AVERAGE NUCLEAR POTENTIALS FROM SELFCONSISTENT SEMICLASSICAL CALCULATIONS*

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Using the selfconsistent semiclassical Extended Thomas–Fermi (ETF) method up to 4^{th} order in connection with Skyrme forces it is demonstrated that the neutron and proton average potentials obtained using the semiclassical functionals $\tau^{(\mathrm{ETF})}[\rho]$ and $\vec{J}^{(\mathrm{ETF})}[\rho]$ reproduce the corresponding Hartree–Fock fields extremely well, except for shell oscillations in the nuclear center.

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The semiclassical Extended Thomas–Fermi method has been extremely successful in describing average nuclear properties [1], of the Liquid-Drop or Droplet-model type, ranging from binding energies over radii, nuclear deformation and fission properties to the description of low-lying collective excitations such as giant resonances. Starting from the Wigner–Kirkwood expansion which expresses densities such as the local density ρ_q, the kinetic energy density τ_q or the spin-orbit density $\vec{J}_q$, $\{q = n,p\}$, in a power series in $\hbar$ and gradient terms of the average potential, one is able to invert these series expansions to express *e.g.* τ_q as a functional of ρ_q. For effective nucleon-nucleon interactions such as those of the Skyrme type [2] which express the total energy of the nuclear system as a functional of the above mentioned densities ρ_q, τ_q and $\vec{J}_q$ one is then able within the ETF approach to write the total energy as a functional of the local densities ρ_n and ρ_p alone. In its selfconsistent version the ETF approach corresponds then to a density-variational calculation where the variational quantities are the neutron and proton densities instead of single-particle wave functions as is the case in the Hartree–Fock (HF) method.

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Whereas nuclear binding energies obtained in this way have been shown to reproduce very well the average Liquid-Drop type energy as can be obtained for a given nucleus and a given nuclear interaction from a Strutinski averaged HF calculation [1, 3], the form of the central potentials V_q, have never been explicitly investigated. It might however be interesting to look at these potentials and their reproduction by semiclassical methods, especially in the perspective of studying their dependence on rotation and nuclear excitation. It would indeed be interesting to know, how to change the parameters of a model potential as widely used as a Woods–Saxon mean field when going from a cold non-rotating nucleus to an excited one (characterized by a nuclear temperature T) [4] which is rotating with an angular frequency ω (angular momentum L) [5].

The present contribution is meant as a first step in this direction, namely to establish the validity and test the quality of the ETF approach what nuclear mean fields are concerned.

For effective nucleon-nucleon interactions of the Skyrme type (see *e.g.* [6] and references therein) the nuclear energy density is written as

$$
\begin{aligned}
\mathcal{E}(\vec{r}) =& \frac{\hbar^2}{2m}\tau + \frac{t_0}{2}\left[\left(1+\frac{x_0}{2}\right)\rho^2 - \left(x_0+\frac{1}{2}\right)(\rho_n^2+\rho_p^2)\right] + \frac{t_3}{12}\rho^\alpha \\
&\times \left[\left(1+\frac{x_3}{2}\right)\rho^2 - \left(x_3+\frac{1}{2}\right)(\rho_n^2+\rho_p^2)\right] + \frac{1}{4}\left[t_1\left(1+\frac{x_1}{2}\right) + t_2\left(1+\frac{x_2}{2}\right)\right] \\
&\times \rho\tau + \frac{1}{4}\left[-t_1\left(x_1+\frac{1}{2}\right) + t_2\left(x_2+\frac{1}{2}\right)\right](\rho_n\tau_n + \rho_p\tau_p) \\
&+ \frac{1}{16}\left[3t_1\left(1+\frac{x_1}{2}\right) - t_2\left(1+\frac{x_2}{2}\right)\right](\vec{\nabla}\rho)^2 \\
&- \frac{1}{16}\left[3t_1\left(x_1+\frac{1}{2}\right) + t_2\left(x_2+\frac{1}{2}\right)\right] \\
&\times \left[(\vec{\nabla}\rho_n)^2 + (\vec{\nabla}\rho_p)^2\right] + \frac{W_0}{2}\left[\vec{J}\cdot\vec{\nabla}\rho + \vec{J}_n\cdot\vec{\nabla}\rho_n + \vec{J}_p\cdot\vec{\nabla}\rho_p\right],
\end{aligned}
$$

where non-indexed quantities like ρ are the sum of neutron and proton densities $\rho = \rho_n + \rho_p$. In the ETF approach the kinetic energy densities τ_q and the spin-orbit densities $\vec{J}_q$, $\{q = n, p\}$ for protons and neutrons can be written as functionals of the corresponding local densities ρ_q

$$
\tau_q^{(\mathrm{ETF})}[\rho_q] = \tau_q^{(\mathrm{TF})}[\rho_q] + \tau_q^{(2)}[\rho_q] + \tau_q^{(4)}[\rho_q]
$$

and

$$
\vec{J}_q^{(\mathrm{ETF})}[\rho_q] = \vec{J}_q^{(2)}[\rho_q] + \vec{J}_q^{(4)}[\rho_q] .
$$

The Thomas–Fermi expression for the kinetic energy density is well known

$$\tau_q^{(\mathrm{TF})}[\rho_q] = \frac{3}{5}(3\pi^2)^{2/3}\,\rho_q^{5/3}\,,$$

whereas the semiclassical correction to τ of order $\hbar^2$ is a sum of 6 terms

$$\begin{aligned}\tau_q^{(2)}[\rho_q] \;=\; & \frac{1}{36}\frac{(\vec{\nabla}\rho_q)^2}{\rho_q} + \frac{1}{3}\Delta\rho_q + \frac{1}{6}\frac{\vec{\nabla}\rho_q\cdot\vec{\nabla}f_q}{f_q} + \frac{1}{6}\rho_q\frac{\Delta f_q}{f_q} - \frac{1}{12}\rho_q\left(\frac{\vec{\nabla}f_q}{f_q}\right)^2 \\ & + \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^2\rho_q\left(\frac{\vec{W}_q}{f_q}\right)^2 .\end{aligned}$$

As the spin is a pure quantal object there is no contribution to the spin-orbit density at the TF level and one has in second order simply

$$\vec{J}_q^{(2)}[\rho_q] = -\frac{2m}{\hbar^2}\frac{\vec{W}_q}{f_q}\rho_q\;.$$

The quantities f_q and $\vec{W}_q$ are the effective mass and spin-orbit form factors which will be defined below. The 4^{th} order corrections to $\tau[\rho]$ and $\vec{J}[\rho]$ are quite lengthy. They had been used in a partial integrated form in [1], but have been derived recently [7] from the semiclassical expansions given in reference [8].

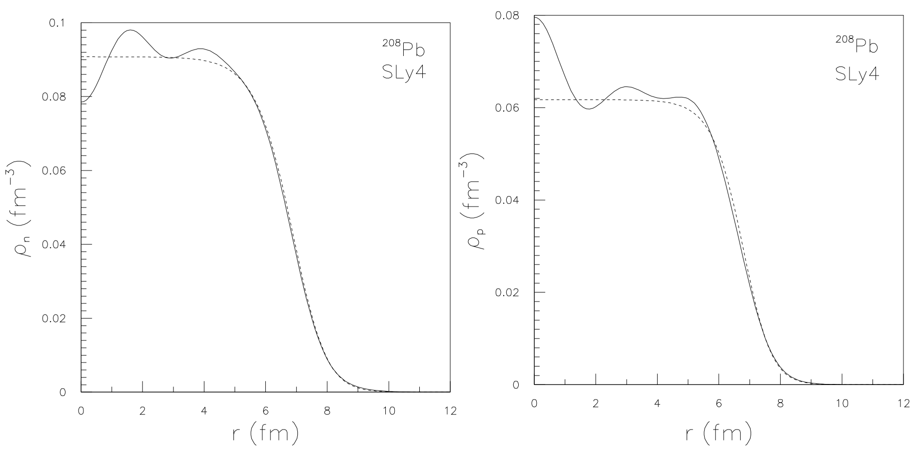

Fig. 1. Comparison of selfonsistent neutron and proton HF (solid line) and ETF denities (dashed line) for ^{208}Pb calculated with the SLy4 Skyrme force.

As mentioned before, selfconsistent semiclassical (density variational) calculations can be performed to obtain ground-state properties of nuclei. The semiclassical densities that minimize the total Skyrme ETF energy are shown in Fig. 1 for ^{208}Pb obtained with the Skyrme force SLy4 [9]. One notices a very reasonable reproduction of the HF densities obtained for the same nucleus with the same force, except for shell oscillations in the nuclear bulk, oscillations which *by definition* are absent from the semiclassical (liquid-drop type) densities. What seems important is that the nuclear surface is very well reproduced. An agreement of the same quality is obtained for other nuclei and other Skyrme forces such as SIII [10] and SkM* [6].

Encouraged by this result one can investigate the reproduction of the HF nuclear central potentials $V_q(\vec{r})$, the spin-orbit and effective-mass form factors $\vec{W}_q(\vec{r})$ and $f_q(\vec{r}) = \frac{m}{m_q^*(\vec{r})}$ mentioned above. They are given by functional derivatives of the above given energy density. One obtains the following expressions

$$
\begin{aligned}
V_q(\vec{r}) = \frac{\delta\mathcal{E}(\vec{r})}{\delta\rho_q(\vec{r})} &= t_0 \left[\left(1+\frac{x_0}{2}\right)\rho - \left(x_0+\frac{1}{2}\right)\rho_q\right] \\
&+\frac{t_3}{6}\rho^\alpha \left[\left(1+\frac{x_3}{2}\right)\rho - \left(x_3+\frac{1}{2}\right)\rho_q\right] + \frac{t_3}{12}\alpha\rho^{\alpha-1} \\
&\times \left[\left(1+\frac{x_3}{2}\right)\rho^2 - \left(x_3+\frac{1}{2}\right)(\rho_n^2+\rho_p^2)\right] \\
&+\frac{1}{4}\left[t_1\left(1+\frac{x_1}{2}\right) + t_2\left(1+\frac{x_2}{2}\right)\right]\tau \\
&+\frac{1}{4}\left[-t_1\left(x_1+\frac{1}{2}\right) + t_2\left(x_2+\frac{1}{2}\right)\right]\tau_q \\
&-\frac{1}{8}\left[3t_1\left(1+\frac{x_1}{2}\right) - t_2\left(1+\frac{x_2}{2}\right)\right]\vec{\nabla}^2\rho \\
&+\frac{1}{8}\left[3t_1\left(x_1+\frac{1}{2}\right) + t_2\left(x_2+\frac{1}{2}\right)\right]\vec{\nabla}^2\rho_q - \frac{W_0}{2}\left[\mathrm{div}\vec{J} + \mathrm{div}\vec{J}_q\right] .
\end{aligned}
$$

$$
\vec{W}_q(\vec{r}) = \frac{\delta\mathcal{E}(\vec{r})}{\delta\vec{J}_q(\vec{r})} = \frac{W_0}{2}\,\vec{\nabla}(\rho+\rho_q)
$$

and

$$
\begin{aligned}
f_q(\vec{r}) \;=\; \frac{2m}{\hbar^2}\frac{\delta\mathcal{E}(\vec{r})}{\delta\tau_q(\vec{r})} &= 1 + \frac{2m}{\hbar^2}\left\{\frac{1}{4}\left[t_1\left(1+\frac{x_1}{2}\right) + t_2\left(1+\frac{x_2}{2}\right)\right]\rho(\vec{r})\right. \\
&\left.-\frac{1}{4}\left[t_1\left(x_1+\frac{1}{2}\right) - t_2\left(x_2+\frac{1}{2}\right)\right]\rho_q(\vec{r})\right\} .
\end{aligned}
$$

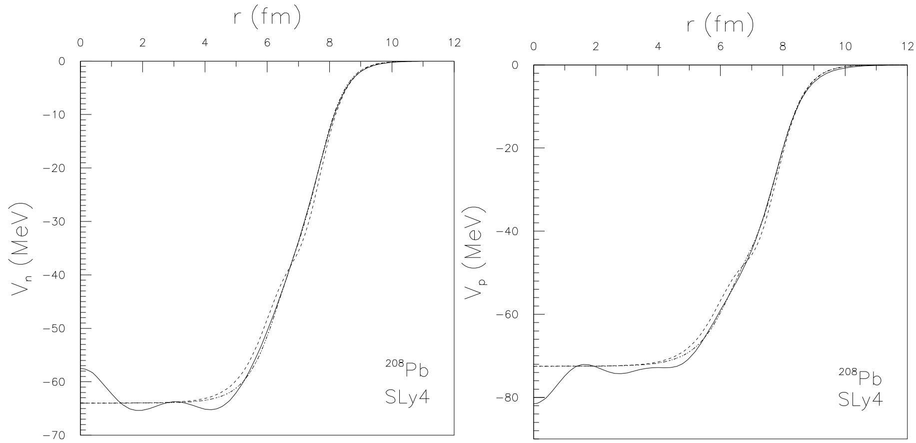

Fig. 2. Same as Fig. 1 for the neutron and proton central potentials V_n and V_p.

That the effective mass form factor $f_q(\vec{r})$ and the spin-orbit potential $\vec{W}_q(\vec{r})$ will be well reproduced is quite obvious from the quality of the agreement of HF and semiclassical densities. The ability of the semiclassical functionals to reproduce to a high degree of accuracy the nuclear mean fields $V_n(\vec{r})$ and $V_p(\vec{r})$ is much less evident. This is however the case as shown on figure 2.

One notices that already at the TF level the semiclassical average potentials look fairly reasonable. Going to second order in the semiclassical correction yield already nuclear mean fields which are almost undistinguishable from the corresponding HF results. Including fourth order corrections turn out to give a practically identical result. The difference between the potentials including up to second or up to forth order terms is invisible on figure 2.

As nuclear structure calculations using semiclassical methods are much more directly obtained than corresponding HF calculations it is now interesting, as already mentioned in the introduction, to study in a systematic way the dependence of nuclear average potentials on both nuclear temperature and angular frequency for rotating nuclei. Investigations along these lines are under way.

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