface depends on the density of states near the Fermi level. Thus we expect β to depend on the interaction merely through the effective mass m^*/m. We have checked that the value $\beta = \frac{1}{9}$, which is in agreement with that of L. Wilets [5] , gives a good overall fit for different schematic interactions, provided that their effective mass is near the value. 75 . A more detailed study (using Skyrme forces

SII, SIII, SV, SVI [9] , Köhler forces Ska, Skb [10] and KT force [7] which cover a range of values of m^*/m from .38 to .95) shows a roughly linear dependence between β and m^*/m of the form :

$$\beta = \frac{1}{9} [\frac{m^*}{m} + \frac{1}{4}]$$

It is worthwhile to compare the results of the present paper to those obtained [3] when one uses, for $\tau_q(r)$, the functional derived from the semi-classical approaches [6] :

$$\tau_q^{ITF}(r) = \frac{\hbar^2}{2m} \left(\alpha_\infty \quad \rho_q^{5/3} + \frac{1}{36} \frac{(\nabla\rho_q)^2}{\rho_q} + \frac{1}{3} \Delta\rho_q \right) \tag{6}$$

The densities, labelled ρ_q^{ITF} , are reproduced in fig.1 : the too small value of β leads to too sharp surfaces and consequently too small surface thickness (see table 1). Indeed, it is known that the semi-classical expansion (6) is not valid beyond the turning point and this is certaintly why the densities are not satisfactory at the surface.

The functional (3) is also well suited to the study of very large systems because it is found that with all the above mentioned forces, radii and surface thicknesses are rather insensitive to the precise value of β . Calculation of a system of 2500 protons and neutrons (without Coulomb forces) is a good approximation to the semi infinite medium ; it shows that a variation of 50 % on β induces a variation of 8 % on the surface thickness a and of 1 % on the radii. This is in agreement with the study of Campi and Stringari [11] which give an approximated expression for a as a function of β and the parameter of the interaction. Thus one can study with this MTF procedure the gross effects of the interaction on the diffuseness . As an example, we give in table (2) the values of the diffuseness a for various

schematic forces in the nucleus $^{2500}_{2500}X$. The role of the two important parameters, m^*/m and the incompressibility K, is not very clear. Nevertheless it seems that for a given effective mass, the surface thickness decreases when K increases and that for a given K, a is rather insensitive to m^*/m when m^*/m is not too small.

Finally, we have tested the dynamical properties of the functional (3) in a simple case, (monopole isoscalar vibration) following a fluid dynamical method proposed in ref.[7]. Table (3) gives the results of three self-consistent calculations[*]. One can see that the agreement between MTF and RPA is very satisfactory. The origin of the discrepancy between ITF and MTF is twofold : i) the compressibility of the nucleus, which is related to the second variation of the hamiltonian with respect to the densities, is of course modified if one changes the functional used for $\tau_q(r)$. ii) the differences in the shape of the equilibrium densities ρ_q^{ITF} and ρ_q^{MTF} play also a certain role in the determination of the energy of the resonance. It can be shown [7] that i) is the most important factor. This favors the use of the functional (3) for practical calculations as it allows a completely self-consistent fluid dynamical treatment.

The (empirical) functional (3) has to be microscopically understood. Work in this direction is in progress, using one-dimensional simplified models.

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Table Captions

Table 1 : Total energy per particle E/A, kinetic energy per
particle T/A, neutron and proton radii r_n and r_p,
neutron and proton surface thicknesses a_n and a_p
in ^{16}O, ^{40}Ca, ^{90}Zr and ^{208}Pb using ITF, MTF and HF
approximations with SIII interaction [9].

Table 2 : Mean square radii and surface thicknesses in $^{2500}_{2500}X$
calculated with various Skyrme interactions [9] and
Köhler force Ska [10]. SC is a Skyrme interaction
with no velocity dependent component.

Table 3 : Energy of the giant monopole resonance in ^{208}Pb ;
comparison between a fluid dynamical calculation using
ITF or MTF approximation and the RPA result.

	^{16}O			^{40}Ca			^{208}Pb		
	ITF	MTF	HF	ITF	MTF	HF	ITF	MTF	HF
E/A	-6.99	-6.81	-6.87	-8.11	-7.90	-7.93	-7.62	-7.22	-7.23
T/A	15.85	14.58	14.89	17.00	16.03	16.27	18.47	17.91	18.15
r_n	2.56	2.64	2.65	3.31	3.37	3.38	5.64	5.71	5.70
r_p	2.58	2.67	2.68	3.35	3.42	3.43	5.55	5.56	5.57
a_n	.33	.43	.45	.35	.46	.47	.43	.58	.55
a_p	.34	.44	.46	.35	.47	.48	.32	.46	.44

^{90}Zr		
ITF	MTF	HF
-8.44	-7.95	-7.93
17.77	17.13	17.42
4.29	4.36	4.37
4.25	4.30	4.30
.39	.52	.48
.35	.47	.49

- Table 1 -

	SII	SIII	SIV	SV	SVI	SC	Ska
K	342	356	325	306	364	307	263
m^*/m	.58	.76	.47	.38	.95	1	.61
a[fm]	.56	.57	.62	.74	.56	.30	.70

– Table 2 –

ITF[7]	MTF	RPA[8]
19.6	17.7	17.9

– Table 3 –

Figure Captions

Fig.1 : Proton density and kinetic energy density plotted
for ^{208}Pb (right) and ^{16}O (left). Full line,
dashed line and dashed-dotted line correspond
respectively to HF, MTF and ITF results.

Fig.2 : Plot of the function $\frac{\alpha(A)}{\alpha_\infty}$. It can be roughly parametrized
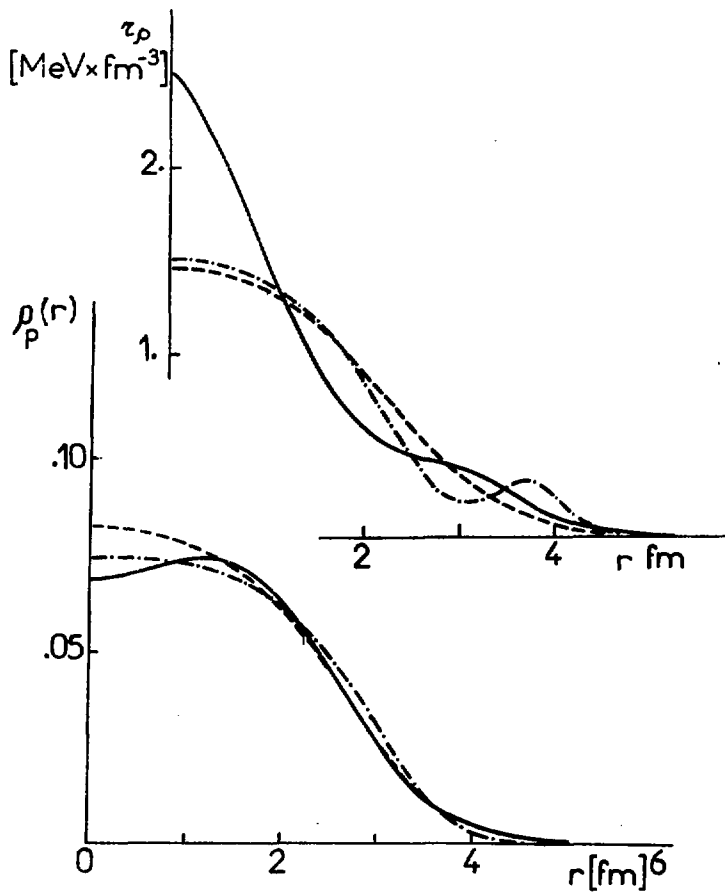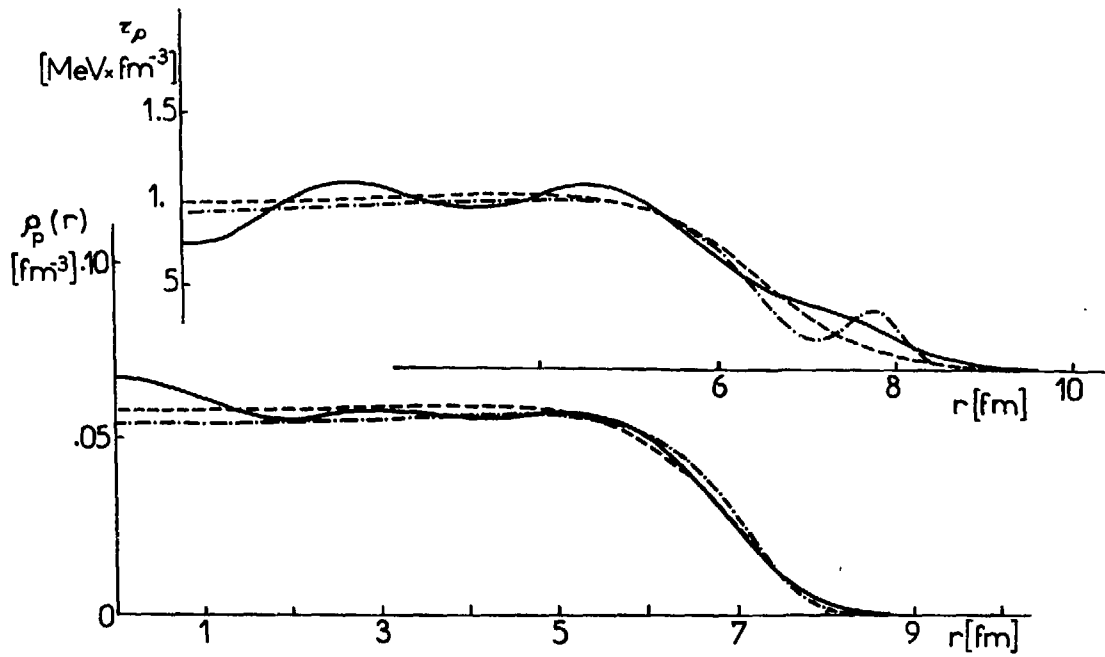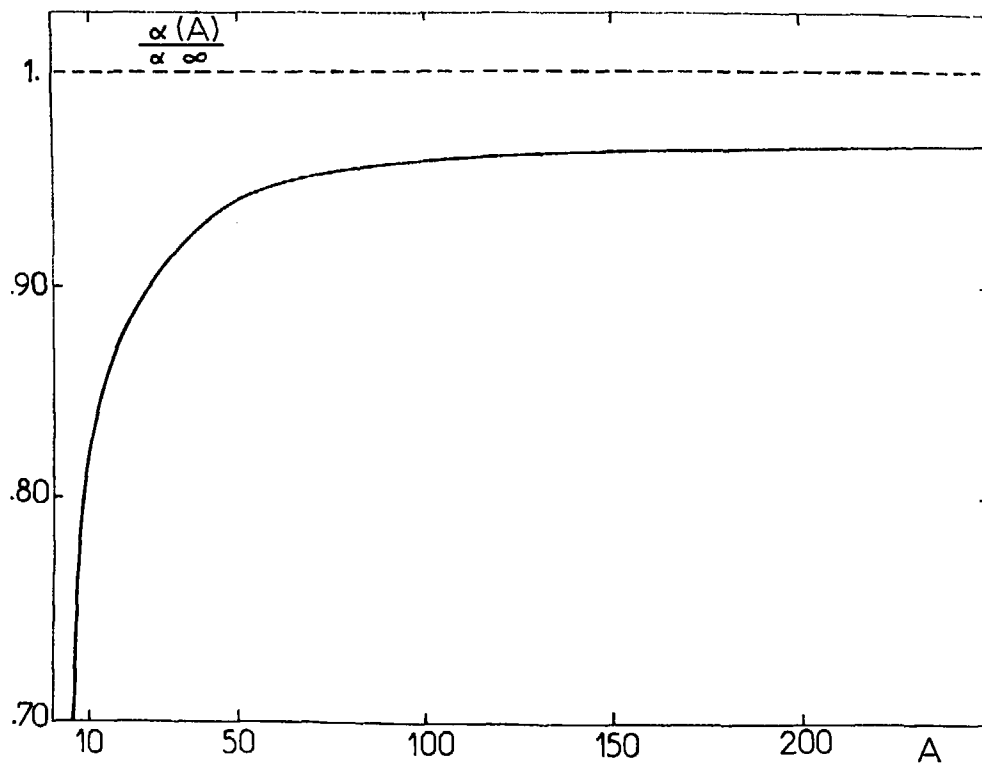by the expression $\frac{\alpha(A)}{\alpha_\infty} = \tanh. 7764 (A-2)^{1/5}$.

Fig. 1a

Fig. 1b

Fig. 2