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Nuclear mean fields through self-consistent semiclassical calculations

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Abstract. Semiclassical expansions derived in the framework of the Extended Thomas-Fermi approach for the kinetic energy density $\tau(\vec{r})$ and the spin-orbit density $\vec{J}(\vec{r})$ as functions of the local density $\rho(\vec{r})$ are used to determine the central nuclear potentials $V_n(\vec{r})$ and $V_p(\vec{r})$ of the neutron and proton distribution for effective interactions of the Skyrme type. We demonstrate that the convergence of the resulting semiclassical expansions for these potentials is fast and that they reproduce quite accurately the corresponding Hartree-Fock average fields.

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1 Introduction

Mean-field calculations have been extremely successful over the last 3 decades to describe the structure of stable as well as radioactive nuclei and this over a very wide range of nuclear masses. Especially effective nucleon-nucleon interactions of the type of Skyrme [1,2] and Gogny forces [3] have been particularly efficient in this context. Such phenomenological effective interactions can be understood as mathematically simple parametrisations of a density-dependent effective G-matrix (see [4] and [5] for a review on such effective forces).

Together with the exact treatment of the mean-field problem in the Hartree-Fock (HF) approach, semiclassical approximations thereof have proven very appropriate. Especially the approach known as the Extended Thomas-Fermi (ETF) method has been shown [6] to describe very accurately average nuclear properties in the sense of the Bethe-Weizsäcker mass formula [7,8]. In their self-consistent version the ETF calculations determine the structure of a given nucleus by minimizing the total energy with respect to a variation of the neutron and proton densities. Such calculations require, however, only *integrated* quantities as, *e.g.*, the total nuclear energy.

The aim of the present paper is, on the contrary, to investigate *local* quantities such as nuclear mean-field potentials, effective mass and spin-orbit form factors which are at the basis of the description of the nuclear structure and which can be obtained as a function of the self-consistent semiclassical densities. The convergence of these local (non-integrated) semiclassical quantities and their comparison to the corresponding HF distributions has, to our knowledge, never been extensively investigated as this will be done here.

This paper is organized as follows. After specifying in sect. 2 the ETF expressions up to order $\hbar^4$ for $\tau[\rho]$ and $\vec{J}[\rho]$ derived from the general but rather cumbersome form of these expressions given in [9,10], we show in sect. 3 that the semiclassical expansions which define these quantities converge rapidly for reasonable forms of the nuclear density $\rho(\vec{r})$. Once these expressions and their convergence established, we compare in sect. 4 the average mean fields obtained using these semiclassical densities to the central potentials resulting from a HF calculation. We finally conclude giving an outlook on how these calculations can be generalized to excited and rotating nuclei.

2 Form factors for Skyrme interactions

For effective nucleon-nucleon interactions of the Skyrme type the total energy of a nucleus is a functional of the local densities $\rho_q(\vec{r})$, the kinetic energy densities $\tau_q(\vec{r})$ and the so-called spin-orbit densities $\vec{J}_q(\vec{r})$ [2]

$$E = \int \mathcal{E}(\rho_q(\vec{r}), \tau_q(\vec{r}), \vec{J}_q(\vec{r}))\, \mathrm{d}^3 r \,, \tag{1}$$

where the subscript q={n, p} denotes the nucleon charge state. In the case of broken time-reversal symmetry the

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energy density depends, in addition, on other local quantities [11,12], such as the current density $\vec{j}(\vec{r})$ and the spin-vector density $\vec{\rho}(\vec{r})$. In what follows we will restrict ourselves to time-reversal symmetric systems leaving the case of broken time-reversal symmetry, particularly encountered in the case of rotating nuclei, to a subsequent publication.

The total energy determined in this way is exact within the HF formalism. A semiclassical approximation thereof is obtained when instead of using the exact quantum-mechanical densities $\rho_q(\vec{r})$, $\tau_q(\vec{r})$, $\vec{J}_q(\vec{r})$, etc. a semiclassical approximation for these quantities is used. The semiclassical densities $\tau_q(\vec{r})$ and $\vec{J}_q(\vec{r})$ are obtained in the so-called *Extended Thomas-Fermi model* [6] as functions of the local density $\rho(\vec{r})$ and of its derivatives. The best known of these functionals is the Thomas-Fermi approximation for the kinetic energy density in the form

$$\tau_q^{(\mathrm{TF})}[\rho_q] = \frac{3}{5}\,(3\pi^2)^{2/3}\,\rho_q^{5/3} \quad , \quad q = \{n,p\}\,. \tag{2}$$

Once these functional expression are given, the total energy of the nuclear system is then uniquely determined by the knowledge of the local densities of protons and neutrons. That such a functional dependence of the total energy on the local densities $\rho_q(\vec{r})$ should exist is guaranteed by the famous theorem by Hohenberg and Kohn [13]. In the most general quantum-mechanical case this functional is, however, perfectly unknown. The great advantage of the semiclassical approach used here, consists in the fact that, in connection with effective interactions of the Skyrme type such an energy functional $\mathcal{E}$ can be derived explicitly. In addition, it is to be noted that the semiclassical functionals obtained in the ETF formalism such as $\tau[\rho]$ are completely general and valid for any local interaction and any nucleus, and can therefore be determined once and forever.

Once the functional of the total energy is known, one is able, due to the Hohenberg-Kohn theorem, to perform density variational calculations, where the local densities $\rho_q(\vec{r})$ are the variational quantities. One should, however, keep in mind that, as the ETF functionals are of semiclassical nature, the density functions $\rho_q(\vec{r})$ obtained as a result of the variational procedure can only be semiclassical in nature, *i.e.* of the liquid-drop type. Taking into account that in such a process the particle numbers N and Z should be conserved, one can formulate the variational principle in the form

$$\frac{\delta}{\delta\rho_q}\int\{\mathcal{E}[\rho_n(\vec{r}),\rho_p(\vec{r})] - \lambda_n\rho_n(\vec{r}) - \lambda_p\rho_p(\vec{r})\}\,\mathrm{d}^3r\,, \tag{3}$$

with the Lagrange multipliers λ_n and λ_p to ensure the conservation of neutron and proton number.

This density variational problem has been solved in two different ways in the past: either by resolving the Euler-Lagrange equation [14,15] resulting from eq. (3) or by carrying out the variational calculation in a restricted subspace of functions adapted to the problem, *i.e.* being of semiclassical nature, free of shell oscillations in the nuclear interior and falling off exponentially in the nuclear surface. It has been shown [6,14] that modified Fermi functions, which for spherical symmetry take the form

$$\rho_q(\vec{r}) = \rho_{0_q}\left[1+\exp\left(\frac{r-R_{0_q}}{a_q}\right)\right]^{-\gamma_q} , \quad q = \{n,p\}\,, \tag{4}$$

are particularly well suited in this context and that the semiclassical energies obtained are, indeed, very close to those resulting from the exact variation [14,15].

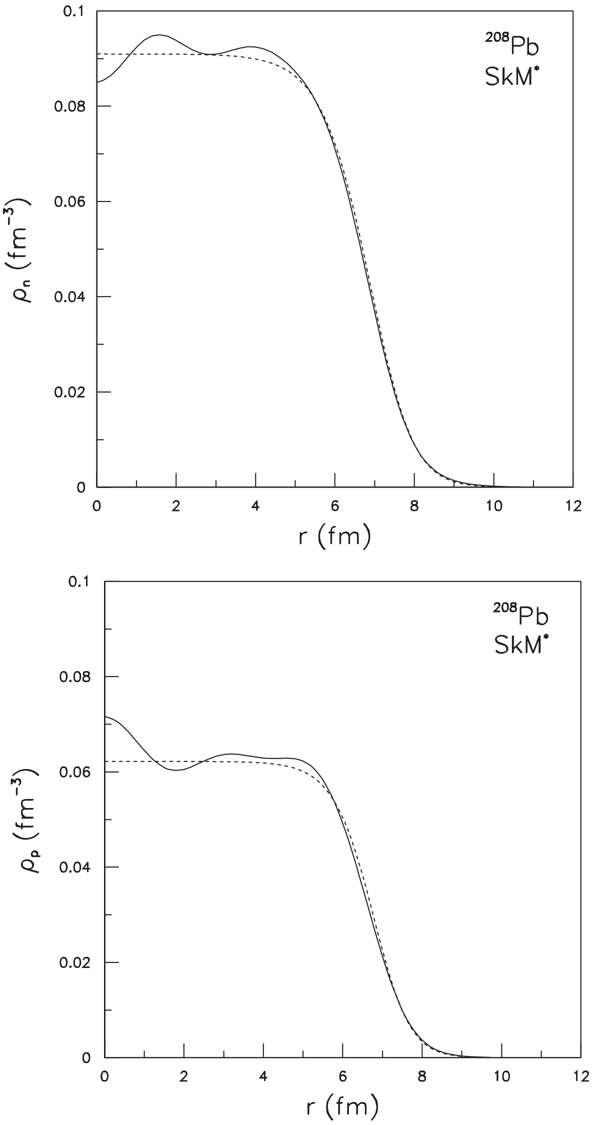

Fig. 1. Comparison of self-consistent neutron and proton HF (solid line) and ETF densities (dashed line) for ^{208}Pb calculated with the SkM* Skyrme force.

As an example of the quality of the semiclassical density obtained by such a restricted variation in the subspace of modified Fermi functions, eq. (4), we show in fig. 1 a comparison of the neutron and proton densities obtained in this way within the ETF approach with the corresponding Hartree-Fock (HF) densities for the nucleus ^{208}Pb calculated with the Skyrme interaction SkM* [16]. It should be emphasized here that a similarly good agreement as

Table 1. Correspondence between the coefficients B_i used in the text and the usual Skyrme force parameters.

B_1	$\frac{1}{2}t_0\left(1+\frac{x_0}{2}\right)$
B_2	$-\frac{t_0}{2}\left(\frac{1}{2}+x_0\right)$
B_3	$\frac{1}{4}\left[t_1\left(1+\frac{x_1}{2}\right)+t_2\left(1+\frac{x_2}{2}\right)\right]$
B_4	$-\frac{1}{4}\left[t_1\left(x_1+\frac{1}{2}\right)-t_2\left(x_2+\frac{1}{2}\right)\right]$
B_5	$-\frac{1}{16}\left[3t_1\left(1+\frac{x_1}{2}\right)-t_2\left(1+\frac{x_2}{2}\right)\right]$
B_6	$\frac{1}{16}\left[3t_1\left(x_1+\frac{1}{2}\right)+t_2\left(x_2+\frac{1}{2}\right)\right]$
B_7	$\frac{1}{12}t_3\left(1+\frac{x_3}{2}\right)$
B_8	$-\frac{1}{12}t_3\left(\frac{1}{2}+x_3\right)$
B_9	$-\frac{1}{2}W_0$

the one shown in fig. 1 is obtained for other nuclei or using other effective interactions such as the Skyrme forces SIII [17] and SLy4 [18].

The energy density $\mathcal{E}$ appearing in eqs. (1) and (3) can be written for a Skyrme interaction as defined in ref. [19] in the compact form [20]

$$\begin{aligned}\mathcal{E}(\vec{r}\,) = &\frac{\hbar^2}{2m}\tau + B_1\rho^2 + B_2(\rho_n^2+\rho_p^2)\\ &+B_3\rho\,\tau + B_4(\rho_n\,\tau_n+\rho_p\,\tau_p)\\ &-B_5(\vec{\nabla}\rho)^2 - B_6\left[(\vec{\nabla}\rho_n)^2+(\vec{\nabla}\rho_p)^2\right]\\ &+\rho^\alpha[B_7\rho^2+B_8(\rho_n^2+\rho_p^2)]\\ &-B_9\left[\vec{J}\cdot\vec{\nabla}\rho+\vec{J}_n\cdot\vec{\nabla}\rho_n+\vec{J}_p\cdot\vec{\nabla}\rho_p\right]+\mathcal{E}_{\rm Coul}(\vec{r}\,)\,,\end{aligned} \tag{5}$$

given in terms of the coefficients B_1–B_9 (see table 1) instead of the usual Skyrme force parameters $t_0, t_1, t_2, t_3, x_0, x_1, x_2, x_3, W_0$.

In eq. (5) non-indexed quantities like ρ correspond to the sum of neutron and proton densities as $\rho = \rho_n + \rho_p$ and $\mathcal{E}_{\rm Coul}$ is the Coulomb energy density which can be written as the sum of the direct and an exchange contribution, the latter being taken into account in the Slater approximation [21,22]

$$\mathcal{E}_{\rm Coul}(\vec{r}\,) = \frac{e^2}{2}\rho_p(\vec{r}\,)\int {\rm d}^3r'\,\frac{\rho_p(\vec{r}\,')}{|\,\vec{r}-\vec{r}\,'\,|} - \frac{3}{4}e^2\left(\frac{3}{\pi}\right)^{1/3}\rho_p^{4/3}(\vec{r}\,)\,. \tag{6}$$

The HF equation is obtained through the variational principle which states that the total energy of eq. (1) should be stationary with respect to any variation of the single-particle wave functions $\varphi_j^{(q)}$:

$$\begin{aligned}\hat{\mathcal{H}}_q\varphi_j^{(q)} &= \left(-\vec{\nabla}\frac{\hbar^2}{2m_q^*(\vec{r}\,)}\vec{\nabla}+V_q(\vec{r}\,)-i\vec{W}_q(\vec{r}\,)\cdot(\vec{\nabla}\times\vec{\sigma})\right)\varphi_j^{(q)}\\ &= \varepsilon_j^{(q)}\varphi_j^{(q)}\,.\end{aligned} \tag{7}$$

Here appear different form factors such as the central one-body potential $V_q(\vec{r}\,)$, the effective mass $m_q^*(\vec{r}\,)$ and the spin-orbit potential $\vec{W}_q(\vec{r}\,)$ which are all defined as functional derivatives of the total energy density. One obtains from eq. (5):

$$\begin{aligned}V_q(\vec{r}\,) = \frac{\delta\mathcal{E}(\vec{r}\,)}{\delta\rho_q(\vec{r}\,)} &= 2(B_1\rho+B_2\rho_q)+B_3\tau+B_4\tau_q\\ &+2(B_5\Delta\rho+B_6\Delta\rho_q)+(2+\alpha)B_7\rho^{\alpha+1}\\ &+B_8\left[\alpha\rho^{\alpha-1}\sum_q\rho_q^2+2\rho^\alpha\rho_q\right]\\ &+B_9({\rm div}\vec{J}+{\rm div}\vec{J}_q)+V_{\rm Coul}(\vec{r}\,)\,\delta_{pq}\,,\end{aligned} \tag{8}$$

$$\begin{aligned}f_q(\vec{r}\,) = \frac{m}{m_q^*(\vec{r}\,)} &= \frac{2m}{\hbar^2}\,\frac{\delta\mathcal{E}(\vec{r}\,)}{\delta\tau_q(\vec{r}\,)}\\ &= 1+\frac{2m}{\hbar^2}\,[B_3\rho(\vec{r}\,)+B_4\rho_q(\vec{r}\,)]\end{aligned} \tag{9}$$

and

$$\vec{W}_q(\vec{r}\,) = \frac{\delta\mathcal{E}(\vec{r}\,)}{\delta\vec{J}_q(\vec{r}\,)} = -B_9\,\vec{\nabla}(\rho+\rho_q)\,. \tag{10}$$

The Coulomb potential in eq. (8) is easily obtained as

$$V_{\rm Coul}(\vec{r}\,) = e\int\frac{\rho_p(\vec{r}\,')}{|\,\vec{r}-\vec{r}\,'\,|}\,{\rm d}^3r\,' - \left(\frac{e}{\pi}\right)^{1/3}\rho_p^{1/3}(\vec{r}\,)\,. \tag{11}$$

It is noteworthy in this connection that for such an effective mass (9) and spin-orbit potential (10) the energy density (5) takes the simple form

$$\begin{aligned}\mathcal{E}(\vec{r}\,) = &\frac{\hbar^2}{2m}\sum_q f_q\,\tau_q + B_1\rho^2 + B_2(\rho_n^2+\rho_p^2)\\ &-B_5(\vec{\nabla}\rho)^2 - B_6\left[(\vec{\nabla}\rho_n)^2+(\vec{\nabla}\rho_p)^2\right]\\ &+\rho^\alpha[B_7\rho^2+B_8(\rho_n^2+\rho_p^2)]\\ &+\sum_q\vec{J}_q\cdot\vec{W}_q+\mathcal{E}_{\rm Coul}(\vec{r}\,)\,,\end{aligned} \tag{12}$$

which simplifies somewhat the calculation.

All the expressions derived so far (eqs. (6)–(12)) are exact and when used with densities constructed from the single-particle wave functions $\varphi_j^{(q)}(\vec{r}\,)$, solutions of the HF equation (7), these quantities contain all the quantum effects of the system. If one is interested in the semiclassical approximation of these form factors one can immediately conclude, from the analytical form of eqs. (9) and (10) and the smooth behavior of the semiclassical densities, as demonstrated in fig. 1, on the smooth behavior of the semiclassical effective mass and spin-orbit form factors. As the nuclear quantal density is well reproduced on the average by the ETF densities it appears evident that the same is going to be the case for the effective mass and the spin-orbit potential, when semiclassical, *i.e.* liquid-drop–type densities are used in eqs. (9) and (10).

Things are, however, less evident for the central nuclear potentials. Not only is the functional expression, eq. (8), much more complicated then those for the effective mass and spin-orbit potential, but the central potential is also the only one of the three functional derivatives that depends not only on the local densities $\rho_q(\vec{r})$ and their derivatives but also on the kinetic energy density $\tau_q(\vec{r})$ and the spin-orbit density $\vec{J}_q(\vec{r})$ which are the quantities for which the Extended Thomas-Fermi approach has written down functional expressions. We, therefore, choose to study the convergence of the semiclassical series corresponding to these functional expressions of $\tau_q[\rho_q]$ and $\vec{J}_q[\rho_q]$ before investigating the quality of the agreement between the HF central potential and the one obtained when using these semiclassical ETF functionals.

3 Convergence of ETF functionals

The semiclassical expansions of kinetic energy density τ_q and spin-orbit density $\vec{J}_q$ as functions of the local density ρ_q are functional expressions with $\hbar$ as order parameter. These expressions can be obtained for instance through the semiclassical $\hbar$ expansions developed by Wigner [23] and Kirkwood [24] or through the semiclassical method of Baraff and Borowitz [25]. In either of the two approaches one obtains functional expressions like

$$\tau_q^{(\mathrm{ETF})}[\rho_q] = \tau_q^{(\mathrm{TF})}[\rho_q] + \tau_q^{(2)}[\rho_q] + \tau_q^{(4)}[\rho_q]\,, \qquad (13)$$

written here for the kinetic energy density $\tau_q(\vec{r})$ where $\tau_q^{(\mathrm{TF})}[\rho_q]$ is the well-known Thomas-Fermi expression already given in eq. (2), $\tau_q^{(2)}[\rho_q]$ the semiclassical correction of second order and $\tau_q^{(4)}[\rho_q]$ is of fourth order in $\hbar$. The ETF expressions such as $\tau_q^{(\mathrm{ETF})}[\rho_q]$, eq. (13), up to order $\hbar^4$ are to be understood as the converging part of an asymptotic series.

The second-order term $\tau_q^{(2)}[\rho_q]$ has already been derived in ref. [26] for a Hamiltonian, eq. (7), with an effective mass $m_q^* = m/f_q$ and a spin-orbit potential $\vec{W}_q$

$$\tau_q^{(2)}[\rho_q] = \frac{1}{36}\frac{(\vec{\nabla}\rho_q)^2}{\rho_q} + \frac{1}{3}\Delta\rho_q + \frac{1}{6}\frac{\vec{\nabla}\rho_q\cdot\vec{\nabla}f_q}{f_q} + \frac{1}{6}\rho_q\frac{\Delta f_q}{f_q} - \frac{1}{12}\rho_q\left(\frac{\vec{\nabla}f_q}{f_q}\right)^2 + \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^2\rho_q\left(\frac{\vec{W}_q}{f_q}\right)^2, \qquad (14)$$

the first term of which is known as the Weizsäcker correction [7]. It was sometimes used in the past with an adjustable parameter (instead of $\frac{1}{36}$) in order to mock up the absence of the other second-order and all of the fourth-order terms. It has, however, been shown (see, *e.g.*, ref. [6]) that such a procedure is unable to correctly describe both the slope of the surface of the nuclear mass or charge density and, at the same time, the height of nuclear fission barriers in the actinide region. From this analysis we conclude that the inclusion of fourth-order terms in the semiclassical functionals is, in fact, without credible alternatives.

In the following we are going to exploit the expressions for the 4th-order functionals τ_q and $\vec{J}_q$ developed by Grammaticos and Voros [9,10]. These authors have taken the convention "that any free-standing gradient operator acts only on the *rightmost* term" (see their remark after eq. (III.13) of ref. [9]). In our present work we prefer to rewrite these terms in a more conventional way and have any free-standing gradient operator act, as usual, on *all* the terms that appear on its right-hand side. We, therefore, write (subscripts GV refer to the Grammaticos-Voros convention)

$$\left[(\vec{\nabla}f_q\cdot\vec{\nabla})^2 f_q\right]_{\mathrm{GV}} = \frac{1}{2}(\vec{\nabla}f_q\cdot\vec{\nabla})(\vec{\nabla}f_q)^2\,,$$

$$\left[(\vec{\nabla}\rho_q\cdot\vec{\nabla})^2 f_q\right]_{\mathrm{GV}} = \vec{\nabla}\rho_q\cdot\vec{\nabla}(\vec{\nabla}f_q\cdot\vec{\nabla}\rho_q) - \frac{1}{2}\vec{\nabla}f_q\cdot\vec{\nabla}(\vec{\nabla}\rho_q)^2\,,$$

and

$$\left[(\vec{\nabla}f_q\cdot\vec{\nabla})(\vec{\nabla}\rho_q\cdot\vec{\nabla})f_q\right]_{\mathrm{GV}} = \frac{1}{2}\vec{\nabla}\rho_q\cdot\vec{\nabla}(\vec{\nabla}f_q)^2\,,$$

plus terms that are obtained from these ones by interchanging the role of f_q and ρ_q. One has also to keep in mind that Grammaticos and Voros use a slightly different definition of the effective-mass and spin-orbit form factors than the ones given in eqs. (9) and (10) above:

$$f_{\mathrm{GV}} = \frac{1}{m}f$$

and

$$\vec{S}_{\mathrm{GV}} = \frac{1}{\hbar^2}\vec{W}\,.$$

Using these expressions we obtain the following form for the 4th-order kinetic energy density, where contributions from the spin-orbit interaction have been, temporarily left out:

$$\tau_q^{(4)}[\rho_q] = (3\pi^2)^{-2/3}\frac{\rho_q^{1/3}}{4320}\Bigg\{24\frac{\Delta^2\rho_q}{\rho_q} - 60\frac{\vec{\nabla}\rho_q\cdot\vec{\nabla}(\Delta\rho_q)}{\rho_q^2} - 28\left(\frac{\Delta\rho_q}{\rho_q}\right)^2 - 14\frac{\Delta(\vec{\nabla}\rho_q)^2}{\rho_q^2} + \frac{280}{3}\frac{(\vec{\nabla}\rho_q)^2\Delta\rho_q}{\rho_q^3} + \frac{184}{3}\frac{\vec{\nabla}\rho_q\cdot\vec{\nabla}(\vec{\nabla}\rho_q)^2}{\rho_q^3} - 96\left(\frac{\vec{\nabla}\rho_q}{\rho_q}\right)^4 - 36\frac{\Delta^2 f_q}{f_q} + 36\frac{\Delta(\vec{\nabla}f_q)^2}{f_q^2} - 18\left(\frac{\Delta f_q}{f_q}\right)^2 - 72\frac{\vec{\nabla}f_q\cdot\vec{\nabla}(\vec{\nabla}f_q)^2}{f_q^3}$$

$$+54\left(\frac{\vec{\nabla} f_q}{f_q}\right)^4 + 12\frac{\Delta(\vec{\nabla} f_q\cdot\vec{\nabla}\rho_q)}{f_q\,\rho_q} + 24\frac{\vec{\nabla} f_q\cdot\vec{\nabla}(\Delta\rho_q)}{f_q\,\rho_q}$$
$$-36\frac{\vec{\nabla}\rho_q\cdot\vec{\nabla}(\Delta f_q)}{f_q\,\rho_q} + 24\frac{\vec{\nabla}\rho_q\cdot\vec{\nabla}(\vec{\nabla} f_q)^2}{f_q^2\,\rho_q}$$
$$-12\frac{(\vec{\nabla} f_q\cdot\vec{\nabla}\rho_q)\Delta f_q}{f_q^2\,\rho_q} - 24\frac{\vec{\nabla} f_q\cdot\vec{\nabla}(\vec{\nabla} f_q\cdot\vec{\nabla}\rho_q)}{f_q^2\,\rho_q}$$
$$-44\frac{\vec{\nabla}\rho_q\cdot\vec{\nabla}(\vec{\nabla} f_q\cdot\vec{\nabla}\rho_q)}{f_q\,\rho_q^2} - 16\frac{\vec{\nabla} f_q\cdot\vec{\nabla}(\vec{\nabla}\rho_q)^2}{f_q\,\rho_q^2}$$
$$-52\frac{(\vec{\nabla} f_q\cdot\vec{\nabla}\rho_q)\Delta\rho_q}{f_q\,\rho_q^2} + 30\frac{(\vec{\nabla} f_q\cdot\vec{\nabla}\rho_q)^2}{f_q^2\,\rho_q^2}$$
$$+\frac{260}{3}\frac{(\vec{\nabla} f_q\cdot\vec{\nabla}\rho_q)(\vec{\nabla}\rho_q)^2}{f_q\,\rho_q^3}\Bigg\}\,. \qquad (15)$$

The interested reader, who might want to use the semiclassical functionals calculated here, will find in the appendix the expression that the 4th-order kinetic energy density takes in the case of spherical symmetry as well as all the other semiclassical functionals developed below.

Until now we have not taken into account the spin-orbit interaction. Its influence on the semiclassical ETF functionals is treated in ref. [10] and its contribution $\tau_q^{(4)\mathrm{so}}$ constitutes simply an additive term to the spin-orbit independent part of the kinetic energy density considered above. According to [10]:

$$\tau_q^{(4)\mathrm{so}}[\rho] = (3\pi^2)^{-2/3}\left(\frac{2m}{\hbar^2}\right)^2\frac{\rho_q^{1/3}}{4f_q^2}\Bigg\{\Bigg[\frac{1}{4}\vec{W}_q\cdot\Delta\vec{W}_q$$
$$+\frac{1}{2}\vec{W}_q\cdot\vec{\nabla}(\mathrm{div}\vec{W}_q)+\frac{1}{8}\Delta(\vec{W}_q^2)+\frac{1}{4}(\mathrm{div}\,\vec{W}_q)^2\Bigg]$$
$$-\frac{1}{2f_q}\Bigg[2\vec{W}_q\cdot(\vec{\nabla} f_q\cdot\vec{\nabla})\vec{W}_q+\mathrm{div}\vec{W}_q\,(\vec{\nabla} f_q\cdot\vec{W}_q)$$
$$+\vec{\nabla} f_q\cdot(\vec{W}_q\cdot\vec{\nabla})\vec{W}_q+\vec{W}_q^2\Delta f_q+\vec{W}_q\cdot\vec{\nabla}(\vec{W}_q\cdot\vec{\nabla} f_q)$$
$$-\frac{1}{2}\vec{\nabla} f_q\cdot\vec{\nabla}(\vec{W}_q^2)\Bigg]+\frac{3}{4f_q^2}\Bigg[(\vec{\nabla} f_q)^2\vec{W}_q^2+(\vec{W}_q\cdot\vec{\nabla} f_q)^2$$
$$-\left(\frac{2m}{\hbar^2}\right)^2\vec{W}_q^4\Bigg]+\frac{1}{6\rho_q}\Bigg[\vec{W}_q\cdot(\vec{\nabla}\rho_q\cdot\vec{\nabla})\vec{W}_q$$
$$+(\vec{W}_q\cdot\vec{\nabla}\rho_q)\,\mathrm{div}\vec{W}_q\Bigg]-\frac{1}{6f_q\rho_q}\Bigg[(\vec{\nabla} f_q\cdot\vec{\nabla}\rho_q)\vec{W}_q^2$$
$$+(\vec{\nabla} f_q\cdot\vec{W}_q)(\vec{\nabla}\rho_q\cdot\vec{W}_q)\Bigg]\Bigg\}\,. \qquad (16)$$

It is now interesting to investigate the relative importance of the different contributions in eqs. (2), (14), (15) and (16) to the kinetic energy density obtained when using the self-consistent semiclassical densities generated by a variational procedure restricted to functions of the type of eq. (4) as explained above. As can be seen in fig. 2 (a) the Thomas-Fermi contribution to $\tau[\rho]$ is largely dominant, at least in the nuclear bulk. Semiclassical corrections play, however, a significant role in the nuclear surface with a second-order correction which is much larger than the fourth-order term (multiplied for better visibility by a factor 10 in fig. 2 (a)). The different contributions to the second- and fourth-order functional are given, respectively, in part (b) and (c) of the figure. We show the contributions coming form gradient terms of ρ (term 1 and 2 in eq. (14)), of f (terms 4 and 5) and the mixed term (term 3) as well as the spin-orbit contribution (last term) and similarly in part (c) of the figure for the fourth-order term. As can be seen, the gradient term of ρ is dominant in 2nd order, whereas in 4th order the spin-orbit contribution becomes also crucial. The self-consistent HF neutron kinetic energy density is also shown in fig. 2 (a). One notices that, except for quantum oscillations in the nuclear interior, the HF kinetic energy density is quite nicely reproduced if the semiclassical corrections τ_2 and τ_4 are taken into account.

It is interesting to note in this connection that, despite the fact that the 2nd-order contribution $\tau_q^{(2)}(\vec{r})$ is one order of magnitude larger than the 4th-order contribution, after integration, the 2nd-order contribution of $\tau[\rho]$ to the total energy, *i.e.* the integral $\sum_q\int f_q(\vec{r})\tau_q^{(2)}(\vec{r})\mathrm{d}^3r$ is of the same order of magnitude than the corresponding 4th-order contribution (see, *e.g.*, [27,6]), which seems to indicate that there is a stronger cancellation taking place in the 2nd-order than in 4th-order contribution.

We have done the same study for the proton distribution, for other nuclei and used other effective interactions of the Skyrme type, namely the Skyrme SIII force [17] and the SLy4 Skyrme force [18]. The conclusions made above remain valid in all these cases, only the relative importance of the semiclassical corrections $\tau^{(2)}[\rho]$ and $\tau^{(4)}[\rho]$ increases slightly when one goes from heavy to light nuclei.

As already discussed above, ETF functionals like $\tau^{(\mathrm{ETF})}[\rho]$, eq. (13), up to order $\hbar^4$ constitute the converging part of an asymptotic expansion which needs to be truncated. Comparing, indeed, the ρ-dependence of the different orders of the semiclassical functional ($\rho^{5/3}$ for $\tau^{(\mathrm{TF})}[\rho]$, ρ for $\tau^{(2)}[\rho]$ and $\rho^{1/3}$ for $\tau^{(4)}[\rho]$) one concludes that a term $\tau^{(6)}[\rho]$ in the ETF functional would show a ρ-dependence of the form $\rho^{-1/3}$ and would therefore diverge in the limit $r\to\infty$ for densities that fall off exponentially at large distances.

Let us now turn to the spin-orbit density $\vec{J}$. It is given in ref. [10] in the form of a second-rank tensor which is related to the components of the vector $\vec{J}$ by the relation

$$J_\lambda = \sum_{\mu\nu}\epsilon_{\lambda\mu\nu}\,J_{\mu\nu}\,,$$

where $\epsilon_{\lambda\mu\nu}$ is the Levi-Civita symbol. The spin being a purely quantal property with no classical analogon, there is no contribution to the semiclassical functional of $\vec{J}$ in lowest order, *i.e.* at the level of the Thomas-Fermi approach whereas one obtains for the 2nd- and 4th-order contributions to the semiclassical expansion of the spin-

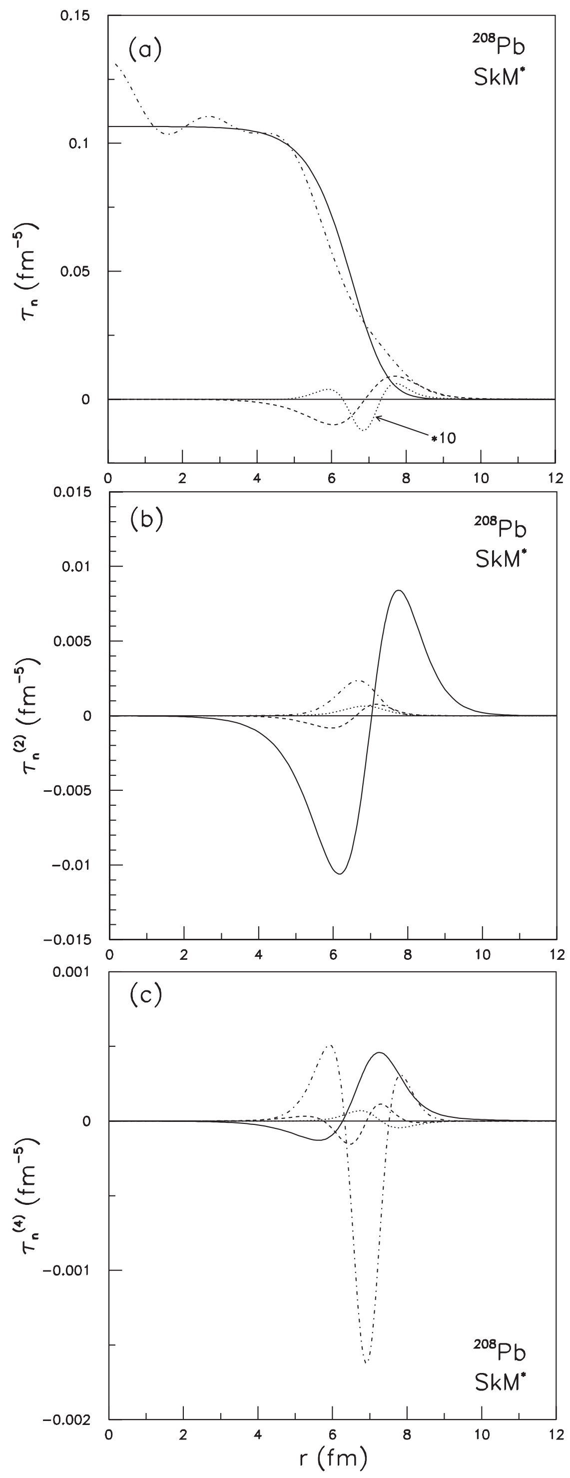

Fig. 2. Contributions from the different orders in the semiclassical expansion to the kinetic energy density $\tau[\rho]$ for the self-consistent neutron density distribution shown in fig. 1 for ^{208}Pb (TF (solid line), 2nd- (dashed line) and 4th-order multiplied (dotted line)) are compared with the corresponding HF density (dash-dotted line) (part (a)). Different contributions to 2nd (part (b)) and 4th order (part (c)) coming from gradient terms of ρ (solid line), of f (dashed line), of mixed terms containing gradient terms of ρ and f (dotted line), and of the spin-orbit coupling (dash-dotted line).

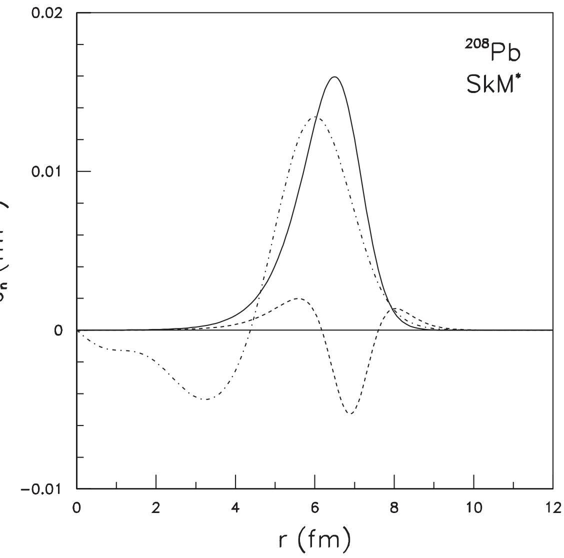

Fig. 3. Contributions from the different orders in the semiclassical expansion (2nd (solid line) and 4th order (dashed line)) to the radial part of the vector field $\vec{J}_q(\vec{r})$ shown here for the self-consistent spherical neutron distribution of ^{208}Pb as compared to the HF spin-orbit density (dash-dotted line).

orbit density

$$\vec{J}_q^{(2)} = -\frac{2m}{\hbar^2}\,\frac{\rho_q}{f_q}\,\vec{W}_q \tag{17}$$

and

$$\begin{aligned}\vec{J}_q^{(4)} = {}& (3\pi^2)^{-2/3}\,\frac{2m}{\hbar^2}\,\frac{\rho_q^{1/3}}{8f_q}\Bigg\{-\Big[\mathit{\Delta}\vec{W}_q + \vec{\nabla}(\mathrm{div}\vec{W}_q)\Big] \\ & +\frac{1}{f_q}\Big[\vec{W}_q\,\mathit{\Delta} f_q + (\vec{W}_q\cdot\vec{\nabla})\vec{\nabla}f_q + (\vec{\nabla}f_q\times\mathrm{rot}\vec{W}_q) \\ & +2(\vec{\nabla}f_q\cdot\vec{\nabla})\vec{W}_q\Big] - \frac{1}{f_q^2}\Bigg[(\vec{\nabla}f_q)^2\vec{W}_q + (\vec{\nabla}f_q\cdot\vec{W}_q)\vec{\nabla}f_q \\ & -2\left(\frac{2m}{\hbar^2}\right)^2\vec{W}_q^3\Bigg] - \frac{1}{3\rho_q}\Bigg[(\vec{\nabla}\rho_q\cdot\vec{\nabla})\vec{W}_q + \mathrm{div}\vec{W}_q\,\vec{\nabla}\rho_q \\ & -\frac{1}{f_q}\Big((\vec{\nabla}f_q\cdot\vec{\nabla}\rho_q)\vec{W}_q + (\vec{\nabla}f_q\cdot\vec{W}_q)\vec{\nabla}\rho_q\Big)\Bigg]\Bigg\}.\end{aligned} \tag{18}$$

Let us again investigate the convergence of the semiclassical expansion associated this time with the vector field $\vec{J}_q[\rho]$ and compare it with the corresponding HF density. We show in fig. 3 the contributions to $\vec{J}_q[\rho]$ from 2nd and from 4th order as well as $\vec{J}_{\mathrm{HF}}$.

We would like to check now that the semiclassical functionals which we have written down up to order $\hbar^4$ are indeed correct. We perform this test numerically in the following way.

One notices that when calculating the total energy through eq. (12) the kinetic energy density τ_q does not appear by itself, but only in connection with the form factor f_q. The τ-dependent part of the total energy is simply obtained through the integral $\int d^3r \sum_q f_q \tau_q$. In the contribution at order $\hbar^4$ to this integral one can then perform integrations by parts to obtain an expression which contains only second-order derivatives of the density ρ_q and the effective-mass form factor f_q [6]:

$$\begin{aligned}\int f_q\,\tau_q^{(4)}\,d^3r = &(3\pi^2)^{-2/3}\int d^3r\,\rho_q^{1/3}\Bigg\{\frac{1}{270}f_q\left(\frac{\Delta\rho_q}{\rho_q}\right)^2\\ &-\frac{1}{240}f_q\,\frac{\Delta\rho_q}{\rho_q}\left(\frac{\vec\nabla\rho_q}{\rho_q}\right)^2+\frac{1}{810}f_q\left(\frac{\vec\nabla\rho_q}{\rho_q}\right)^2-\frac{1}{240}\frac{(\Delta f_q)^2}{f_q}\\ &+\frac{1}{120}\frac{\Delta f_q\,(\vec\nabla f_q)^2}{f_q^2}-\frac{1}{240}\frac{(\vec\nabla f_q)^4}{f_q^3}+\frac{1}{360}\Delta f_q\,\frac{(\vec\nabla f_q\cdot\vec\nabla\rho_q)}{f_q\rho_q}\\ &-\frac{1}{360}\Delta\rho_q\,\frac{(\vec\nabla f_q)^2}{f_q\,\rho_q}-\frac{7}{2160}\Delta f_q\left(\frac{\vec\nabla\rho_q}{\rho_q}\right)^2\\ &+\frac{1}{540}\left(\frac{\vec\nabla\rho_q}{\rho_q}\right)^2\frac{(\vec\nabla f_q)^2}{f_q}+\frac{7}{2160}\frac{(\vec\nabla f_q\cdot\vec\nabla\rho_q)}{f_q\,\rho_q^2}\\ &-\frac{11}{3240}\left(\frac{\vec\nabla\rho_q}{\rho_q}\right)^2\frac{(\vec\nabla f_q\cdot\vec\nabla\rho_q)}{\rho_q}\\ &+\frac{7}{1080}\,\Delta\rho_q\,\frac{(\vec\nabla f_q\cdot\vec\nabla\rho_q)}{\rho_q^2}+\frac{1}{180}\,\Delta f_q\,\frac{\Delta\rho_q}{\rho_q}\Bigg\},\end{aligned} \quad (19)$$

where $\tau_q^{(4)}$ is the spin-independent part of the kinetic energy density.

The dependence of the total energy density on the spin degrees of freedom enters in two different ways: through the spin-orbit part of the kinetic energy density τ_q^{so} and through a term $\vec J_q\cdot\vec W_q$. This total spin dependence is then given by $\sum_q\int\left(\frac{\hbar^2}{2m}f_q\tau_q^{\mathrm{so}}[\rho]+\vec W_q\cdot\vec J_q[\rho]\right)d^3r$. It can be shown after some integration by parts with eqs. (14), (16), (17) and (18) that in the different orders of the semiclassical expansion this integral takes on the simple form [6]

$$\begin{aligned}\int\left[\frac{\hbar^2}{2m}f_q\,\tau_q^{(2)\mathrm{so}}[\rho]+\vec W_q\cdot\vec J_q^{(2)}[\rho]\right]d^3r =\\ -\frac{m}{\hbar^2}\sum_q\int\frac{\rho_q}{f_q}\,\vec W_q^2 d^3r\end{aligned} \quad (20)$$

and that

$$\begin{aligned}&\int\left[\frac{\hbar^2}{2m}f_q\tau_q^{(4)\mathrm{so}}[\rho]+\vec W_q\cdot\vec J_q^{(4)}[\rho]\right]d^3r =\\ &(3\pi^2)^{-2/3}\,\frac{m}{\hbar^2}\int\frac{\rho_q^{1/3}}{f_q}\Bigg\{\frac14(\mathrm{div}\,\vec W_q)^2-\frac38\,\mathrm{div}\,\vec W_q\,\frac{(\vec\nabla f_q\cdot\vec W_q)}{f_q}\\ &+\frac{1}{16}\vec W_q^2\,\frac{\Delta f_q}{f_q}+\frac18\frac{(\vec\nabla f_q\cdot\vec W_q)^2}{f_q^2}+\frac{1}{24}\,\mathrm{div}\,\vec W_q\,\frac{(\vec\nabla\rho_q\cdot\vec W_q)}{\rho_q}\\ &+\frac{1}{48}\,\vec W_q^2\,\frac{\Delta\rho_q}{\rho_q}-\frac{1}{72}\,\vec W_q^2\left(\frac{\vec\nabla\rho_q}{\rho_q}\right)^2+\frac12\left(\frac{m}{\hbar^2}\right)^2\frac{\vec W_q^4}{f_q^2}\Bigg\}d^3r\,.\end{aligned} \quad (21)$$

We have tested the semiclassical functionals given above by verifying numerically that these integral relations (19), (20) and (21) hold true.

We have also evaluated different integrals involving these functionals and which have been calculated in ref. [15]. We obtain agreement with their results of the order of 1 to 2%, which is of the same order as their agreement between the results of a full variational calculation and one in the restricted subspace of modified Fermi functions.

As can be seen in eq. (8) only the divergence of the vector field $\vec J$ is present in the expression of the central one-body potential. One obtains from eqs. (17) and (18), respectively, the contributions to 2nd order

$$\mathrm{div}\vec J_q^{(2)} = -\frac{2m}{\hbar^2}\frac{1}{f_q}\left[\rho_q\mathrm{div}\vec W_q+(\vec\nabla\rho_q\cdot\vec W_q)-\frac{\rho_q}{f_q}(\vec\nabla f_q\cdot\vec W_q)\right] \quad (22)$$

and, after some lengthy but straightforward calculation, to 4th order

$$\begin{aligned}\mathrm{div}\vec J_q^{(4)} = &(3\pi^2)^{-2/3}\,\frac{2m}{\hbar^2}\,\frac{\rho_q^{1/3}}{8f_q}\Bigg\{-2\mathrm{div}\Big[\vec\nabla(\mathrm{div}\vec W_q)\Big]\\ &+\frac{1}{2f_q}\Big[2\Delta f_q\mathrm{div}\vec W_q+(\vec\nabla^3 f_q\cdot\vec W_q)+3\Delta(\vec\nabla f_q\cdot\vec W_q)\\ &+(\vec\nabla f_q\cdot\Delta\vec W_q)+4\vec\nabla f_q\cdot\vec\nabla(\mathrm{div}\vec W_q)\Big]-\frac{1}{f_q^2}\Bigg[(\vec\nabla f_q)^2\mathrm{div}\vec W_q\\ &+3\Delta f_q(\vec\nabla f_q\cdot\vec W_q)+5\vec\nabla f_q\cdot(\vec W_q\cdot\vec\nabla)\vec\nabla f_q\\ &+5\vec\nabla f_q\cdot(\vec\nabla f_q\cdot\vec\nabla)\vec W_q)+2\vec\nabla f_q\cdot(\vec\nabla f_q\times\mathrm{rot}\vec W_q)\\ &-2\left(\frac{2m}{\hbar^2}\right)^2\Big(\vec W_q^2\mathrm{div}\vec W_q+\vec W_q\cdot\vec\nabla(\vec W_q^2)\Big)\Bigg]\\ &+\frac{6}{f_q^3}\left[(\vec\nabla f_q)^2(\vec\nabla f_q\cdot\vec W_q)-\left(\frac{2m}{\hbar^2}\right)^2\vec W_q^2(\vec\nabla f_q\cdot\vec W_q)\right]\\ &-\frac{1}{6\rho_q}\Big[\Delta(\vec\nabla\rho_q\cdot\vec W_q)+(\vec\nabla\rho_q\cdot\Delta\vec W_q)-(\vec\nabla^3\rho_q\cdot\vec W_q)\\ &+2\Delta\rho_q\,\mathrm{div}\vec W_q+6\vec\nabla\rho_q\cdot\vec\nabla(\mathrm{div}\vec W_q)\Big]\\ &+\frac{1}{3f_q\rho_q}\Big[2(\vec\nabla f_q\cdot\vec\nabla\rho_q)\mathrm{div}\vec W_q+\vec W_q\cdot\vec\nabla(\vec\nabla f_q\cdot\vec\nabla\rho_q)\\ &+\Delta\rho_q(\vec\nabla f_q\cdot\vec W_q)+2\vec\nabla\rho_q\cdot\vec\nabla(\vec\nabla f_q\cdot\vec W_q)+\Delta f_q(\vec\nabla\rho_q\cdot\vec W_q)\\ &+\vec\nabla\rho_q\cdot(\vec\nabla f_q\times\mathrm{rot}\vec W_q)+2\vec\nabla\rho_q\cdot(\vec\nabla f_q\cdot\vec\nabla)\vec W_q)\Big]\\ &-\frac{1}{3f_q^2\rho_q}\Bigg[5(\vec\nabla f_q\cdot\vec\nabla\rho_q)(\vec\nabla f_q\cdot\vec W_q)+(\vec\nabla f_q)^2(\vec\nabla\rho_q\cdot\vec W_q)\\ &-2\left(\frac{2m}{\hbar^2}\right)^2\vec W_q^2(\vec\nabla\rho_q\cdot\vec W_q)\Bigg]+\frac{2}{9\rho_q^2}\Big[\vec\nabla\rho_q\cdot(\vec\nabla\rho_q\cdot\vec\nabla)\vec W_q)\\ &+(\vec\nabla\rho_q)^2\mathrm{div}\vec W_q\Big]-\frac{2}{9f_q\rho_q^2}\Big[(\vec\nabla f_q\cdot\vec\nabla\rho_q)(\vec\nabla\rho_q\cdot\vec W_q)\\ &+(\vec\nabla\rho_q)^2(\vec\nabla f_q\cdot\vec W_q)\Big]\Bigg\}\;.\end{aligned} \quad (23)$$

4 Average nuclear potentials

One now controls all the ingredients which enter into the calculation of the nuclear central potentials, eq. (8), for effective interactions of the Skyrme type. It is now interesting to look at the *convergence* of the expressions which define these average fields calculated with the semiclassical functionals $\tau_q[\rho]$ and $\vec{J}_q[\rho]$ and to check how these potentials compare with the ones obtained in the HF approach.

We, therefore, show in fig. 4 the neutron and proton nuclear central potentials for the nucleus ^{208}Pb obtained for the Skyrme interaction SkM*. The Coulomb potential $V_{\rm Coul}$ for the proton field has been left out in this investigation, because it is directly given through the proton density (see eq. (11)). As the latter is very well reproduced, except for quantum oscillations in the nuclear interior, we already know that the Coulomb potential calculated through this semiclassical density will, indeed, reproduce on the average the exact one calculated from the quantum-mechanical densities.

We show a comparison between the HF neutron and proton central potentials with the ones obtained using the self-consistent semiclassical densities ρ_n and ρ_p but restricting ourselves to the TF approximations for the functional $\tau[\rho]$, eq. (2), and $\vec{J}[\rho]$ (which is zero as explained above). We do not want to call this the Thomas-Fermi approximation to the nuclear central fields since even if we have used the above-mentioned functionals in their Thomas-Fermi approximation, the nuclear structure has been determined through a full variational calculation including the functionals up to order $\hbar^4$.

As seen in fig. 4 the reproduction of the HF self-consistent fields is already quite remarkable at the lowest (TF) order in the semiclassical expansion. Apart from shell oscillations in the nuclear interior and a small wiggle in the TF potential in the surface region the agreement seems very satisfactory.

It is now interesting to study the contributions to the nuclear central fields coming from higher orders in the semiclassical expansion. For this reason we show in fig. 5 the corrections $\delta V_n^{(2)}$ and $\delta V_n^{(4)}$ defined as (see eq. (8))

$$\begin{aligned}\delta V_n^{(2)} &= (B_3+B_4)\tau_n^{(2)} + B_3\tau_p^{(2)} \\ &\quad + B_9(2\,\mathrm{div}\vec{J}_n^{(2)} + \mathrm{div}\vec{J}_p^{(2)})\,, \\ \delta V_n^{(4)} &= (B_3+B_4)\tau_n^{(4)} + B_3\tau_p^{(4)} \\ &\quad + B_9(2\,\mathrm{div}\vec{J}_n^{(4)} + \mathrm{div}\vec{J}_p^{(4)})\ , \end{aligned} \tag{24}$$

together with the semiclassical TF potential already shown in fig. 4. It turns out that these corrections are rather small and we have to multiply $\delta V_n^{(2)}$ by a factor of 10 and $\delta V_n^{(4)}$ by a factor of 100 to make their relative importance better visible in fig. 5.

It can be seen that both these terms give a contribution in the nuclear surface where the lowest-order term showed some deviation from the HF potentials. It is therefore to be expected that potential using the second-order functionals

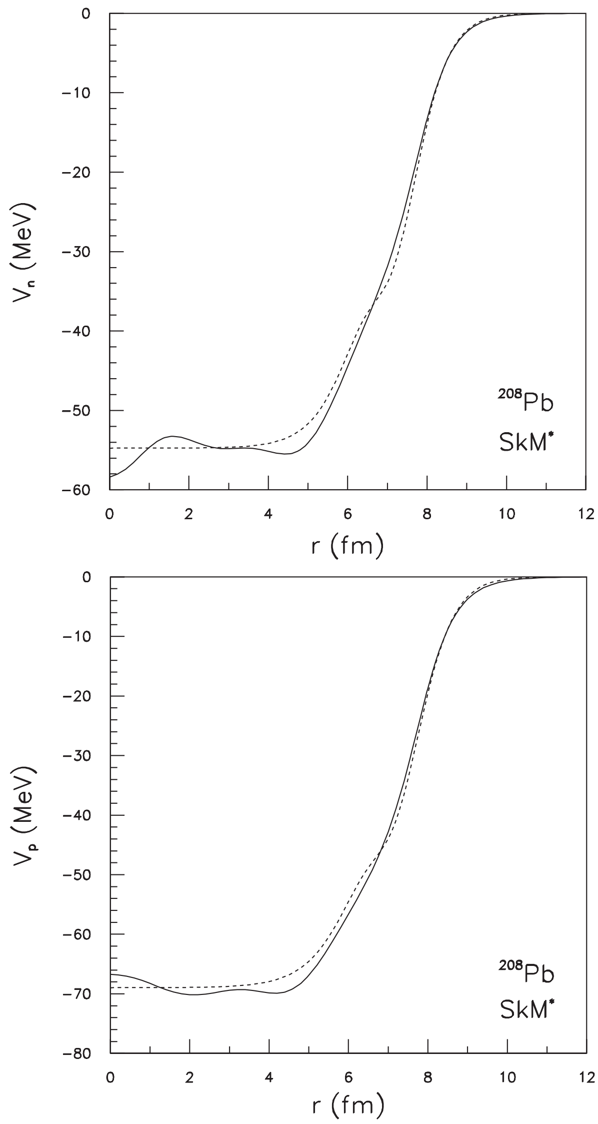

Fig. 4. Comparison of the Hartree-Fock central nuclear potentials (solid line) for protons and neutrons with the corresponding semiclassical potentials (dashed line) obtained using the Thomas-Fermi approximation for the functionals $\tau[\rho]$ and $\vec{J}[\rho]$.

$\tau^{(2)}[\rho]$ and $\vec{J}^{(2)}[\rho]$ will partially correct for this deficiency and be quite close to the self-consistent HF potentials. Due to the smallness of the 4th-order term in fig. 5 we can expect the semiclassical potentials obtained using the full semiclassical functionals up to 4th order to be practically indistinguishable from the ones using the 2nd-order corrections only. This conclusion is, indeed, confirmed in fig. 6.

The same kind of calculations have been performed also for lighter nuclei down to ^{40}Ca. The quality of the agreement between HF and semiclassical potentials is the same as the one obtained for the nucleus ^{208}Pb studied above. As already mentioned, the effective-mass form factor $f_q(\vec{r})$, eq. (9) and the spin-orbit potential $\vec{W}_q(\vec{r})$, eq. (10) are, except for shell oscillations in the nuclear interior, very well reproduced, since the nuclear densities

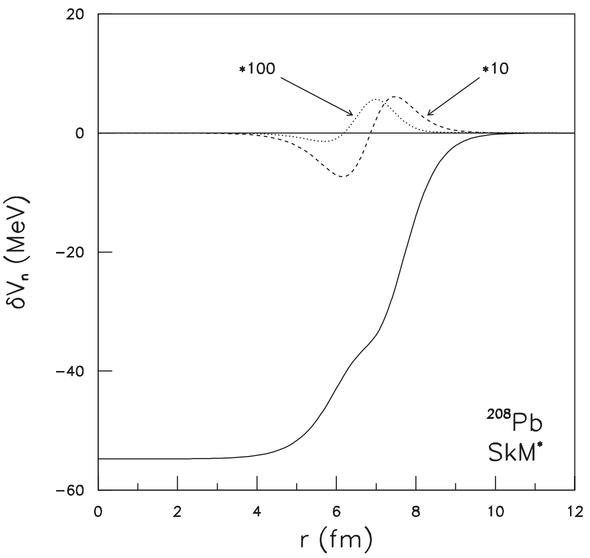

Fig. 5. Semiclassical neutron potential using the TF approximation (solid line) of the semiclassical functionals $\tau[\rho]$, and $\vec{J}[\rho]$ and corrections coming from second (dashed line) and fourth order (dotted line) in the semiclassical expansion. For better visibility the second-order correction has been multiplied by a factor of 10 and the fourth order by a factor of 100.

which directly determine these quantities are well reproduced. For this reason we do not explicitly show these quantities. These conclusions remain valid when other effective interactions of the Skyrme type are used.

5 Summary and conclusions

We have demonstrated that using the Extended Thomas-Fermi approach one is not only able to give a very precise description of average nuclear properties but that this method is also able to reproduce quite nicely local quantities, not only neutron and proton density distributions but also the corresponding nuclear central potentials, effective-mass form factors and spin-orbit potentials. These are precisely the ingredients of the Schrödinger-like Hartree-Fock equation, eq. (7), which arises from the variational principle. Within this semiclassical approach which relies on a density variational calculation one should therefore be able to solve in an approximate way the quantum-mechanical problem without having to go through the full self-consistency problem of the HF approach. This is the essential idea of an approximate solution of the HF problem known as the "expectation value method" (EVM) [28]. It consists in constructing the ground-state Slater determinant from the eigenfunctions of eq. (7) using the ETF fields $V_q(\vec{r})$, $m_q^*(\vec{r})$ and $\vec{W}_q(\vec{r})$ (to second order in the ETF expansions) and calculating with this Slater determinant the expectation value of the total Skyrme Hamiltonian. The rapid convergence of the ETF functionals demonstrated above explains, *a posteriori*, the success of this approach.

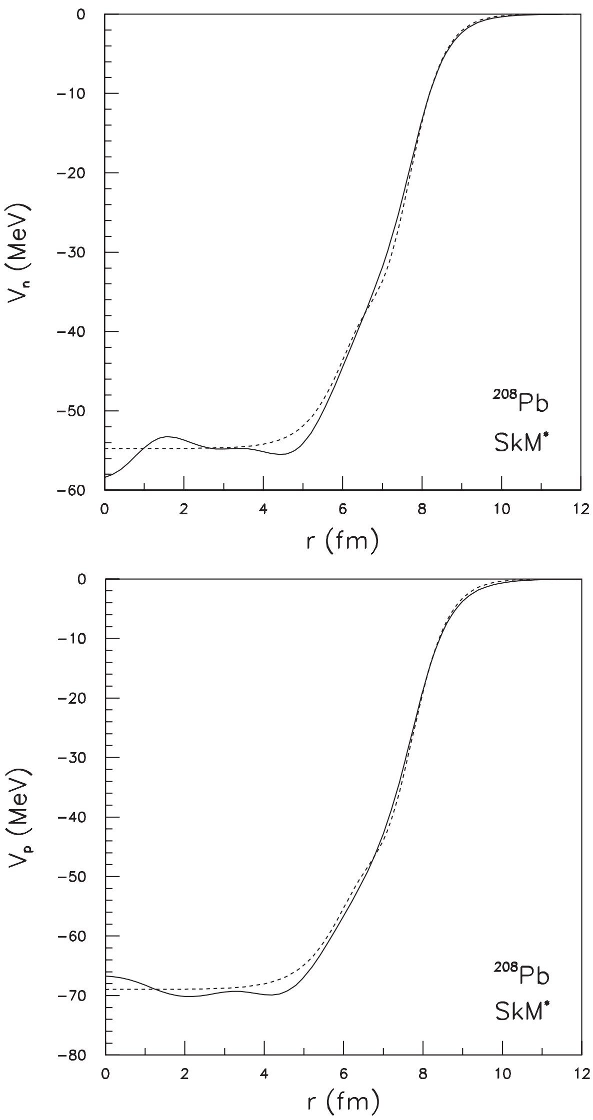

Fig. 6. Comparison of the Hartree-Fock central nuclear potentials (solid line) for protons and neutrons with the semiclassical potentials (dashed line) obtained by using the semiclassical functionals $\tau[\rho]$ and $\vec{J}[\rho]$ up to order $\hbar^2$ (dashed line). The semiclassical potentials including the functionals up to order $\hbar^4$ are indistinguishable from the latter ones.

The interested reader might object that nowadays, where computational power has been increased tremendously, there is no real need for semiclassical approximations, but all calculations of nuclear structure should be directly performed at the level of the Hartree-Fock model (or beyond). The point, however, is that as soon as one is interested in nuclear systematics where one is looking at the behavior of nuclei over a wide range of the nuclear chart, semiclassical approximations are without any credible substitute.

A point that might, *e.g.*, be interesting to study is the variation of the diffuseness of the nuclear densities and central potentials when increasing the nuclear excitation and/or when going to rotating nuclei. The approach we have developed here is, indeed, easily generalized to the description of excited or rotating nuclei. If one is interested in *hot* nuclear systems one simply need to replace the semiclassical functionals for $\tau[\rho]$ and $\vec{J}[\rho]$ which we have developed by those derived in ref. [14] for the ETF approach at finite temperature. In this case the coefficients in the semiclassical expansions, eqs. (2), (14), (15), (16) etc. are to be replaced by a combination of Fermi integrals [14].

If, on the other hand, one is interested in the description of systems breaking time-reversal symmetry, the energy density, eq. (5), will be changed [11,12] and some additional densities will appear, such as the current density $\vec{j}(\vec{r})$ or the spin-vector density $\vec{\rho}(\vec{r})$ which, in the case of rotations, are a manifestation of the time-odd part of the density matrix generated by the cranking piece of the Hamiltonian. This causes not only a change in the analytical form of quantities such as the average potentials $V_q(\vec{r})$ which are now going to depend on these additional densities but also leads to the appearance of additional terms in the functionals $\tau[\rho]$ and $\vec{J}[\rho]$. These functionals have already been determined in [12] which makes it quite straightforward to calculate self-consistent semiclassical fields such as $V_q(\vec{r})$ for rotating nuclei very similarly to what we have done here in the static case and investigate the dependence of these quantities with increasing angular momentum. Investigations along these lines are currently in progress.

The present method can also be profitably exploited to establish some easy to use parametrization (as a function of mass number A and isospin parameter $I = (N-Z)/A$) of central and spin-orbit potential and effective mass and this over a wide region of the nuclear chart [29]. Such an investigation could be the ideal starting point for Strutinski shell correction calculations as, *e.g.*, formulated in the so-called Extended Thomas-Fermi plus Strutinski integral (ETFSI) method (see ref. [30] and references given therein) where average mean fields like the ones investigated here are used to determine shell corrections.

The authors are grateful to K. Pomorski for having suggested the investigation undertaken here and for his constant interest in this work. The authors have also benefitted from fruitful discussions with P. Quentin. One of us (KB) gratefully acknowledges the hospitality extended to him during his stay at the Institut de Recherches Subatomiques of Strasbourg. This work is supported in part by the French-Algerian CNRS/DEF scientific research agreement under Contract No. PNC 10090.

Appendix A.

As mentioned in the text we gather here the expressions the ETF functionals take in the case of spherical symmetry.

For the 4th-order spin-independent part of the kinetic energy density, eq. (15), one obtains (primes denoting derivatives with respect to the radial variable r):

$$\begin{aligned}
\tau_q^{(4)}[\rho] = {} & (3\pi^2)^{-2/3}\frac{\rho_q^{1/3}}{4320}\Bigg\{\frac{24}{\rho_q}\left[\rho_q^{(4)} + \frac{4}{r}\rho_q'''\right] \\
& -\frac{8}{\rho_q^2}\left[11\rho_q'''\rho_q' + 7(\rho_q'')^2 + \frac{36}{r}\rho_q''\rho_q' - \frac{1}{r^2}(\rho_q')^2\right] \\
& +\frac{8}{3\,\rho_q^3}\left[81\rho_q''(\rho_q')^2 + \frac{70}{r}(\rho_q')^3\right] - \frac{96}{\rho_q^4}(\rho_q')^4 \\
& -\frac{36}{f_q}\left[f_q^{(4)} + \frac{4}{r}f_q'''\right] + \frac{18}{f_q^2}\left[4f_q'''f_q' + 3(f_q'')^2 + \frac{4}{r}f_q''f_q'\right. \\
& \left.-\frac{4}{r^2}(f_q')^2\right] - \frac{144}{f_q^3}f_q''(f_q')^2 + \frac{54}{f_q^4}(f_q')^4 + \frac{12}{f_q\,\rho_q} \\
& \times\left[3f_q'\rho_q''' + 2f_q''\rho_q'' - 2f_q'''\rho_q' + \frac{6}{r}f_q'\rho_q'' - \frac{4}{r}f_q''\rho_q' + \frac{2}{r^2}f_q'\rho_q'\right] \\
& +\frac{12}{f_q^2\,\rho_q}\left[f_q'f_q''\rho_q' - 2(f_q')^2\rho_q'' - \frac{2}{r}(f_q')^2\rho_q'\right] \\
& -\frac{4}{f_q\,\rho_q^2}\left[11f_q''(\rho_q')^2 + 32f_q'\rho_q'\rho_q'' + \frac{26}{r}f_q'(\rho_q')^2\right] \\
& +\frac{30}{f_q^2\,\rho_q^2}(f_q')^2(\rho_q')^2 + \frac{260}{3\,f_q\,\rho_q^3}f_q'(\rho_q')^3\Bigg\}. \qquad \text{(A.1)}
\end{aligned}$$

When giving the spin-dependent part of $\tau_q^{(4)}[\rho]$ we take advantage of the fact that the spin-orbit potential $\vec{W}_q$ has for Skyrme forces the simple form of eq. (10) which allows us to introduce the quantity

$$A_q = \rho + \rho_q \qquad \Longrightarrow \qquad \vec{W}_q = -B_9\vec{\nabla}A_q\,. \qquad \text{(A.2)}$$

Using the vector identity

$$\mathrm{rot}(\mathrm{rot}\,\vec{a}) = \vec{\nabla}(\mathrm{div}\,\vec{a}) - \Delta\,\vec{a}\,,$$

one shows that because of the form of the spin-orbit potential, eq. (10), one simply has

$$\vec{W}\cdot\Delta\vec{W} = \vec{W}\cdot\vec{\nabla}(\mathrm{div}\vec{W})\,,$$

which then allows us to write the spin-dependent part of $\tau_q^{(4)\mathrm{so}}$ in the form of the local densities ρ_n and ρ_p and of their derivatives:

$$\tau_q^{(4)\mathrm{so}}[\rho]=(3\pi^2)^{-2/3}\left(\frac{mW_0}{\hbar^2}\right)^2\frac{\rho_q^{1/3}}{4f_q^2}\Bigg\{\Bigg[\frac{3}{4}\vec\nabla A_q\cdot\vec\nabla^3 A_q +\frac{1}{8}\Delta(\vec\nabla A_q)^2+\frac{1}{4}(\Delta A_q)^2\Bigg]-\frac{1}{2f_q}\Bigg[\Delta A_q(\vec\nabla f_q\cdot\vec\nabla A_q) +2\vec\nabla A_q\cdot(\vec\nabla f_q\cdot\vec\nabla)\vec\nabla A_q+\vec\nabla f_q\cdot(\vec\nabla A_q\cdot\vec\nabla)\vec\nabla A_q +\Delta f_q(\vec\nabla A_q)^2+\vec\nabla A_q\cdot\vec\nabla(\vec\nabla A_q\cdot\vec\nabla f_q)-\frac{1}{2}\vec\nabla f_q\cdot\vec\nabla(\vec\nabla A_q)^2\Bigg] +\frac{3}{4f_q^2}\Bigg[(\vec\nabla f_q)^2(\vec\nabla A_q)^2+(\vec\nabla f_q\cdot\vec\nabla A_q)^2-\left(\frac{mW_0}{\hbar^2}\right)^2(\vec\nabla A_q)^4\Bigg] +\frac{1}{6\rho_q}\Big[\vec\nabla A_q\cdot(\vec\nabla\rho_q\cdot\vec\nabla)\vec\nabla A_q+\Delta A_q(\vec\nabla\rho_q\cdot\vec\nabla A_q)\Big] -\frac{1}{6f_q\rho_q}\Big[(\vec\nabla f_q\cdot\vec\nabla\rho_q)(\vec\nabla A_q)^2+(\vec\nabla f_q\cdot\vec\nabla A_q)(\vec\nabla\rho_q\cdot\vec\nabla A_q)\Big]\Bigg\}, \tag{A.3}$$

which for spherical symmetry reads

$$\tau_q^{(4)\mathrm{so}}[\rho]=(3\pi^2)^{-2/3}\left(\frac{mW_0}{\hbar^2}\right)^2\frac{\rho_q^{1/3}}{4f_q^2}\Bigg\{\frac{1}{2}\Bigg[2A_q'A_q'''+(A_q'')^2 +\frac{6}{r}A_q'A_q''-\frac{1}{r^2}(A_q')^2\Bigg]-\frac{A_q'}{f_q}\Bigg[f_q''A_q'+2f_q'A_q''+\frac{2}{r}f_q'A_q'\Bigg] +\frac{3(A_q')^2}{4f_q^2}\Bigg[2(f_q')^2-\left(\frac{mW_0}{\hbar^2}\right)^2(A_q')^2\Bigg] +\frac{\rho_q'A_q'}{3f_q\rho_q}\Bigg[f_q(A_q''+\frac{1}{r}A_q')-f_q'A_q'\Bigg]\Bigg\}\ . \tag{A.4}$$

The 4th-order spin-orbit density $\vec J_q^{(4)}[\rho]$, eq. (18) written in terms of the function A_q defined above is given by

$$\vec J_q^{(4)}[\rho]=(3\pi^2)^{-2/3}\,\frac{mW_0}{\hbar^2}\,\frac{\rho_q^{1/3}}{8f_q}\Bigg\{-2\vec\nabla^3A_q +\frac{1}{f_q}\Big[\Delta f_q\,\vec\nabla A_q+(\vec\nabla A_q\cdot\vec\nabla)\vec\nabla f_q+2(\vec\nabla f_q\cdot\vec\nabla)\vec\nabla A_q\Big] -\frac{1}{f_q^2}\Bigg[(\vec\nabla f_q)^2\vec\nabla A_q+(\vec\nabla f_q\cdot\vec\nabla A_q)\vec\nabla f_q-2\left(\frac{mW_0}{\hbar^2}\right)^2 \times(\vec\nabla A_q)^3\Bigg]-\frac{1}{3\rho_q}\Big[(\vec\nabla\rho_q\cdot\vec\nabla)\vec\nabla A_q+\Delta A_q\vec\nabla\rho_q\Big] +\frac{1}{3f_q\rho_q}\Big[(\vec\nabla f_q\cdot\vec\nabla\rho_q)\vec\nabla A_q+(\vec\nabla f_q\cdot\vec\nabla A_q)\vec\nabla\rho_q\Big]\Bigg\}, \tag{A.5}$$

which in the case of a spherically symmetric system takes the form

$$\vec J_q^{(4)}[\rho]=(3\pi^2)^{-2/3}\,\frac{mW_0}{\hbar^2}\,\frac{\rho_q^{1/3}}{4f_q}\Bigg\{-\Bigg[A_q'''+\frac{2}{r}A_q''-\frac{2}{r^2}A_q'\Bigg] +\frac{1}{f_q}\Bigg[f_q''A_q'+f_q'A_q''+\frac{1}{r}f_q'A_q'\Bigg] -\frac{A_q'}{f_q^2}\Bigg[(f_q')^2-\left(\frac{mW_0}{\hbar^2}\right)^2(A_q')^2\Bigg] -\frac{\rho_q'}{3f_q\rho_q}\Bigg[f_q\left(A_q''+\frac{1}{r}A_q'\right)-f_q'A_q'\Bigg]\Bigg\}\vec u_r \tag{A.6}$$

with the unit vector in radial direction $\vec u_r$.

The corresponding expressions for $\mathrm{div}\vec J_q^{(4)}[\rho]$ are the following:

$$\mathrm{div}\vec J_q^{(4)}[\rho]=(3\pi^2)^{-2/3}\,\frac{mW_0}{\hbar^2}\,\frac{\rho_q^{1/3}}{8f_q}\Bigg\{-2\Delta^2A_q +\frac{1}{2f_q}\Big[2\,\Delta f_q\,\Delta A_q+\vec\nabla^3 f_q\cdot\vec\nabla A_q+3\Delta(\vec\nabla f_q\cdot\vec\nabla A_q) +5\vec\nabla f_q\cdot\vec\nabla^3A_q\Big]-\frac{1}{f_q^2}\Bigg[(\vec\nabla f_q)^2\Delta A_q+3\Delta f_q(\vec\nabla f_q\cdot\vec\nabla A_q) +5\vec\nabla f_q\cdot(\vec\nabla A_q\cdot\vec\nabla)\vec\nabla f_q+5\vec\nabla f_q\cdot(\vec\nabla f_q\cdot\vec\nabla)\vec\nabla A_q) -2\left(\frac{mW_0}{\hbar^2}\right)^2\Big(\Delta A_q(\vec\nabla A_q)^2+\vec\nabla A_q\cdot\vec\nabla(\vec\nabla A_q)^2\Big)\Bigg] +\frac{6}{f_q^3}\Bigg[(\vec\nabla f_q)^2(\vec\nabla f_q\cdot\vec\nabla A_q)-\left(\frac{mW_0}{\hbar^2}\right)^2(\vec\nabla A_q)^2(\vec\nabla f_q\cdot\vec\nabla A_q)\Bigg] -\frac{1}{6\rho_q}\Big[\Delta(\vec\nabla\rho_q\cdot\vec\nabla A_q)+7\vec\nabla\rho_q\cdot\vec\nabla^3A_q-\vec\nabla^3\rho_q\cdot\vec\nabla A_q +2\Delta\rho_q\,\Delta A_q\Big]+\frac{1}{3f_q\rho_q}\Big[2(\vec\nabla f_q\cdot\vec\nabla\rho_q)\Delta A_q +\vec\nabla A_q\cdot\vec\nabla(\vec\nabla f_q\cdot\vec\nabla\rho_q)+\Delta\rho_q(\vec\nabla f_q\cdot\vec\nabla A_q)+ +2\vec\nabla\rho_q\cdot\vec\nabla(\vec\nabla f_q\cdot\vec\nabla A_q)+\Delta f_q(\vec\nabla\rho_q\cdot\vec\nabla A_q) +2\vec\nabla\rho_q\cdot(\vec\nabla f_q\cdot\vec\nabla)\vec\nabla A_q\Big]-\frac{1}{3f_q^2\rho_q}\Bigg[5(\vec\nabla f_q\cdot\vec\nabla\rho_q)(\vec\nabla f_q\cdot\vec\nabla A_q) +(\vec\nabla f_q)^2(\vec\nabla\rho_q\cdot\vec\nabla A_q)-2\left(\frac{mW_0}{\hbar^2}\right)^2(\vec\nabla A_q)^2(\vec\nabla\rho_q\cdot\vec\nabla A_q)\Bigg] +\frac{2}{9\rho_q^2}\Big[\vec\nabla\rho_q\cdot(\vec\nabla\rho_q\cdot\vec\nabla)\vec\nabla A_q+(\vec\nabla\rho_q)^2\Delta A_q\Big] -\frac{2}{9f_q\rho_q^2}\Big[(\vec\nabla f_q\cdot\vec\nabla\rho_q)(\vec\nabla\rho_q\cdot\vec\nabla A_q)+(\vec\nabla\rho_q)^2(\vec\nabla f_q\cdot\vec\nabla A_q)\Big]\Bigg\}. \tag{A.7}$$

and in the case of spherical symmetry

$$
\begin{aligned}
\mathrm{div}\vec{J}_q^{(4)}[\rho] &= (3\pi^2)^{-2/3}\,\frac{mW_0}{\hbar^2}\,\frac{\rho_q^{1/3}}{4f_q} \\
&\times\Bigg\{-\Big(A_q^{(4)}+\frac{4}{r}A_q'''\Big)+\frac{1}{f_q}\Bigg[f_q'''A_q'+2f_q''A_q''+2f_q'A_q''' \\
&+\frac{5}{r}f_q'A_q''+\frac{3}{r}f_q''A_q'-\frac{1}{r}f_q'A_q'\Bigg]-\frac{1}{f_q^2}\Bigg[3(f_q')^2A_q'' \\
&+4f_q'f_q''A_q'+\frac{4}{r}(f_q')^2A_q'-\left(\frac{mW_0}{\hbar^2}\right)^2(A_q')^2\Big(3A_q''+\frac{2}{r}A_q'\Big)\Bigg] \\
&+\frac{3}{f_q^3}f_q'A_q'\Bigg[(f_q')^2-\left(\frac{mW_0}{\hbar^2}\right)^2(A_q')^2\Bigg] \\
&-\frac{1}{3\rho_q}\Bigg[2\rho_q'A_q'''+\rho_q''A_q''+\frac{1}{r}\rho_q''A_q'+\frac{5}{r}\rho_q'A_q''+\frac{1}{r^2}\rho_q'A_q'\Bigg] \\
&+\frac{1}{3f_q\rho_q}\Bigg[3f_q'\rho_q'A_q''+f_q'\rho_q''A_q'+2f_q''\rho_q'A_q'+\frac{4}{r}f_q'\rho_q'A_q'\Bigg] \\
&-\frac{1}{3f_q^2\rho_q}\rho_q'A_q'\Bigg[3(f_q')^2-\left(\frac{mW_0}{\hbar^2}\right)^2(A_q')^2\Bigg] \\
&+\frac{2}{9\rho_q^2}(\rho_q')^2\left(A_q''+\frac{1}{r}A_q'\right)-\frac{2}{9f_q\rho_q^2}f_q'(\rho_q')^2A_q'\Bigg\} \qquad \text{(A.8)}
\end{aligned}
$$

which can also be obtained directly from eq. (A.6), remembering that the divergence of a vector field $\vec{a}$ that has only a radial component a_r is given by

$$\mathrm{div}\,\vec{a} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 a_r)\ .$$

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