EXTENSIONS OF THE THOMAS-FERMI APPROXIMATION FOR FINITE NUCLEI

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Abstract

Inhomogeneity terms in the expansion of the kinetic energy density are included and the Euler-Lagrange equations solved. Shell effects may be incorporated in a simple way. The study of spherical shapes of large systems is given as an illustration of the method proposed.

In recent years, the description of bulk properties of nuclei has met considerable success by the use of the static Hartree-Fock (HF) method. Recently, also dynamical calculations have been attempted. Although the use of schematic effective forces [1-4] drastically simplifies the calculations, they still remain very involved, especially if one is interested in the description of heavy nuclei, or, even more, in the decription of fission barriers, heavy ion collisions etc... It is then natural to ask, especially if one keeps in mind the schematic nature of the forces used, wether a procedure like HF or its time dependent version is not actually anoverdetailed one. Surprisingly enough, the complexity of the calculations using simplified effective forces is due, to a large extent, not to the interaction term, but to the kinetic energy one. It seems thus worthwhile to look for approximate treatments of the kinetic energy that may introduce essential simplifications in the whole approach.

The Thomas-Fermi (TF) approximation is a well known alternative procedure to the HF method. One approximates* the kinetic energy density $\tau(r) = (\hbar^2/2m) \sum_i |\nabla \phi_i|^2$, where i labels occupied states ϕ_i , by $\tau_{TF} \propto \rho^{5/3}$, where ρ is the one-body density. If the TF approximation is used in conjunction with the above mentioned schematic forces, one is lead to an energy density formalism [5] , in which the energy E is a functional of the density ρ . Instead of dealing, as in the HF method, with as many functions as single-particle occupied states, one deals only with one function ρ . Among the drawbacks of the TF approximation let us mention its well known failure to correctly describe the nuclear surface as well as its unability to include shell effects.

The purpose of the present work is to go as far as we can from the results obtained in some improved TF (ITF) approximation towards static HF ones, with special emphasis on the simplicity of the procedure. Only interactions leading to a local energy density formalism shall be treated. We want to stress the following two points :

i) when an ITF approximation is used (essentially by including the Weizsäcker [6] term), one obtains solutions ρ_{TF} that have the exponential fall off at large distances and the Euler equation can be integrated over the whole range of values of r (from zero to infinity).

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* Although in the numerical applications we treat protons (with the Coulomb force) and neutrons, the discussion and notation will be simpler by treating identical particles.

ii) if one wishes to further improve the treatment, in particular by including shell effects, one takes the functions ρ_{ITF} and τ_{ITF} thus obtained to calculate a one-body potential and solve a Schrödinger equation once for each s.p. state.

Our starting point is the semi-classical expansion (in powers of $\hbar^2$) of the kinetic energy density $\tau(r)$ in terms of ρ as explained in ref. [7] (the same expansion has been recently obtained [8,9] using the method proposed by Bhaduri and Ross [10]). If, for a system of particles in a central local field, one keeps the first two terms in this expansion, the resulting approximate kinetic energy density, that we shall denote by τ_{ITF}, reads

$$\tau_{ITF} = \frac{\hbar^2}{2m}\left(\alpha\rho^{5/3} + \beta\frac{(\nabla\rho)^2}{\rho} + \gamma\,\Delta\rho\right) \qquad (1)$$

where $\alpha = (3/5)(3\pi^2)^{2/3}$, $\beta = 1/3$ and $\gamma = 1/3$. The first term in (1) corresponds to the standard TF approximation and the second one is the modified Weizsäcker term [5].

When using the approximation $\tau \simeq \tau_{ITF}$ and restricting to spherically symmetric systems, the Hamiltonian density H(r) we deal with can be written as

$$H(r) \simeq P(\rho) + |\nabla\rho|^2\left(d + \frac{\hbar^2}{2m}\frac{\beta}{\rho}\right) + \frac{\hbar^2}{2m}\gamma\,\Delta\rho\,, \qquad (2)$$

where $P(\rho)$ is a sum of powers ν of ρ, with $\nu > 1$; to $P(\rho)$ contribute genuine interaction terms, the TF kinetic energy term $\alpha\rho^{5/3}$ as well as terms of the form $\rho\tau$ induced by a momentum-dependent interaction, leading to $\alpha\rho^{5/3}$ by use of (1) ; similarly, to the constant d may contribute genuine interaction terms as well as terms induced by β and γ in (1) through such momentum-dependent interactions. We look for the function ρ that minimizes the energy E with respect to variations of ρ and with the constraint of keeping the number A of particles constant. The Euler-Lagrange equation has the form

$$\frac{\partial P}{\partial\rho} + \frac{\hbar^2}{2m}\beta\frac{|\nabla\rho|^2}{\rho^2} - 2\,\Delta\rho\left(d + \frac{\hbar^2}{2m}\frac{\beta}{\rho}\right) = \lambda \qquad (3)$$

The Lagrange multiplier λ is equal to $\partial E/\partial A$, i.e. corresponds to the one particle separation energy. We look for solutions of (3) that vanish at large distances. The asymptotic form (see also ref. [11]) of (3) is

$$\frac{|\nabla\rho|^2}{\rho} - 2\Delta\rho = \frac{2m}{\hbar^2}\frac{\lambda}{\beta}\rho \quad , \qquad (4)$$

which leads to

$$\rho \underset{r\to\infty}{\sim} \frac{1}{r^2}\exp\left(-\sqrt{\frac{2m}{\hbar^2}\frac{\lambda}{\beta}}\,r\right) = \frac{1}{r^2}\exp\left(-6\sqrt{-\frac{2m}{\hbar^2}\lambda}\,r\right), \qquad (5)$$

i.e., there are solutions with the exponential fall-off appropriate for a finite quantum-mechanical system. It is worth noticing that this asymptotic behaviour is due to the inhomogeneity Weizsäcker term : without it ($\beta=0$), the asymptotic form of (3) would be $\Delta\rho$ = constant, which has no physical acceptable solution over the whole space. The presence in (3) of a $\Delta\rho$ term, when limiting to regular solutions of ρ at any point, insures that $\rho'=0$ at the origin.

It is in order here to compare the asymptotic behaviour given by equation (5) to the one corresponding to a shell model wave function whose least bound orbital has energy ε, which is $(1/r^2)\exp(-2\sqrt{-(2m/\hbar^2)\varepsilon}\,r)$. As can be seen, (5) goes faster to zero than the shell model wave function and the substitution $\beta \to 9\beta$, that would correspond to the original strength of the Weizsäcker term [6], would insure precisely the shell model fall-off. In the present work, we have not taken β as a parameter, despite the above mentioned observation, but rather kept the terms (1) as given in the theoretical derivation [7-9]. We are aware that this discussion may be questioned because the expansion (1) is not valid beyond the classical turning point. However, as will be seen in what follows, one can take a more practical view and consider (1) and (3) just as a very convenient way of getting solutions that are well behaved over the whole space.

Let us now describe the method we have followed to solve equation (3). As it stands, it is a highly non-linear differential equation. In order to proceed, we write (3) in the form

$$A(\rho)\rho + B(\rho,\rho')\rho' + C(\rho,\rho')\rho'' = \lambda\rho \qquad (6)$$

where A, B and C are known functions of ρ and ρ'. Equation (6) can be considered as an eigen-value equation ; it is similar to the usual HF equation. It can be solved by an iterative procedure : start from some function $\rho_0(r)$, compute A, B and C with ρ and ρ' replaced by ρ_0 and ρ_0' respectively, integrate (6) with the above mentioned boundary conditions

using a method similar to the one described in ref.[12], and iterate. In all cases studied, no problem of numerical instabilities has been found and the convergence is satisfactory. Provided that λ is negative, we always obtain a single solution which happens to be positive definite. The solution of (6) is denoted by ρ_{ITF}, from which τ_{ITF} is constructed through expression (1).

To illustrate the method described, let us now present some results. We leave the neutron ρ_n and proton ρ_p distributions free, apart from the normalisation to the correct number of particles, and include self-consistently the direct Coulomb term (the small exchange one is neglected as in ref.[2]). The spin-orbit force, for simplicity, has also been neglected, although it can be included also in $\tau(r)$ in the same semi-classical way [9]. Instead of solving, as described before, an equation of the form (6), we solve two coupled equations of essentially the same type, producing two eigen-values λ_n and λ_p and two functions $\rho_{ITF,n}$, $\rho_{ITF,p}$. The interaction SVI of the Skyrme type has been used [13]. It has been prefered to others because, having an effective mass $m^*(r)$ which is practically constant, it gives rise to an almost local potential, and the conditions under which expansion (1) has been derived are fulfilled. Otherwise, correction terms [9] depending on $m^*(r)$ and its derivatives should be included in (1).

Results for ^{40}Ca, ^{90}Zr and ^{208}Pb are presented in Table 1 and Fig. 1 ; the ones corresponding to the solution of eq. (6) are labelled ITF and for comparison HF results obtained under the same conditions (only direct Coulomb term included, spin-orbit term omitted) are also shown. Concerning the total energy E (see Table 1) the ITF approximation can be seen to be good to within 0.5MeV/particle. Both kinetic and potential energies are overestimated (in absolute value), the net result beeing an overbinding. Consequently, the r.m.s. radii (r_n and r_p) are slightly underestimated. The ITF proton and neutron densities ($\rho_{ITF,p}$ and $\rho_{ITF,n}$) compare rather well with the HF ones, except that the former have a sharper surface and no shell effects. The absence of shell effects is, of course inherent to the semi-classical approach ; the sharpness of the surface is directly connected to the value of the constant β in (1). The ITF curve corresponding to the kinetic energy density shows some structure beyond the mean radius ; this is essentially due to the term $\Delta\rho$ in (1). Consequently, attention should not be payed to it, because it does not contribute, after integration, to the kinetic energy and its contribution to the potential energy is negligible.

Several ways of improving the procedure described above

can be explored. One would be to keep further terms in the expansion of τ [9]. This would presumably lead to a better description of the mean or liquid drop properties, but shell effects would still be missing. We use a different method which, still preserving simplicity, incorporates shell effects (and also effective mass ones). It consists in solving the HF equation [2]

$$\left(-\underset{\sim}{\nabla}\cdot\frac{\hbar^2}{2m^*(r)}\underset{\sim}{\nabla}+U(r)\right)\phi_i=\varepsilon_i\phi_i \qquad (7)$$

where the HF effective mass m^* and the one-body potential U are given functions of ρ and τ (see eqs. (21) and (22a) of ref.[2]), not as a non-linear equation (requiring iterations) as it is, but as an ordinary Schrödinger equation (no iteration), with m^* and U computed using the functions ρ_{ITF} and τ_{ITF} determined before. This way of proceeding can be viewed essentially as treating $(\tau-\tau_{ITF})$ as a perturbation and allows to regain the single-particle features lost in the semi-classical treatment.

Results obtained in this way and denoted "Improved Thomas-Fermi plus shell corrections" (ITF+SC) are given in Table 1 and Fig. 1. When compared to the HF results, one can see that the agreement is very good : the energies are very similar, the surface of the densities are almost identical and the shell effects corresponding to the approximate treatment are at the correct place, although small discrepancies in their amplitudes are present.

Having checked its accuracy, let us illustrate the ITF approximation by studying the geometrical configuration of systems having very many nucleons. We restrict ourselves to configurations having spherical symmetry. From arguments based essentially on the Bethe-Weizsäcker mass formula [14], when the mass number increases sufficiently, the spherical configuration having the lowest energy is expected to be a shell (or bubble), because the gain in the Coulomb repulsion will compensate the lost due to the increase of the surface energy. We have solved eq. (6) for systems having $A\simeq 1000$. We give in Fig.2 results corresponding to $^{960}X_{294}^{696}$ which in our approximation is stable against particle-emission as well as β-stable. As can be seen, the lowest spherical solution is a "bubble", with a density close to the nuclear matter saturation density and with one interior and one exterior surfaces that are quite similar. The energy per particle (-3.5 Mev) is of the same order of magnitude as the estimate given by Bethe and Siemens [14]. Shell corrections as described before have also been included and drawn on the figure ; they reduce the binding by 0.2 Mev per particle. Of course, the main question is the stability of this configuration against deformations. Work in this direction is in progress.

The results presented in this letter are illustrative and serve mainly to check the accuracy of the method proposed. We think that, when applied to more complex problems, the simplification it will introduce may be essential.

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Table Caption

Table 1 Comparison of the results for the total and kinetic energies per particle and r.m.s. neutron and proton radii obtained using different approximations

Figure Captions

Figure 1 Comparison of the particle and kinetic energy densities for neutrons and protons in ^{208}Pb, using different approximations.

Figure 2 Neutron and proton densities for a system of A=980 nucleons, using different approximations.

	^{40}Ca			^{90}Zr			^{208}Pb		
	ITF	ITF+SC	HF	ITF	ITF+SC	HF	ITF	ITF+SC	HF
E/A (MeV)	-8.17	- 7.86	-7.91	-8.46	- 7.95	-7.93	-7.64	- 7.25	-7.24
E_{kin}/A (MeV)	17.03	16.59	16.24	17.80	17.63	17.43	18.50	18.36	18.20
r_n (fm)	3.32	3.35	3.38	4.29	4.35	4.37	5.63	5.67	5.69
r_p (fm)	3.35	3.40	3.43	4.26	4.27	4.31	5.56	5.56	5.59

Table 1

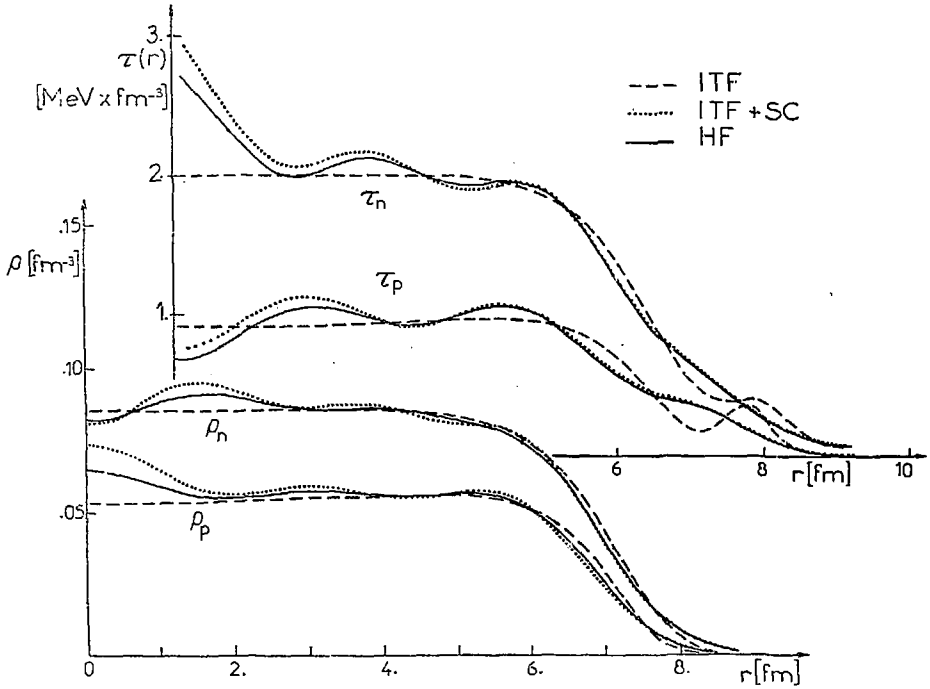
3.
τ(r)
[MeV x fm⁻³]
2.
1.
ITF
ITF + SC
HF
τn
τp
.15
ρ [fm⁻³]
.10
.05
ρn
ρp
6
8
r[fm]
10
0
2.
4.
6.
8.
r[fm]

Fig. 1

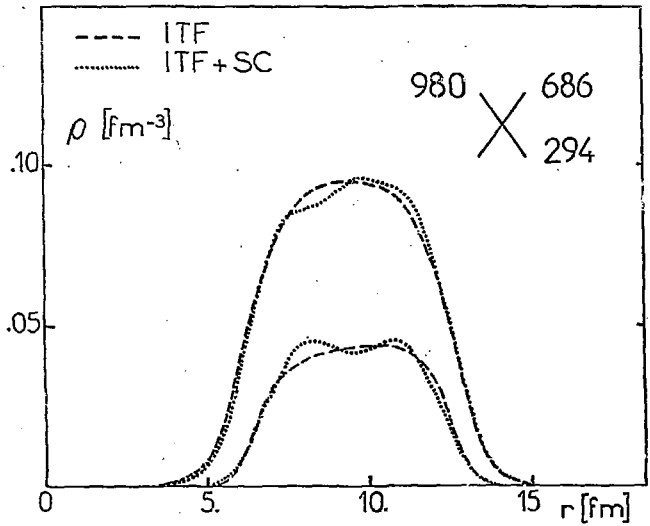

Fig. 2