Extended Thomas-Fermi density functionals in the presence of a tensor interaction in spherical symmetry

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For a one-body Hamiltonian obtained from the energy-density functional associated with a Skyrme effective interaction, including a tensor force, semiclassical functional densities are derived in the framework of the Extended Thomas-Fermi method, in spherical symmetry, for the kinetic energy and spin-orbit density. The structure of the self-consistent mean-field potentials constructed with such semiclassical functionals is studied. The impact of the tensor force in particular on the spin-orbit form factor clearly indicates the necessity of including such tensor-force terms in the theoretical description of atomic nuclei and their possible influence on the shell structure of exotic nuclei.

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I. INTRODUCTION

In the recent experimental effort of synthesizing nuclei far from the β stability line, the possibility of a different shell closure and thus the appearance of new magic numbers have been widely discussed [1–3]. Experiments on properties of low-lying collective states of neutron-rich even-even titanium nuclei [4,5] seem to indicate, in addition to the standard $N = 28$ shell closure, the existence of a closed $N = 32$ subshell. Such an additional shell structure can be generated if the neutron single-particle $f_{5/2}$ state is shifted upward, thus leaving a gap between spin-orbit partners $p_{3/2}$ and $p_{1/2}$. Another prominent candidate for a modified shell structure is the relative shift of the $1g_{7/2}$ and $1h_{11/2}$ proton levels in tin isotopes, an effect that is interpreted [6] by a reduction, with increasing neutron numbers, of the spin-orbit splitting of both single-particle levels with their respective spin-orbit partners. From the theoretical point of view the spin-orbit splitting in nuclei has its origin in the two-body spin-orbit and tensor interactions [7–9], which contribute differently to spin-saturated and spin-unsaturated nuclei. Whereas the genuine spin-orbit interaction is, indeed, weakly dependent on the nuclear shell structure, the spin-orbit splitting induced by the tensor force leads to a strong dependence on the filling of neutron and proton single-particle states. Even though the tensor terms in the interaction were long known, this part of the nucleon-nucleon force has generally been neglected in mean-field-type calculations [10–13].[1] Very recently the important role of the so-far neglected tensor terms for spin nonsaturated systems, as they are encountered for neutron-deficient or neutron-rich light nuclei, was largely discussed in the framework of schematic calculations in Refs. [17–19]. The inclusion of such tensor terms in the two-body effective nucleon-nucleon interaction has been worked out in the framework of the Skyrme Hartree-Fock approximation in Ref. [20] when limited to spherically symmetric systems, and, more generally, for time-reversal symmetric even-even systems in Ref. [21]. It is now interesting to develop the semiclassical counterpart of such an approach in the framework of the so-called Extended Thomas-Fermi (ETF) approximation [22,23]. It has, in fact, been shown in Ref. [24] that the mean-field Skyrme form factors obtained through the use of the semiclassical ETF functional densities do, indeed, reproduce their Hartree-Fock counterparts to considerable accuracy. Because this former study was carried out in the absence of any tensor terms (such terms having, at that time, also been neglected in virtually all Hartree-Fock type calculations), the derivation of the semiclassical density-functional expressions taking the tensor interaction explicitly into account therefore becomes of great interest and the present study is devoted to this subject.

The present paper is organized as follows. After giving a brief outline of the energy-density functional associated with a Skyrme effective nucleon-nucleon interaction including a zero-range two-body tensor force in Sec. II, we derive the mean-field Hamiltonian and the various involved form factors. The semiclassical ETF method is then used in Sec. III to obtain explicit density functionals for the kinetic-energy and spin-orbit densities in the presence of a tensor interaction. Using these ETF functionals, we examine the impact of the tensor force on the mean-field form factors in Sec. IV. Some conclusions are given in Sec. V.

[1] For a recent review on effective interactions and mean-field theories, see Refs. [14–16] and references therein.

II. SKYRME ENERGY-DENSITY FUNCTIONAL WITH A TENSOR FORCE

Let us start from the standard effective nucleon-nucleon interaction of the Skyrme type consisting of a density-dependent central force v_c, a standard spin-orbit term v_{so}, and a zero-range two-body tensor interaction v_t:

$$v_{\rm Sky}(\mathbf{r}_1,\mathbf{r}_2) = v_c(\mathbf{r}_1,\mathbf{r}_2) + v_{so}(\mathbf{r}_1,\mathbf{r}_2) + v_t(\mathbf{r}_1,\mathbf{r}_2) \tag{1}$$

with the central force [10,25]

$$\begin{aligned} v_c(\mathbf{R},\mathbf{s}) = {} & t_0(1+x_0P_\sigma)\,\delta(\mathbf{s}) + \frac{t_1}{2}(1+x_1P_\sigma) \\ & \times [\mathbf{k}'^2\,\delta(\mathbf{s}) + \delta(\mathbf{s})\mathbf{k}^2] + t_2(1+x_2P_\sigma)\mathbf{k}'\cdot\delta(\mathbf{s})\mathbf{k} \\ & + \frac{t_3}{6}(1+x_3P_\sigma)\,\rho_0^\alpha(\mathbf{R})\delta(\mathbf{s}) \end{aligned} \tag{2}$$

and the spin-orbit interaction

$$v_{so}(\mathbf{s}) = iW_0\,(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\cdot\mathbf{k}'\times\delta(\mathbf{s})\,\mathbf{k}, \tag{3}$$

where $\mathbf{R}$ and $\mathbf{s}$ are, respectively, the center of mass and relative coordinate, P_σ is the spin exchange operator, and $\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_2$ is the operator of relative momentum with the Hermitian adjoint operator $\mathbf{k}'$. The tensor part of the interaction is defined as [7,26]

$$\begin{aligned} v_t(\mathbf{s}) = {} & \frac{T_E}{2}\{[3(\boldsymbol{\sigma}_1\cdot\mathbf{k}')(\boldsymbol{\sigma}_2\cdot\mathbf{k}') - (\boldsymbol{\sigma}_1\cdot\sigma_2)\mathbf{k}'^2]\,\delta(\mathbf{s}) \\ & + \delta(\mathbf{s})\,[3(\boldsymbol{\sigma}_1\cdot\mathbf{k})(\boldsymbol{\sigma}_2\cdot\mathbf{k}) - (\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\mathbf{k}^2]\} \\ & + T_0[3(\boldsymbol{\sigma}_1\cdot\mathbf{k}')\,\delta(\mathbf{s})(\boldsymbol{\sigma}_2\cdot\mathbf{k}) - (\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\,\mathbf{k}'\cdot\delta(\mathbf{s})\mathbf{k}]. \end{aligned} \tag{4}$$

The energy-density functional $\mathcal{E}_{\rm Sky}$ associated with such a general Skyrme effective interaction is given for a time-reversal symmetric system, for which the time-odd local components of the density matrix vanish, by the following expression [20,27]:

$$\begin{aligned} & \mathcal{E}_{\rm Sky}(\mathbf{r}) \\ & = \frac{\hbar^2}{2m}\tau_0 + \sum_{t=0,1}\Bigg\{ C_t^\rho[\rho_0]\rho_t^2 - C_t^{\Delta\rho}(\nabla\rho_t)^2 + C_t^\tau\rho_t\tau_t \\ & \quad - C_t^T\sum_{\mu\nu}J_{t_{\mu\nu}}J_{t_{\mu\nu}} - \frac{1}{2}C_t^F\left[\left(\sum_\mu J_{t_{\mu\nu}}\right)^2 + \sum_{\mu\nu}J_{t_{\mu\nu}}J_{t_{\mu\nu}}\right] \\ & \quad + C_t^{\nabla J}\rho_t\nabla\cdot\mathbf{J}_t\Bigg\}, \end{aligned} \tag{5}$$

where the indices $t = 0$ and $t = 1$ stand for the isoscalar and isovector part of the corresponding densities, as, for example,

$$\begin{aligned} \rho_0(\mathbf{r}) &= \rho_n(\mathbf{r}) + \rho_p(\mathbf{r}), \\ \rho_1(\mathbf{r}) &= \rho_n(\mathbf{r}) - \rho_p(\mathbf{r}). \end{aligned} \tag{6}$$

How the coefficients of the energy-density functional $\mathcal{E}_{\rm Sky}$ are related to the coefficients t_k, x_k, W_0, α, T_E, and T_0 of the effective interaction, Eqs. (2)–(4), will be explicitly written down further on.

In the following we would like to investigate, in particular, the contribution of the spin-current pseudotensor density $J_{t_{\mu\nu}}$ to the total energy, but also to the mean-field form factors, such as the one-body potential and, in particular, to the spin-orbit potential, which, as pointed out in the introduction, determines to a large extent the shell closure and the magic numbers. For a given sort of particles (neutrons or protons) this quantity can be written as

$$J_{\mu\nu}(\mathbf{r}) = -\frac{i}{2}(\nabla_\mu - \nabla'_\mu)\sum_{\sigma,\sigma'}\rho(\mathbf{r}\sigma,\mathbf{r}'\sigma')|_{\mathbf{r}=\mathbf{r}'}\langle\sigma'|\sigma_\nu|\sigma\rangle \tag{7}$$

(where for the time being we drop the charge index $q = \{n, p\}$). Using the fact that the Cartesian components of the spin-current pseudotensor density $J_{\mu\nu}$ can be decomposed into a pseudoscalar, an antisymmetric vector, and a symmetric pseudotensor contribution (with well-defined transformation properties under rotation), namely [20]

$$J_{\mu\nu}(\mathbf{r}) = \frac{1}{3}\delta_{\mu\nu}J^{(0)}(\mathbf{r}) + \frac{1}{2}\sum_\lambda\epsilon_{\mu\nu\lambda}J_\lambda^{(1)}(\mathbf{r}) + J_{\mu\nu}^{(2)}(\mathbf{r}) \tag{8}$$

with

$$\begin{aligned} J^{(0)}(\mathbf{r}) &= \sum_\lambda J_{\lambda\lambda}(\mathbf{r}), \\ J_\lambda^{(1)}(\mathbf{r}) &= \sum_{\mu\nu}\epsilon_{\lambda\mu\nu}J_{\mu\nu}(\mathbf{r}), \\ J_{\mu\nu}^{(2)}(\mathbf{r}) &= \frac{1}{2}[J_{\mu\nu}(\mathbf{r}) + J_{\nu\mu}(\mathbf{r})] - \frac{1}{3}\delta_{\mu\nu}\sum_\lambda J_{\lambda\lambda}(\mathbf{r}), \end{aligned} \tag{9}$$

allows us to rewrite the J-dependent terms appearing in Eq. (5) in the form [20]

$$\sum_{\mu\nu}J_{\mu\nu}J_{\mu\nu} = \frac{1}{3}[J^{(0)}]^2 + \frac{1}{2}\mathbf{J}^2 + \sum_{\mu\nu}J_{\mu\nu}^{(2)}J_{\mu\nu}^{(2)} \tag{10}$$

and

$$\begin{aligned} \frac{1}{2}\left[\left(\sum_\mu J_{t_{\mu\nu}}\right)^2 + \sum_{\mu\nu}J_{t_{\mu\nu}}J_{t_{\mu\nu}}\right] &= \frac{2}{3}[J^{(0)}]^2 - \frac{1}{4}\mathbf{J}^2 \\ & + \frac{1}{2}\sum_{\mu\nu}J_{\mu\nu}^{(2)}J_{\mu\nu}^{(2)}, \end{aligned} \tag{11}$$

where $\mathbf{J}$ is the well-known spin-orbit density [10] with the Cartesian components $J_\lambda^{(1)}$ given in Eq. (9). The Skyrme energy density of Eq. (5) then takes the form

$$\begin{aligned} \mathcal{E}_{\rm Sky}(\mathbf{r}) = {} & \frac{\hbar^2}{2m}\tau_0 + \sum_{t=0,1}\Bigg\{ C_t^\rho[\rho_0]\rho_t^2 - C_t^{\Delta\rho}(\nabla\rho_t)^2 + C_t^\tau\rho_t\tau_t \\ & + \frac{1}{3}C_t^{J_0}\left[J_t^{(0)}\right]^2 + \frac{1}{2}C_t^{J_1}\mathbf{J}_t^2 + C_t^{J_2}\sum_{\mu\nu}J_{t_{\mu\nu}}^{(2)}J_{t_{\mu\nu}}^{(2)} \\ & + C_t^{\nabla J}\rho_t\,\nabla\cdot\mathbf{J}_t\Bigg\}, \end{aligned} \tag{12}$$

where we have defined the coefficients

$$\begin{aligned} C_t^{J_0} &= -\left(2C_t^F + C_t^T\right), \quad C_t^{J_1} = \left(\tfrac{1}{2}C_t^F - C_t^T\right), \\ C_t^{J_2} &= -\left(\tfrac{1}{2}C_t^F + C_t^T\right). \end{aligned}$$

To obtain the one-body Hamiltonian for a nucleon of type $q = \{n, p\}$, one has to carry out the following minimization

procedure (with $N_q = \{\frac{N}{2}, \frac{Z}{2}\}$):

$$\frac{\delta}{\delta\varphi_i^*(\mathbf{r},\sigma,q)} \times \int \left[\mathcal{E}_{\rm Sky}(\mathbf{r}) - \sum_q \sum_{j=1}^{N_q} \sum_{\sigma'} \varepsilon_j^{(q)} \, |\varphi_j(\mathbf{r},\sigma',q)|^2\right] d^3r = 0, \tag{13}$$

which for the energy density here can be written as

$$\frac{\partial \mathcal{E}_{\rm Sky}}{\partial \varphi_i^*(\mathbf{r},\sigma,q)} - \boldsymbol{\nabla}\left[\frac{\partial \mathcal{E}_{\rm Sky}}{\partial \boldsymbol{\nabla}\varphi_i^*(\mathbf{r},\sigma,q)}\right] = \mathcal{H}_q\varphi_i(\mathbf{r},\sigma,q) = \varepsilon_i^{(q)}\varphi_i(\mathbf{r},\sigma,q). \tag{14}$$

Since the derivative in Eqs. (13) and (14) is with respect to the single-particle wave function φ_j of a nucleon of type q we prefer, for better transparency, to write down the Skyrme energy-density functional in terms of the neutron and proton densities instead of the isoscalar and isovector densities of Eq. (6). As a first step in the treatment of the tensor interaction, we shall, as was also done in Ref. [20], restrict ourselves in the following to spherically symmetric nuclear systems. It is now interesting to note that, when imposing spherical symmetry, only one out of the nine components of the tensor $J_{\mu\nu}$ survives. One can, indeed, show that in that case the scalar part $J^{(0)}$ and the symmetric part $J^{(2)}_{\mu\nu}$ of the second ranked tensor vanish and only the (radial part of the) vector $\mathbf{J}$ survives. The Skyrme energy-density functional can then be simply written as

$$\begin{aligned}\mathcal{E}_{\rm Sky}(\mathbf{r}) = \sum_q \Big\{ &\frac{\hbar^2}{2m} f_q\tau_q + \big(C_0^\rho + C_1^\rho\big)\rho_q^2 + \big(C_0^\rho - C_1^\rho\big)\rho_q\rho_{\bar q} \\ &- \big(C_0^{\Delta\rho} + C_1^{\Delta\rho}\big)\big(\boldsymbol{\nabla}\rho_q\big)^2 - \big(C_0^{\Delta\rho} - C_1^{\Delta\rho}\big)\boldsymbol{\nabla}\rho_q\cdot\boldsymbol{\nabla}\rho_{\bar q} \\ &+ \frac{1}{2}\big(C_0^J + C_1^J\big)\mathbf{J}_q^2 + \frac{1}{2}\big(C_0^J - C_1^J\big)\mathbf{J}_q\cdot\mathbf{J}_{\bar q} \\ &- \big[\big(C_0^{\nabla J} + C_1^{\nabla J}\big)\boldsymbol{\nabla}\rho_q + \big(C_0^{\nabla J} - C_1^{\nabla J}\big)\boldsymbol{\nabla}\rho_{\bar q}\big]\cdot\mathbf{J}_q \Big\},\end{aligned} \tag{15}$$

where we have slightly changed the last term by moving through an integration by parts the gradient operator from the spin-orbit density $\mathbf{J}$ onto the local density ρ. Since for spherical systems no confusion is possible, and to simplify the notation, we have also written C_t^J instead of $C_t^{J_1}$ in this equation. The effective-mass form factor $f_q(\mathbf{r})$ is here defined in the usual way as

$$f_q = 1 + \frac{2m}{\hbar^2}\big[\big(C_0^\tau + C_1^\tau\big)\rho_q + \big(C_0^\tau - C_1^\tau\big)\rho_{\bar q}\big]. \tag{16}$$

The coefficients C_t^x appearing in the energy-density functional $\mathcal{E}_{\rm Sky}$, Eq. (15), are related to the coefficients t_k, x_k, W_0, α, T_E, and T_0 of Eqs. (2)–(4) in the following way [20,27]:

$$\begin{aligned} C_0^\rho &= \tfrac{3}{8}t_0 + \tfrac{3}{48}t_3\rho_0^\alpha(\mathbf{r}), \\ C_1^\rho &= -\tfrac{1}{8}t_0(2x_0+1) - \tfrac{1}{48}t_3(2x_3+1)\rho_0^\alpha(\mathbf{r}), \\ C_0^{\Delta\rho} &= \tfrac{1}{64}[-9t_1 + t_2(4x_2+5)], \\ C_1^{\Delta\rho} &= \tfrac{1}{64}[3t_1(2x_1+1) + t_2(2x_2+1)], \\ C_0^\tau &= \tfrac{1}{16}\left[3t_1 + t_2(4x_2+5)\right], \\ C_1^\tau &= \tfrac{1}{16}[-t_1(2x_1+1) + t_2(2x_2+1)], \\ C_0^{\nabla J} &= -\tfrac{3}{4}W_0, \quad C_1^{\nabla J} = -\tfrac{1}{4}W_0, \\ C_0^J &= -\tfrac{1}{16}\left[t_1(2x_1-1) + t_2(2x_2+1) - 5(T_E+3T_0)\right], \\ C_1^J &= -\tfrac{1}{16}\left[-t_1 + t_2 + 5(T_E - T_0)\right]. \end{aligned} \tag{17}$$

For what follows it will be useful to write down in some detail the Cartesian components of the spin-orbit density vector $\mathbf{J}$ as obtained from Eqs. (7) and (9):

$$\mathbf{J}_q = -\frac{i}{2}\sum_k \sum_{\sigma'\sigma''}[\varphi_k^*(\mathbf{r},\sigma'',q)\,\boldsymbol{\nabla}\varphi_k(\mathbf{r},\sigma',q) - \boldsymbol{\nabla}\varphi_k^*(\mathbf{r},\sigma'',q)\,\varphi_k(\mathbf{r},\sigma',q)] \times \langle\sigma''|\boldsymbol{\sigma}|\sigma'\rangle. \tag{18}$$

Through the functional derivative in Eq. (14) the one-body Hamiltonian $\mathcal{H}_q$ is obtained. The calculation of the different contributions is straightforward. The contributions [the so-called $\mathbf{J}^2$ terms [20] proportional to the C_t^T coefficients in Eq. (5)] arising from the tensor force but also from the exchange part of the central interaction are explicitly derived in the Appendix. Summing all the terms appearing in the functional derivative one obtains the following mean-field Hamiltonian $\mathcal{H}_q$ of Eq. (14):

$$\mathcal{H}_q = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}\cdot f_q(\mathbf{r})\boldsymbol{\nabla} + V_q(\mathbf{r}) - \frac{i}{2}\sum_{\sigma'}[\mathbf{W}_q\cdot(\boldsymbol{\nabla}\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle) + (\boldsymbol{\nabla}\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle)\cdot\mathbf{W}_q], \tag{19}$$

where the effective mass form factor $f_q(\mathbf{r})$ is given by Eq. (16) and where the central mean-field potential $V_q(\mathbf{r})$ and the spin-orbit type potential $\mathbf{W}_q(\mathbf{r})$ are obtained in the usual way as functional derivatives of the energy density $\mathcal{E}_{\rm Sky}$ with respect to the local density ρ_q and the spin-orbit density $\mathbf{J}_q$, respectively,

$$\begin{aligned} V_q(\mathbf{r}) = &\big(C_0^\tau + C_1^\tau\big)\tau_q + \big(C_0^\tau - C_1^\tau\big)\tau_{\bar q} + 2\big[\big(C_0^\rho + C_1^\rho\big)\rho_q \\ &+ \big(C_0^\rho - C_1^\rho\big)\rho_{\bar q}\big] + \left[\left(\frac{\partial C_0^\rho}{\partial\rho_0} + \frac{\partial C_1^\rho}{\partial\rho_0}\right)\rho_q^2 \right. \\ &\left. + \left(\frac{\partial C_0^\rho}{\partial\rho_0} - \frac{\partial C_1^\rho}{\partial\rho_0}\right)\rho_q\rho_{\bar q}\right] + 2\big[\big(C_0^{\Delta\rho} + C_1^{\Delta\rho}\big)\boldsymbol{\nabla}^2\rho_q \\ &+ \big(C_0^{\Delta\rho} - C_1^{\Delta\rho}\big)\boldsymbol{\nabla}^2\rho_{\bar q}\big] + \big(C_0^{\nabla J} + C_1^{\nabla J}\big)\mathrm{div}\mathbf{J}_q \\ &+ \big(C_0^{\nabla J} - C_1^{\nabla J}\big)\mathrm{div}\mathbf{J}_{\bar q} \end{aligned} \tag{20}$$

and

$$\mathbf{W}_q(\mathbf{r}) = -\big(C_0^{\nabla J} + C_1^{\nabla J}\big)\boldsymbol{\nabla}\rho_q - \big(C_0^{\nabla J} - C_1^{\nabla J}\big)\boldsymbol{\nabla}\rho_{\bar q} + \big(C_0^J + C_1^J\big)\mathbf{J}_q + \big(C_0^J - C_1^J\big)\mathbf{J}_{\bar q}. \tag{21}$$

At this point one could be tempted to conclude that, using this definition of $\mathbf{W}_q$, the spin-orbit dependent part of the energy density could be simply written in the form $\sum_q \mathbf{J}_q\cdot\mathbf{W}_q$, as this was the case before the introduction of the tensor terms [22]. This is, however, not possible because the terms

in C_t^J and $C_t^{\nabla J}$ appear in Eq. (15) with a different coefficient (1 versus 1/2).

Since the energy density functional $\mathcal{E}_{\rm Sky}$, Eq. (15), for a Skyrme effective interaction depends only on the local densities ρ_q, τ_q, and $\mathbf{J}_q$, and consequently the resulting mean-field potentials $V_q(\mathbf{r})$, Eq. (20), and $\mathbf{W}_q(\mathbf{r})$, Eq. (21), simple and useful approximate functionals for $\tau[\rho]$ and $\mathbf{J}[\rho]$ in terms of the particle density ρ and its derivatives can be obtained through the semiclassical Extended Thomas-Fermi method [22]. This then allows us to express the total energy as a functional of the neutron and proton densities only, which are obtained by a density variational calculation. Such an approach can be considered as an approximate treatment of the Hohenberg-Kohn method [28] in density functional theory. For a standard Skyrme force [i.e., without any tensor term and with the $\mathbf{J}_q$ and $\mathbf{J}_{\bar{q}}$ terms in Eq. (21) ignored], explicit ETF density functionals for $\tau[\rho]$ and $\mathbf{J}[\rho]$ up to fourth order in the semiclassical $\hbar$ expansion are given in integrated form (to calculate semiclassical energies) in Ref. [22] and locally [to be able to determine the form factors $V_q(\mathbf{r})$ and $\mathbf{W}_q(\mathbf{r})$] in Ref. [24]. Full ETF density functionals that take into account all the terms of Eq. (15), including the tensor term, are derived, up to order $\hbar^2$, in the next section.

III. SEMICLASSICAL FUNCTIONALS IN THE PRESENCE OF A TENSOR INTERACTION

At this stage we would like to insist on the point that the single-particle Hamiltonian (19) is exactly of the same form that it was before the inclusion of the tensor terms in the two-body interaction. The only thing that has changed is the fact that the central mean-field potential V_q and the spin-orbit potential $\mathbf{W}_q$ are of a slightly different form, now containing additional terms (depending on the coefficients C_0^J and C_1^J). We can therefore conclude that for a one-body Hamiltonian of the form (19) the ETF spin-orbit density functional $\mathbf{J}_q[\rho]$ obtained at lowest order (order $\hbar^2$) in the semiclassical expansion is of the usual form [22]

$$\mathbf{J}_q = -\frac{2m}{\hbar^2 f_q}\rho_q \mathbf{W}_q. \tag{22}$$

Here $\mathbf{W}_q$ as given by Eq. (21) now has a much richer structure than in the absence of the tensor terms. One thus obtains the following expression:

$$\begin{aligned}\mathbf{J}_q = -\frac{2m}{\hbar^2 f_q}\rho_q \big[&\left(C_0^J + C_1^J\right)\mathbf{J}_q + \left(C_0^J - C_1^J\right)\mathbf{J}_{\bar{q}} \\ &- \left(C_0^{\nabla J} + C_1^{\nabla J}\right)\nabla\rho_q - \left(C_0^{\nabla J} - C_1^{\nabla J}\right)\nabla\rho_{\bar{q}}\big].\end{aligned} \tag{23}$$

Because the final aim of the ETF approach is to express quantities such as the spin-orbit densities $\mathbf{J}_n$ and $\mathbf{J}_p$ as functions of the local densities ρ_n and ρ_p and its derivatives, one then simply has to solve the following system of linear equations:

$$\begin{aligned}&\left[\frac{\hbar^2}{2m}f_n + \left(C_0^J + C_1^J\right)\rho_n\right]\mathbf{J}_n + \left(C_0^J - C_1^J\right)\rho_n\mathbf{J}_p \\ &\quad = \left(C_0^{\nabla J} + C_1^{\nabla J}\right)\rho_n\nabla\rho_n + \left(C_0^{\nabla J} - C_1^{\nabla J}\right)\rho_n\nabla\rho_p,\end{aligned}$$

$$\begin{aligned}&\left[\frac{\hbar^2}{2m}f_p + \left(C_0^J + C_1^J\right)\rho_p\right]\mathbf{J}_p + \left(C_0^J - C_1^J\right)\rho_p\mathbf{J}_n \\ &\quad = \left(C_0^{\nabla J} + C_1^{\nabla J}\right)\rho_p\nabla\rho_p + \left(C_0^{\nabla J} - C_1^{\nabla J}\right)\rho_p\nabla\rho_n.\end{aligned} \tag{24}$$

Notice at this point that in the absence of the aforementioned $\mathbf{J}^2$ terms in the Skyrme energy-density functional, the ETF spin-orbit density recovers, of course, the usual simple form [22,24]. The question now also arises whether this treatment of the spin-orbit density can be easily carried on to the fourth order in the semiclassical expansion. This is, however, not the case, since the fourth-order counterpart of Eq. (22) involves not only the spin-orbit potential but also its first and second derivatives [24], which through Eq. (21) would then lead to a differential equation for the spin-orbit density. We will therefore, in the following, neglect the influence of the tensor terms on the fourth-order spin-orbit density functional. Such an approximation should be quite reasonable since it fully includes the impact of the $\mathbf{J}^2$ terms in the secnd-order functionals and only neglects its influence on the fourth-order terms, which have been explicitly shown in Ref. [24] to be small as compared to the second-order terms (and the Thomas-Fermi term, when present, as for the functional $\tau[\rho]$). Since the tensor term itself yields an important, yet in no way dominant, contribution to the nuclear structure, the introduced approximation should be largely sufficient to take its influence into account in our Extended Thomas-Fermi calculations.

When calculating the central mean-field potential $V_q(\mathbf{r})$ through Eq. (20) the divergence of the vector fields $\mathbf{J}_n(\mathbf{r})$ and $\mathbf{J}_p(\mathbf{r})$ is needed. These quantities are easily obtained by taking the divergence of Eq. (24) and solving a system of linear equations, which is straightforward but somewhat lengthy to write down and which we therefore do not display here. It is, however, in all points similar to the one here for the fields $\mathbf{J}_q(\mathbf{r})$.

One might wonder in which way the ETF kinetic-energy density $\tau[\rho]$ will change by the inclusion of the tensor terms in the energy-density functional. The answer is *not at all*, except that the spin-orbit form factor $\mathbf{W}_q$ in Eq. (21) now has a richer structure, as previously mentioned. Limiting ourselves again to the lowest nontrivial order beyond the Thomas-Fermi approximation (order $\hbar^2$) one obtains, as usual [22],

$$\begin{aligned}\tau_q[\rho_q] = &\frac{3}{5}(3\pi^2)^{2/3}\rho_q^{5/3} + \frac{1}{36}\frac{(\nabla\rho_q)^2}{\rho_q} + \frac{1}{3}\Delta\rho_q \\ &+ \frac{1}{6}\frac{\nabla\rho_q\cdot\nabla f_q}{f_q} + \frac{1}{6}\rho_q\frac{\Delta f_q}{f_q} - \frac{1}{12}\rho_q\left(\frac{\nabla f_q}{f_q}\right)^2 \\ &+ \frac{1}{2}\left(\frac{2m}{\hbar^2}\right)^2\rho_q\left(\frac{\mathbf{W}_q}{f_q}\right)^2, \\ q = &\{n, p\}.\end{aligned} \tag{25}$$

Since the spin-orbit form factor $\mathbf{W}_q$ is given by Eq. (21) as a function of the spin-orbit densities $\mathbf{J}_q$, which are themselves determined through the system of linear equations (24), the kinetic-energy density is known. It is understood that the full 4th order kinetic energy density is used in the calculations presented in the following.

IV. IMPACT OF THE TENSOR FORCE ON MEAN-FIELD POTENTIALS IN THE SEMICLASSICAL ETF APPROACH

It will now be interesting to investigate the impact of the tensor terms on a large variety of nuclear quantities that can be determined or, at least, constrained by available experimental data. At this point we do not aim at a full self-consistent semiclassical treatment, which would include the full effective interaction as presented earlier. Such a complete approach has been presented in Ref. [20]. Here we will rather treat the influence of the tensor terms perturbatively, performing a full selfconsistent ETF calculation (up to order $\hbar^4$) with a Skyrme effective interaction limited to the central force and spin-orbit term, Eqs. (2) and (3), and setting, as usually done, the coefficients C_t^J equal to zero, and add the contributions of the terms that were left out to the thus obtained fields. Such an approach is in the same spirit as the perturbative treatment of the tensor terms in Refs. [29,30].

We will in the following investigate in particular the impact of the tensor terms on the total energy, central mean-field, and spin-orbit potential. One should first notice that, even in the absence of a genuine tensor force, that is, with the coefficients T_E and T_0 equal to zero, the resolution of the system of linear equations for the $\mathbf{J}_n(\mathbf{r})$ and $\mathbf{J}_p(\mathbf{r})$ will *not* lead to the traditional ETF expression

$$\mathbf{J}_q = -\frac{2m}{\hbar^2}\frac{\rho_q}{f_q}\frac{W_0}{2}\nabla(\rho_0+\rho_q), \tag{26}$$

which has its origin in the neglect of $\mathbf{J}^2$ in the energy-density functional. A comparison between the two spin-orbit densities is shown in Fig. 1 for the neutron densities obtained in ^{208}Pb with the Skyrme interactions SkM* [22,31] and SLy4 [32]. The effect is clearly visible, with a decrease of the spin-orbit densities by about 10% when the contribution of the $\mathbf{J}^2$ terms, which have their origin in the exchange part of the central force, are consistently taken into account. An effect of the same order of magnitude is observed for the proton densities.

It is now interesting to investigate the impact of a genuine tensor force. To that aim we choose one of the parameter sets proposed in Ref. [20], namely the T42 parametrization, which, according to Figs. 27 to 32 of that publication, seems to be among the best candidates for an effective interaction of the Skyrme type that takes a tensor term consistently into account. The result is even more striking here, as can be seen in Fig. 2, since the inclusion of the $\mathbf{J}^2$ terms leads to a reduction of the spin-orbit densities by approximately a factor of 2.

Such a very noticeable change in the spin-orbit density raises the question of to what extent the inclusion of the $\mathbf{J}^2$ terms will modify the spin-orbit potential and thereby have an impact on the spin-orbit splitting. To answer this question we display in Fig. 3 the neutron spin-orbit potential obtained in ^{208}Pb with the T42 Skyrme interaction with and without the inclusion of the $\mathbf{J}$-dependent terms in Eq. (21). Since it is interesting to investigate how such a behavior varies when going from light to heavy nuclei, we are also showing, in Fig. 3, the same quantity for the nucleus ^{90}Zr. One concludes from both cases that the effect is dramatic, leading to a reduction of the spin-orbit potential by practically

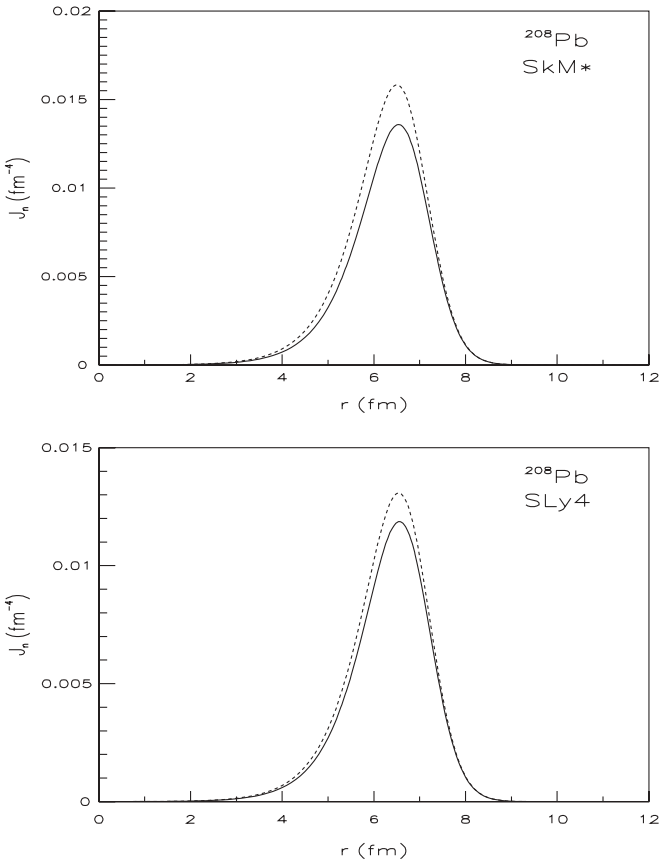

FIG. 1. Radial component of the ETF neutron spin-orbit density $J_n(r)$ in ^{208}Pb obtained with the Skyrme interactions SkM* (upper part) and SLy4 (lower part) by solving the system of linear equations (21) (solid line) and by Eq. (26), that is, by neglecting the coefficients of the $\mathbf{J}^2$ terms in the energy-density functional (dashed line).

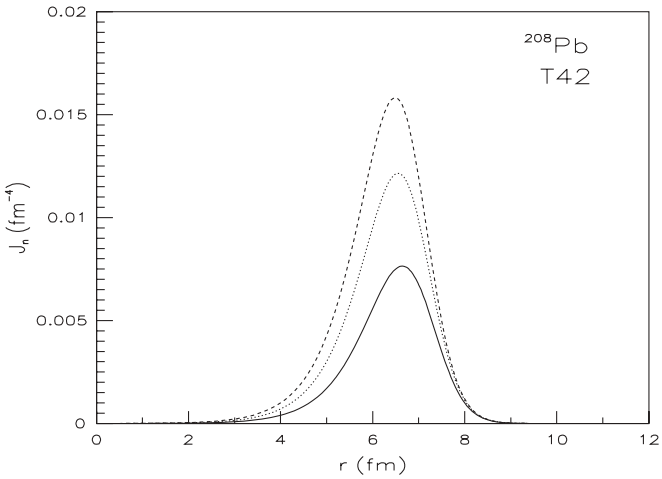

FIG. 2. Same as Fig. 1, but obtained with the T42 parametrization of Ref. [20] through the solution of the system of linear equations (21) (solid line), by solving that system with the tensor-force coefficients (T_0 and T_E) set to zero (dotted line) and by neglecting the $\mathbf{J}^2$ coefficients altogether (dashed line).

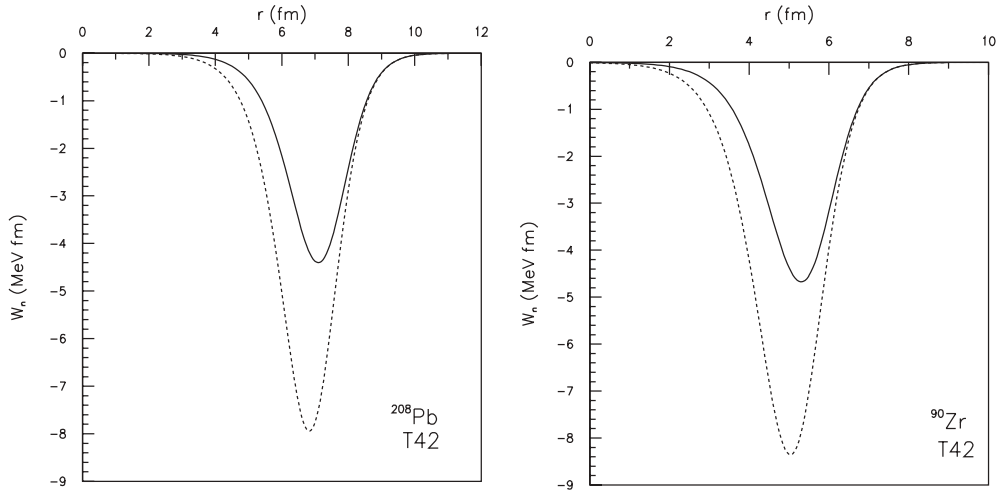

FIG. 3. Neutron spin-orbit potential obtained in ^{208}Pb (left) and ^{90}Zr (right) with the T42 Skyrme parametrization with (solid line) and without (dashed line) the $\mathbf{J}$-dependent terms.

a factor of 2, owing to a large cancellation that takes place between the *old* and the *new* terms in Eq. (21). Such a reduction has been also observed for a chain of Ni isotopes in the Hartree-Fock-Bogoliubov calculations of Ref. [20].

It is now also interesting to investigate the impact on the additional $\mathbf{J}$ terms on the central mean-field potentials $V_n(\mathbf{r})$ and $V_p(\mathbf{r})$. Such terms do not *explicitly* show up in the Hartree-Fock approach, but there the changes in the central potentials come about through the impact that these terms generate in the self-consistent procedure on the local densities ρ_q, τ_q, and $\mathbf{J}_q$. One therefore expects the impact on the semiclassical central potentials to be rather small. In the ETF approach an additional contribution is generated through the changes that the inclusion of these additional terms are bringing about in the ETF kinetic-energy and spin-orbit density functionals. It is also clear that the change of the spin-orbit potential discussed here will be carried onto the ETF kinetic-energy density (last term) of Eq. (25). The div $\mathbf{J}_q$ terms in Eq. (18) will, obviously, also be modified, since these terms are found, as previously mentioned, by calculating the divergence of both Eqs. (24). The thus generated changes in the central mean fields $V_q(\mathbf{r})$ are expected to be rather small since both of these changes correspond to corrections in the semiclassical functionals of order $\hbar^2$ and it has been shown in Ref. [24] (see in particular Fig. 2 there) that those corrections are themselves quite small as compared to the dominant Thomas-Fermi contribution. To be more specific, it is found that the corrections generated by the new terms never exceed 0.4 MeV in amplitude in either of neutron and proton potentials calculated in ^{208}Pb for either of the two Skyrme interactions used here (SkM* and SLy4), in which case the change is not visible on the figure when displaying the mean-field potentials $V_q(\mathbf{r})$. For the T42 parametrization, however, this difference reaches 1.6 MeV (0.6 MeV) for the neutron (proton) central field in ^{208}Pb and even slightly more in the case of ^{90}Zr. We therefore show the neutron central mean field for this latter nucleus in Fig. 4. As can be seen from the figure such corrections are limited to the surface region where they cause, after all, a small change. What exclusively the mean-field potentials are concerned, such a change should have little influence on the location of single-particle states in such a potential, a location that is, however, also largely determined by the strength of the spin-orbit field, and we expect the effect of the latter, as shown on Fig. 3, to have a rather noticeable effect on the precise location of single-particle states and thereby on the associated shell structure.

All of these investigations rely on a perturbative treatment of the previously neglected $\mathbf{J}^2$ terms, which have their origin in the exchange part of the central nucleon-nucleon force and in a genuine tensor interaction. We would like to close the present study by assessing the validity of such an approximation through a fully self-consistent semiclassical ETF calculation in which the aforementioned terms are fully included in the variational treatment. The result of such an investigation is shown in Fig. 5. The fully self-consistent treatment, where all of the terms in the energy-density functional are included in the semiclassical density variational calculation leads to a spin-orbit form factor that is slightly smaller than the one obtained in the approach where these terms are taken into account perturbatively. The two curves are, however, very close

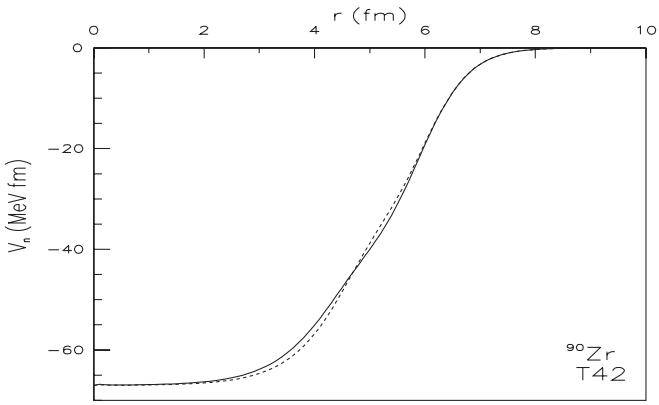

FIG. 4. Neutron central mean-field potential obtained with the T42 Skyrme parametrization for the nucleus ^{90}Zr with (solid line) and without (dashed line) the $\mathbf{J}^2$ terms in the energy-density functional.

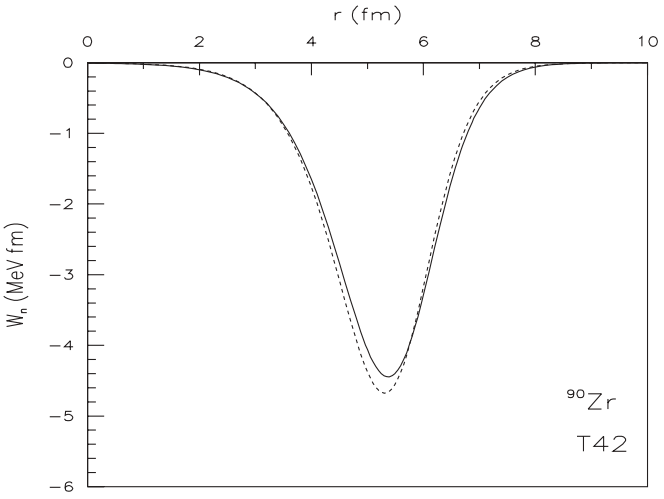

FIG. 5. Neutron spin-orbit potential obtained with the T42 Skyrme parametrization for the nucleus ^{90}Zr with a fully self-consistent (solid line) and a perturbative treatment (dashed line) of the $\mathbf{J}^2$ terms in the energy-density functional.

to each other, with a deviation of less than 5%. Such a behavior therefore justifies, a posteriori, the perturbative treatment that was at the base of our study.

V. CONCLUSIONS

For the case that a tensor force is included in the two-body interaction of an N-particle system, Extended Thomas-Fermi functional expressions are derived, for the first time, for the kinetic-energy density τ and spin-orbit density $\mathbf{J}$ as functions of the local matter density ρ and its derivatives for spherically symmetric systems. It is shown that in the case of a Skyrme-type effective interaction, the tensor terms as well as the previously neglected $\mathbf{J}$-dependent terms, originating from the exchange part of the central force, have a strong influence on the spin-orbit mean-field potential and could, therefore, have a substantial influence on the shell structure of exotic nuclei. We conclude that such terms therefore need to be taken into account in any future adjustments of the effective nucleon-nucleon interaction.

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APPENDIX: $\mathbf{J}^2$ CONTRIBUTIONS TO THE ONE-BODY HAMILTONIAN

As pointed out in the main text the one-body Hamiltonian of Eq. (19) is obtained through the functional derivative of the total energy-density functional as given by Eq. (15) for a Skyrme effective interaction in the case where the system is time reversal invariant and spherically symmetric. Let us carry out the functional derivative of the different $\mathbf{J}$ dependent terms of Eq. (15) one by one we obtain

$$\begin{aligned}
&\frac{\delta}{\delta\varphi_j^*(\mathbf{r},\sigma,q)}\int d^3r'\left[\mathbf{J}_q^2(\mathbf{r}')\right]\\
&= 2\mathbf{J}_q\cdot\frac{\partial\mathbf{J}_q}{\partial\varphi_j^*(\mathbf{r},\sigma,q)} - 2\sum_\lambda\nabla_\lambda\left[\sum_\kappa J_{q_\kappa}\frac{\partial J_{q_\kappa}}{\partial\nabla_\lambda\varphi_j^*(\mathbf{r},\sigma,q)}\right]\\
&= -i\sum_\kappa J_{q_\kappa}\sum_{\sigma'}\sum_{\mu\nu}\epsilon_{\mu\nu\kappa}\nabla_\mu\varphi_j(\mathbf{r},\sigma',q)\langle\sigma|\sigma_\nu|\sigma'\rangle\\
&\quad - i\sum_{\mu,\nu,\kappa}\sum_{\sigma'}\nabla_\mu\left[\epsilon_{\mu\nu\kappa}J_{q_\kappa}\,\varphi_j(\mathbf{r},\sigma',q)\,\langle\sigma|\sigma_\nu|\sigma'\rangle\right]\\
&= -i\mathbf{J}_q\cdot\sum_{\sigma'}(\nabla\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle)\varphi_j(\mathbf{r},\sigma',q)\\
&\quad - i\sum_{\sigma'}(\nabla\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle)\cdot\mathbf{J}_q\varphi_j(\mathbf{r},\sigma',q),
\end{aligned}\tag{A1}$$

$$\begin{aligned}
&\frac{\delta}{\delta\varphi_j^*(\mathbf{r},\sigma,q)}\int d^3r'[\mathbf{J}_q(\mathbf{r}')\cdot\mathbf{J}_{\bar q}(\mathbf{r}')]\\
&\quad = -\frac{i}{2}\left[\mathbf{J}_{\bar q}\cdot\sum_{\sigma'}(\nabla\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle)\varphi_j(\mathbf{r},\sigma',q)\right.\\
&\qquad\left.+\sum_{\sigma'}(\nabla\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle)\cdot\mathbf{J}_{\bar q}\varphi_j(\mathbf{r},\sigma',q)\right],
\end{aligned}\tag{A2}$$

$$\begin{aligned}
&\frac{\delta}{\delta\varphi_j^*(\mathbf{r},\sigma,q)}\int d^3r'[\nabla_{r'}\rho_q\cdot\mathbf{J}_q(\mathbf{r}')]\\
&= \frac{\partial(\nabla\rho_q\cdot\mathbf{J}_q)}{\partial\varphi_j^*(\mathbf{r},\sigma,q)} - \sum_{\lambda,\kappa}\nabla_\lambda\left[\frac{\partial(\nabla_\kappa\rho_q J_{q_\kappa})}{\partial\nabla_\lambda\varphi_j^*(\mathbf{r},\sigma,q)}\right]\\
&= \nabla\varphi_j(\mathbf{r},\sigma,q)\cdot\mathbf{J}_q - \frac{i}{2}\sum_\kappa\nabla_\kappa\rho_q\\
&\quad\times\sum_{\sigma',\sigma''}\sum_k\sum_{\mu,\nu}\epsilon_{\mu\nu\kappa}\nabla_\mu\varphi_j(\mathbf{r},\sigma',q)\langle\sigma|\sigma_\nu|\sigma'\rangle\delta_{kj}\delta_{\sigma\sigma''}\\
&\quad - \sum_{\lambda,\kappa}\nabla_\lambda\left[J_{q_\kappa}\delta_{\lambda,\kappa}\varphi_j(\mathbf{r},\sigma,q)\right] - \frac{i}{2}\sum_{\kappa\lambda}\nabla_\kappa\nabla_\lambda\rho_q\\
&\quad\times\sum_{\sigma'}\sum_{\mu,\nu}\epsilon_{\mu\nu\lambda}\,\varphi_j(\mathbf{r},\sigma',q)\langle\sigma|\sigma_\nu|\sigma'\rangle\delta_{\mu\kappa}\\
&= -(\mathrm{div}\mathbf{J}_q)\varphi_j(\mathbf{r},\sigma,q) - \frac{i}{2}\sum_{\sigma'}[\nabla\rho_q\cdot(\nabla\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle)\\
&\quad + \nabla\cdot(\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle\times\nabla\rho_q)]\varphi_j(\mathbf{r},\sigma',q),
\end{aligned}\tag{A3}$$

$$\begin{aligned}
&\frac{\delta}{\delta\varphi_j^*(\mathbf{r},\sigma,q)}\int d^3r'[\nabla_{r'}\rho_{\bar q}\cdot\mathbf{J}_q(\mathbf{r}')]\\
&\quad = \frac{\partial(\nabla\rho_{\bar q}\cdot\mathbf{J}_q)}{\partial\varphi_j^*(\mathbf{r},\sigma,q)} - \sum_{\lambda,\kappa}\nabla_\lambda\left[\frac{\partial(\nabla_\kappa\rho_{\bar q}J_{q_\kappa})}{\partial\nabla_\lambda\varphi_j^*(\mathbf{r},\sigma,q)}\right]\\
&\quad = -\frac{i}{2}\sum_{\sigma'}[\nabla\rho_{\bar q}\cdot(\nabla\times\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle)\\
&\qquad + \nabla\cdot(\langle\sigma|\boldsymbol{\sigma}|\sigma'\rangle\times\nabla\rho_{\bar q})]\varphi_j(\mathbf{r},\sigma',q).
\end{aligned}\tag{A4}$$

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