Extended Thomas-Fermi approximation to the one-body density matrix

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Abstract

The one-body density matrix is derived within the Extended Thomas-Fermi approximation. This has been done starting from the Wigner-Kirkwood distribution function for a non-local single-particle potential. The links between this new approach to the density matrix with former ones available in the literature are widely discussed. The semiclassical Hartree-Fock energy at Extended Thomas-Fermi level is also obtained in the case of a non-local one-body Hamiltonian. Numerical applications are performed using the Gogny and Brink-Boeker effective interactions. The semiclassical binding energies and root mean square radii are compared with the fully quantal ones and with those obtained using the Strutinsky averaged method.
1 Introduction

The one-body density matrix (DM) $\rho(r, r') = \sum_\alpha \phi_\alpha^*(r) \phi_\alpha(r')$ or equivalently its Wigner transform the distribution function $f(R, p)$ (defined below), plays a crucial role in the Hartree-Fock (HF) calculations. If zero-range Skyrme forces \cite{1} are used, only the diagonal part of the DM is needed. However, full knowledge of $\rho(r, r')$ (or $f(R, p)$) is necessary if one considers finite-range effective nuclear forces which are derived from G-matrix calculations in nuclear matter through the local density approximation \cite{2, 3, 4, 5} or postulated empirically with their parameters fitted to reproduce some properties of nuclear matter and finite nuclei \cite{6, 7}.

The full calculation of the density matrix (or the distribution function) is not an easy task and requires some computational effort \cite{7, 8}. Consequently, approximations which simplify the calculation and, at the same time, show more clearly the physical content of the DM are in order. The simplest one is to replace the non-diagonal part of the DM by its value in nuclear matter (Slater approach). Finite size effects are added using the density matrix expansion (DME), either that due to Negele and Vautherin (NV) \cite{9, 10} or the modified expansion due to Campi and Bouyssy (CB) \cite{11}. Very recently, the CB approach has been applied to HF calculations of finite nuclei \cite{12} using a density-dependent version of the M3Y interaction \cite{4, 5}.

On the other hand, semiclassical methods \cite{13} are very useful for describing nuclear properties of a global character such as binding energies or nuclear densities and their moments. Concerning the nuclear ground state properties at HF level, semiclassical approaches are based on the Wigner-Kirkwood (WK) $\hbar$-expansion of the distribution function which for a set of nucleons moving in a local external potential $V(r)$ up to second order is given by \cite{13}:

\begin{equation}
 f_{WK}(R, p) = \Theta(\lambda - H_W) - \frac{\hbar^2}{8m} \Delta V \delta'(\lambda - H_W) \\
 + \frac{\hbar^2}{24m} |(\nabla V)^2 + \frac{1}{m} (p, \nabla)^2 V| \delta''(\lambda - H_W) + \mathcal{O}(\hbar^4),
 \end{equation}

where $\lambda$ is the chemical potential and $H_W$ is the Wigner transform \cite{13} of the one-body Hamiltonian, which reads

\begin{equation}
 H_W = \frac{p^2}{2m} + V(R).
 \end{equation}

The semiclassical distribution function $f(R, p)$ is a representation of the true phase-space function in terms of distributions and is very efficient in order to obtain semiclassical expectation values by integrals over the whole phase-space \cite{14, 15}.
The main purpose of this paper is to derive the explicit expression of the DM in the Extended Thomas-Fermi (ETF) approximation \[16\] starting from the very recently presented WK expansion up to $\hbar^2$ order of the distribution function for non-local potentials \[15\]. On one hand, we want to establish a link between the NV (and CB) expansions of the DM with this semiclassical approach and, on the other, to apply this ETF DM to derive the exchange HF energy when finite range forces are used. The paper is organized as follows: In the first section we compare the semiclassical ETF density matrix with the former approximations of NV and CB in the case of a local potential. In the second section we derive the density matrix and the HF energy in the ETF approximation for a non-local potential. We also perform restricted HF variational calculations for some selected spherical nuclei using the Gogny [7] and Brink-Boeker [6] effective forces. We compare these HF ETF results with those obtained quantally, with those obtained with the Strutinsky average method [19] and with those which result from the NV and CB approaches to the DM. In the last section we give our conclusions and outlook. Technical details concerning the calculation of the DM and HF energy in the ETF approach for a non-local potential are given in the Appendix.

2 Extended Thomas-Fermi Density Matrix

The first step is to perform the inverse Wigner transform of (1) to obtain the semiclassical WK density matrix in coordinate space. The definition used here for the Wigner transform of the one-body density matrix is [13]:

$$f(R,p) = \int ds e^{-ip s/\hbar} \rho(R + \frac{s}{2}, R - \frac{s}{2}),$$

(3)

where $R = (r_1 + r_2)/2$, $s = r_1 - r_2$ and $p$ are, respectively, the centre-of-mass, the relative coordinates and the phase-space momentum.

After some lengthy but straightforward algebra the semiclassical DM in terms of $R$ and $s$ at WK level is given by:

$$\rho(R, s) = \frac{g k_F^2}{6\pi^2} \frac{3j_1(k_F s)}{k_F s} + \frac{g}{24\pi^2} \Delta k_F [j_0(k_F s) - k_F s j_1(k_F s)]$$

$$+ \frac{g}{48\pi^2} \frac{(\nabla k_F)^2}{k_F} [j_0(k_F s) - 4k_F s j_1(k_F s) + k_F^2 s^2 j_2(k_F s)]$$
\[-\frac{g}{48\pi^2} \frac{1}{k_F} \nabla [k_F \nabla k_F s s] \gamma [ - 3k_F s j_1(k_F s) + k_F^2 s^2 j_2(k_F s)] + O(h^4), \quad (4)\]

where \( k_F = \sqrt{\frac{2m}{\hbar^2}(\lambda - V(R))} \) is the local Fermi momentum, \( j_l(k_F s) \) are the spherical Bessel functions and \( g \) stands for the degeneracy.

This expression, although written in a slightly different way, coincides with the ones obtained previously by Dreizler and Gross [17] and Jennings [18]. The first term of the expansion (4) corresponds to the Slater approach, whereas the \( \hbar^2 \) terms are the part that take into account quantal finite-size effects.

The WK density matrix in coordinate space depends on the angle between \( R \) and \( s \), however for practical purposes and following previous literature [9, 11, 10] we perform the angular average of eq.(4) obtaining:

\[
\tilde{\rho}(R, s) = \tilde{\rho}_0(R, s) + \tilde{\rho}_2(R, s) \\
= \frac{gk_F^3}{6\pi^2} \frac{3j_1(k_F s)}{k_F s} + \frac{g}{144\pi^2} \Delta k_F \left[ 6j_0(k_F s) - 3k_F s j_1(k_F s) - k_F^2 s^2 j_2(k_F s) \right] \\
+ \frac{g}{144\pi^2} \left( \frac{\nabla k_F}{k_F} \right)^2 \left[ 3j_0(k_F s) - 9k_F s j_1(k_F s) + 2k_F^2 s^2 j_2(k_F s) \right]. \quad (5)
\]

The diagonal part \((s=0)\) of eq.(5) is the well-known WK expression for the local density (with degeneracy \( g \)) [13, 15]:

\[
\rho(R) = \frac{gk_F^3}{6\pi^2} + \frac{g}{144\pi^2} \left( \frac{\nabla k_F}{k_F} \right)^2 + 2\Delta k_F. \quad (6)
\]

To obtain the DM in the ETF approach we shall express the Fermi momentum and its derivatives in terms of the local density and its gradients. First, the local Fermi momentum is obtained by inverting eq.(3):

\[
k_F = k_0 - \frac{1}{24} \left[ \left( \nabla k_0 \right)^2 \frac{k_0^3}{k_0^3} + 2\Delta k_0 \frac{k_0^3}{k_0^3} \right], \quad (7)
\]

where \( k_0 = (6\pi^2 \rho/g)^{1/3} \). Notice that for inverting the gradient terms in eq.(3) it is enough to replace \( k_F \) by \( k_0 \) to be consistent with the \( \hbar \)-order in the expansion of the Fermi momentum (7). Writing the gradients of \( k_0 \) in terms of the spatial derivatives of the local density

\[
k_0(\nabla k_0)^2 = \frac{2\pi^2}{3g} \left( \frac{\nabla \rho}{\rho} \right)^2 \quad (8)
\]

\[
k_0^3 \Delta k_0 = \frac{2\pi^2}{g} \left[ \Delta \rho - \frac{2}{3} \left( \frac{\nabla \rho}{\rho} \right)^2 \right] \quad (9)
\]
one finally obtains the Fermi momentum as:

\[ k_F = \left( \frac{6\pi^2}{g} \right)^{1/3} + \frac{1}{72} \left( \frac{6\pi^2}{g} \right)^{-1/3} \left( \frac{\nabla \rho}{\rho^2} - 2 \frac{\Delta \rho}{\rho} \right), \]  

(10)

where the first term of the right-hand side is the pure Thomas-Fermi part and the second term, which contains derivatives of the local density, is the \( \hbar^2 \) contribution. The semiclassical density matrix for a local potential in the ETF approach is obtained from (5) by expanding consistently the Fermi momentum \( k_F \) up to \( \hbar^2 \)-order with the help of eqs.(8 - 10):

\[ \tilde{\rho}_{ETF}(R, s) = \rho^3 \int d^3 p \frac{3 j_1(k_{FS})}{k_{FS}} \rho(r, r') \big|_{r=r'} = j_0(s\hat{p}/\hbar)\rho(r, r') \big|_{r=r'}, \]  

(12)

where now \( k_F = k_0 = \left( \frac{6\pi^2}{g} \right)^{1/3} \).

Let us now analyze the main properties of this semiclassical approach as compared with the quantal case. Following refs.\([8, 9]\), the quantal DM averaged over the \( s \) direction can be approximated by:

\[ \rho(R, s) = \frac{1}{4\pi} \int d\Omega e^{is\hat{p}/\hbar} \rho(r, r') \big|_{r=r'} = j_0(s\hat{p}/\hbar)\rho(r, r') \big|_{r=r'}, \]  

(12)

where \( \hat{p} = -i\hbar(\nabla_1 - \nabla_2)/2 \) is the relative momentum operator. Expanding the Bessel function in a Taylor series one gets:

\[ \rho(R, s) = \sum_{n=0}^{\infty} \frac{(-1)^n s^{2n}}{(2n + 1)!} \left( \frac{\hat{p}}{\hbar} \right)^{2n} \rho(r, r') \big|_{r=r'} = \sum_{n=0}^{\infty} \frac{(-1)^n s^{2n}}{(2n + 1)!} M_{2n}, \]  

(13)

where \( M_{2n} \) are the momentum weighted integrals defined as \([8]\):

\[ M_{2n} = \frac{1}{(2\pi\hbar)^3} \int d\mathbf{p} \left( \frac{\mathbf{p}}{\hbar} \right)^{2n} f(R, \mathbf{p}) = \left( \frac{\mathbf{p}}{\hbar} \right)^{2n} \rho(r, r') \big|_{r=r'} = R. \]  

(14)

It should be pointed out that series (13) as it stands is not useful because it converges very slowly and cannot be truncated for large \( s \)-values if the even moments are different from zero.

At this point there are two possibilities for approximating the exact DM. One is to sum the series (13) using some approach for evaluating the momentum weighted integrals and the other is to rearrange the series (13) in such a way that truncation is possible.

First of all, we will show that the semiclassical ETF approach to the DM eq.(11) corresponds to the whole sum of the series eq.(13) if the moments \( M_{2n} \) are calculated in the ETF approximation. Starting from the semiclassical distribution function, eq.(11), the WK momentum weighted
integrals up to $\hbar^2$-order are easily derived. Expanding consistently the Fermi momentum with the help of (10) and using eqs.(8-9) one finally obtains the ETF weighted integrals in terms of the local density and its gradients:

$$M_{ETF}^{2n} = \frac{3}{2n+3} \rho k_F^{2n} + nk_F^{2n-2} \left\{ \frac{8n-5 (\nabla \rho)^2}{108 \rho} - \frac{2n-5}{36} \Delta \rho \right\}, \quad (15)$$

where again $k_F = k_0 = (6\pi^2 \rho/g)^{1/3}$.

The first term of the right-hand side of (15) is the Thomas-Fermi weighted integral while the second term is just the $\hbar^2$ correction in the ETF approach. For $n = 0$ and $n = 2$ one obtains:

$$M_{ETF}^{0} = \rho$$

$$M_{ETF}^{2} = \frac{3}{5} \rho k_F^2 + \frac{1}{36} (\nabla \rho)^2 + \frac{1}{12} \Delta \rho, \quad (17)$$

which are just the semiclassical counterparts (at ETF-$\hbar^2$ level) of the zeroth and second-order quantal momentum weighted integrals: $M_0 = \rho$ and $M_2 = \tau - \Delta \rho/4$, where $\tau$ is the kinetic energy density. Notice that in the ETF-$\hbar^2$ approach only second-order gradients of the local density appear in $M_{ETF}^{2n}$ for any value of $n$. However, higher order derivatives will appear in the moments if the ETF expansion is pushed to higher powers in $\hbar$.

Taking into account the Taylor expansion of the Bessel functions in eq. (11) and after some algebra one finds:

$$\rho_{ETF}(\mathbf{R}, s) = \frac{3 j_1(k_F s)}{k_F s} - \sum_{n=0}^{\infty} \frac{(-1)^n s^{2n+2}}{(2n+3)!} (n+1) k_F^{2n} \left\{ \frac{8n+3 (\nabla \rho)^2}{108 \rho} - \frac{2n-3}{36} \Delta \rho \right\}$$

$$= \frac{3 \rho}{\sum_{n=0}^{\infty} \frac{(-1)^n s^{2n}}{(2n+3)(2n+1)!} + \sum_{n=1}^{\infty} \frac{(-1)^n s^{2n}}{(2n+1)!} [M_{ETF}^{2n} - \frac{3}{2n+3} \rho k_F^{2n}]}$$

$$= \sum_{n=0}^{\infty} \frac{(-1)^n s^{2n}}{(2n+1)!} M_{ETF}^{2n}. \quad (18)$$

From this result it is clear that in the ETF approximation to the DM all the momentum weighted integrals appearing in eq.(13), evaluated within the same semiclassical approach, are consistently summed.

Another possibility for approximating the quantal DM is to rearrange the terms in eq.(13) in such a way that the leading term is the Slater term. This is, actually, the way in which the NV and CB approaches to the DM are done. For the sake of completeness we shall once again briefly derive the NV and CB approaches to the DM following the method outlined in ref. [8].
The starting point is the identity
\[ j_0(ab) = \sum_{n=0}^{\infty} (-1)^n (4n + 3) \frac{j_{2n+1}(ak) P_{2n+1}(b/k)}{ak b/k} \] (19)
valid for any \( k \) such that \(-1 \leq b/k \leq 1\) and where \( P_{2n+1}(x) \) are the Legendre polynomials
\[ P_{2n+1}(x) = \sum_{m=0}^{n} a_m^n x^{2(n-m)+1} \] (20)

Using eq. (19) in eq. (12), the angular averaged DM eq. (13) is also written as:
\[ \rho(R, s) = \sum_{n=0}^{\infty} (-1)^n (4n + 3) \frac{j_{2n+1}(ks)}{ks} \frac{P_{2n+1}(\hat{p}/\hbar k)}{\hat{p}/\hbar k} \rho(r, r')|_{r=r'=R} \]
\[ = \sum_{n=0}^{\infty} (-1)^n \frac{j_{2n+1}(ks) s^{2n}}{(2n + 1)!} \sum_{m=0}^{n} a_m^n a_0^n M_{2(n-m)} k^{2m}, \] (21)
where \( \hat{j}_{2n+1}(ks) = (4n + 3)!! j_{2n+1}(ks)/(ks)^{2n+1} \) are the spherical Bessel functions normalized to unity at \( s = 0 \).

Of course, the semiclassical \( \tilde{\rho}_{ETF}(R, s) \) (18) also fulfills eq. (21). Starting from this equation if the moments are obtained in the ETF approximation (15), the Bessel functions \( \hat{j}_{2n+1}(ks) \) are expanded in a Taylor series and the even powers of \( s \) are properly sorted out, one recovers (18).

The NV approach consists of keeping the two first terms of the expansion (21) and taking \( k = k_F \). In this case the DM reads:
\[ \tilde{\rho}_{NV}(R, s) = \rho \frac{3 j_1(k_F s)}{k_F s} - \frac{35}{2} \frac{j_3(k_F s)}{k_F s} \frac{3}{5} \frac{k_F^2 M_0 - M_2}{M_2} \] (22)
The CB approximation keeps only the first term of (21) but with k fixed in such a way that the second term of (21) identically vanishes:
\[ \tilde{\rho}_{CB}(R, s) = \rho \frac{3 j_1(k_F s)}{k_F s}, \] (23)
where \( \tilde{k}_F = \sqrt{5 M_2/3 \rho} \).

The NV and CB approaches are truncations of the true expansion of the quantal DM eq. (13). As is discussed in [8], in these approximations only the \( M_0 \) and \( M_2 \) momentum weighted integrals correspond to those obtained with the exact DM, whereas any higher momentum weighted integral in these approaches \( M_{2\lambda} (\lambda > 1) \) has little to do with its exact quantal value.
Let us now discuss the results obtained using the different approaches to the DM analyzed previously. To do this we consider a $^{40}\text{Ca}$ nucleus described using harmonic oscillator (HO) wavefunctions with an oscillator parameter $\alpha = \sqrt{m\omega/\hbar} = 0.516 \text{ fm}^{-1}$. Figure 1 displays the ratio of the off-diagonal to diagonal DM $\rho(\mathbf{R}, s)/\rho(\mathbf{R})$ as a function of the interparticle distance $s$ for selected values of the distance from the centre-of-mass $\mathbf{R}$. The different curves shown in this figure correspond to the quantal DM (black dots), the NV (dashed-dotted line) and CB (dashed line) approximations and the semiclassical ETF approach calculated using the quantal local density (solid line). As general trends the approximations to the DM considered here reproduce reasonably well the quantal values in the range of $R = 1 - 3 \text{ fm}$, they show some deficiencies at $R = 0 \text{ fm}$ and clearly start to separate from the quantal values for $R > 4 \text{ fm}$. However, in the whole range of $R$-values analyzed, the quantal approaches NV and CB reproduce the quantal DM better than the semiclassical ETF calculation.

At this point two comments are in order. First of all, it should be pointed out that all the approaches to the DM considered in this paper are, in fact, distributions (see eq. (1) for the ETF DM and ref. [8] for the discussion of the NV and CB cases) and consequently, the only meaningful comparison should be done through the moments in $k$ and $R$ spaces.

On the other hand, the semiclassical approaches to the DM are obtained by switching off shell effects. Consequently, the Slater and ETF approximations to the DM should be compared with the smoothed DM obtained using the Strutinsky averaged occupation numbers [19] rather than with the quantal DM. To do this, one starts from the smooth distribution function, which for closed HO shells reads [20]:

$$\tilde{f}_{St}(\mathbf{R}, \mathbf{p}) = 8 \sum_{K} (-1)^K \tilde{n}_K \exp^{-\varepsilon} L^2_{K}(2\varepsilon),$$

where $\varepsilon = \frac{p^2}{m} + m\omega^2 R^2$, $L^0_K$ are the generalized Laguerre polynomials and $\tilde{n}_K$ the Strutinsky occupation numbers [19]. Performing the inverse Wigner transform of (24) and averaging over the angles, one obtains the Strutinsky DM in coordinate space to which the semiclassical approximations (Slater and ETF) should be compared.

$$\tilde{\rho}_{St}(\mathbf{R}, s) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \tilde{f}_{St}(\mathbf{R}, \mathbf{p}) e^{i\mathbf{p}s/\hbar^3} \alpha^2 \sum_{K=0}^{\infty} (-1)^K L^{1/2}_{K_1} L^{1/2}_{K-K_1} \frac{\alpha^2 s^2}{2},$$

where $\varepsilon = \frac{p^2}{m} + m\omega^2 R^2$, $L^0_K$ are the generalized Laguerre polynomials and $\tilde{n}_K$ the Strutinsky occupation numbers [19].
The NV and CB expansions of the DM can also be considered within the semiclassical framework if the $M_2$ moment is calculated in the ETF approach. From (18), it is clear that in this case NV and CB become truncations of the ETF density matrix. It is interesting to look at the quality of these approximations because they have been used for calculating the exchange part of the nucleus-nucleus potential (see [21] and references quoted therein).

The Strutinsky DM [23] for $^{40}$Ca is obtained with a HO parameter $\alpha=0.516$ fm$^{-1}$ and with a smoothing parameter [13, 19] $\gamma=1.25$ $\hbar \omega$. Figure 2 collects the semiclassical results where the ratio $\tilde{\rho}(R, s)/\rho(R)$ is displayed for the Strutinsky smoothed DM (black dots) and for the ETF DM (solid line) as well as for the semiclassical NV (dashed line) and CB (dashed-dotted line) truncations of the ETF DM. Notice that in order to completely remove the shell effects, the ETF, NV and CB density matrices have to be obtained using the Strutinsky local density [22]. From this Figure it can be seen that the ETF ratio reproduces reasonably well the Strutinsky result. The ETF quotient is better than the NV result in the whole range of $R$ and $s$ distances analyzed and better than the CB for small values of $R$. The difference between ETF and Strutinsky ratios indicates that the $\hbar$- expansion in ETF does not fully converged. Consequently, it would be necessary to add $\hbar^4$ contributions to the ETF DM to obtain ETF expectation values in good agreement with the corresponding Strutinsky results.

3 Restricted variational energy calculations

The second part of this paper is devoted to discussion of the ability of the ETF approach to the DM for describing the HF binding energy of finite nuclei when effective finite-range nuclear interactions are considered.

First, we derive the ETF approximation to the DM starting from the non-local HF potential:

$$V^{HF}(r, r') = V^H(r, r')\delta(r - r') - V^F(r, r'),$$

(26)

where $V^H$ and $V^F$ are the direct and exchange parts of the HF potential. In Wigner representation eq. (26) becomes:

$$V(R, k) = V_{dir}(R) - V_{ex}(R, k),$$

(27)

where

$$V_{dir}(R) = \int dR' v(R, R')\rho(R')$$

(28)
\[
V_{\text{ex}}(\mathbf{R}, \mathbf{k}) = g \int \frac{d\mathbf{k}'}{(2\pi)^3} w(\mathbf{k}, \mathbf{k}') f(\mathbf{R}, \mathbf{k}').
\] (29)

In these equations \(v(\mathbf{R}, \mathbf{R}')\) is the two-body effective interaction, \(w(\mathbf{k}, \mathbf{k}')\) is its Fourier transform and \(g\) stands for the degeneracy (for the sake of simplicity we consider a simple Wigner force in eqs. (28) and (29)). Consequently, the Wigner transform of the one-body Hamiltonian will be;

\[
H_W(\mathbf{R}, \mathbf{k}) = \frac{\hbar^2 k^2}{2m} + V(\mathbf{R}, \mathbf{k}).
\] (30)

If the HF potential is spherically symmetric in \(\mathbf{k}\), i.e. \(V(\mathbf{R}, \mathbf{k})\), the WK distribution function required for semiclassical calculations is \[13\];

\[
\tilde{f}_{WK}(\mathbf{R}, k) = \frac{1}{4\pi} \int f_{WK}(\mathbf{R}, k) d\Omega_k
\]

\[= \Theta(\lambda - H_W) - \frac{\hbar^2}{8m} \delta'(\lambda - H_W) F_1(\mathbf{R}, k) + \frac{\hbar^2}{24m} \delta''(\lambda - H_W) F_2(\mathbf{R}, k), \] (31)

where the functions \(F_1(\mathbf{R}, k)\) and \(F_2(\mathbf{R}, k)\) are given by:

\[
F_1(\mathbf{R}, k) = \frac{\hbar^2}{3m} \frac{m}{\hbar^2} \Delta V (3f + kf_k) - k^2(\nabla f)^2 \]

\[F_2(\mathbf{R}, k) = \frac{\hbar^2}{3m} \left( \frac{m}{\hbar^2} \nabla V \right)^2 (3f + kf_k) + k^2 f^2 \Delta V - 2k^2 f \nabla V \nabla f. \] (32)

In eqs. (32-33), \(f\) is the inverse of the position and momentum dependent effective mass:

\[
f(\mathbf{R}, k) = \frac{m}{m^*(\mathbf{R}, k)} = 1 + \frac{m}{\hbar^2 k} V_{\text{ex}, k}(\mathbf{R}, k), \] (34)

where the subscript \(k\) indicates a partial derivative with respect to \(k\).

Due to the fact that the effective-mass corrections are included in the \(\hbar^2\) part of the distribution function \[31\], they are calculated using the \(\hbar^0\) order exchange potential in eq. \[34\] to be consistent with the \(\hbar\)-order in the expansion of the WK distribution function.

Following the steps indicated in the Appendix, the ETF density matrix for each kind of nucleon in the case of a non-local potential can be written as:

\[
\tilde{\rho}(\mathbf{R}, s) = \rho \left\{ \frac{3j_1(k_F s)}{k_F s} + \frac{s^2}{216} \left\{ \left( 9 - 2k_F \frac{f_k}{f} - 2k^2_f \frac{f_{kk}}{f^2} + k^2_f \frac{f_{kk}}{f^2} \right) \frac{j_1(k_F s)}{k_F s} - 4j_0(k_F s) \right] \frac{(\nabla \rho)^2}{\rho} \right\}
\]

\[\quad - \left[ (18 + 6k_F \frac{f_k}{f}) \frac{j_1(k_F s)}{k_F s} - 3j_0(k_F s) \right] \Delta \rho - \left[ 18 \rho \frac{\Delta f}{f} + (18 - 6k_F \frac{f_k}{f}) \frac{\nabla \rho \cdot \nabla f}{f} + 12k_F \frac{\nabla \rho \cdot \nabla f_k}{f} - 9 \rho \frac{(\nabla f)^2}{f^2} \frac{j_1(k_F s)}{k_F s} \right], \] (35)

\[10\]
where now \( k_F = (3\pi^2\rho)^{1/3} \) and the inverse effective mass \( f \) and its derivatives are computed at \( k = k_F \). We use here \( g=2 \) because in this way the ETF DM eq.\((34)\) can be directly applied to non-symmetric nuclei.

If all the spatial and momentum derivatives of the inverse effective mass are dropped in eq.\((34)\) one recovers the ETF DM for the local case eq.\((11)\). If only the momentum derivatives of \( f \) are eliminated, one obtains the ETF DM corresponding to the case of a position-dependent effective mass. This latter case is just the situation that appears when one uses zero-range forces such as the Skyrme interactions.

The next step is to obtain the ETF approach to the HF energy, which for an uncharged and spin-saturated nucleus can be written as:

\[
E_{HF} = \sum_q \int dR \left[ \frac{\hbar^2}{2m} \tau_{ETF}(R) + \frac{1}{2} \rho(R) V_{dir}(R) - \frac{1}{2} \int ds V_{ex}(R,s) \rho(R + \frac{s}{2}, R - \frac{s}{2}) \right]_q, \tag{36}
\]

where the subindex \( q \) stands for each kind of nucleon.

The HF energy in the ETF approximation is obtained as explained in the Appendix and reads:

\[
\tilde{E}_{ETF} = \sum_q \int dR \left[ \frac{\hbar^2}{2m} \tau_{ETF}(R) + \frac{1}{2} \rho(R) V_{dir}(R) - \varepsilon_{ex}^{ETF}(R) \right]_q. \tag{37}
\]

In this equation \( \tau_{ETF}(R) \) is the kinetic energy up to \( \hbar^2 \) order for each kind of nucleon in the ETF approximation and reads

\[
\tau_{ETF}(R) = \tau_{ETF,0}(R) + \tau_{ETF,2}(R)
= \frac{3}{5} k_F^2 \rho + \frac{1}{36} \frac{\nabla \rho}{\rho} \left[ 1 + \frac{2}{3} k_F \frac{f_k}{f} + \frac{2}{3} k_F^2 \frac{f_{kk}}{f^2} - \frac{1}{3} \frac{k_F^2 f_k}{f^2} \right] + \frac{1}{12} \Delta \rho [4 + \frac{2}{3} k_F f_k]
+ \frac{1}{6} \rho \frac{\Delta f}{f} + \frac{1}{6} \frac{\nabla \rho \cdot \nabla f}{f} \left[ 1 - \frac{1}{3} k_F \frac{f_k}{f} \right] + \frac{1}{9} \frac{\nabla \rho \cdot \nabla f}{f} - \frac{1}{12} \rho \left( \frac{\nabla f}{f} \right)^2, \tag{38}
\]

and \( \varepsilon_{ex}^{ETF}(R) \) is the exchange energy density for each kind of nucleon in the same approximation given by

\[
\varepsilon_{ex}^{ETF}(R) = \varepsilon_{ex,0}^{ETF}(R) + \varepsilon_{ex,2}^{ETF}(R) = \frac{1}{2} \rho(R) \int ds v(s) \frac{9 j^2_{f}(k_F s)}{k_F^2 s^2}
+ \frac{\hbar^2}{2m} [(f - 1) (\tau_{ETF} - \frac{3}{5} k_F^2 \rho - \frac{1}{4} \Delta \rho) + k_F f_k (\frac{1}{27} \frac{(\nabla \rho)^2}{\rho} - \frac{1}{36} \Delta \rho)], \tag{39}
\]

where \( v(s) \) is the central nucleon-nucleon interaction, \( k_F = (3\pi^2\rho)^{1/3} \) and \( f \) and its \( k \) derivatives are calculated at \( k = k_F \). For Gaussian type forces such as the Gogny or Brink-Boeker interac-
tions used in this paper, the explicit form of the lowest order exchange energy \( \varepsilon_{\text{ex,0}}^{\text{ETF}}(R) \) can be found in ref. [23].

In the special case of a local potential the \( h^2 \) part of the kinetic energy density eq. (38) reduces to the well-known result

\[
\tau_{\text{ETF,2}} = \frac{1}{36} \frac{(\nabla \rho)^2}{\rho} + \frac{1}{3} \Delta \rho,
\]

if the effective mass is not momentum dependent, one recovers the result of [15]

\[
\tau_{\text{ETF,2}} = \frac{1}{36} \frac{(\nabla \rho)^2}{\rho} + \frac{1}{3} \Delta \rho + \frac{1}{6} \frac{\nabla \rho \nabla f}{f} - \frac{1}{12} \frac{\rho (\nabla f)^2}{f^2}.
\]

For the particular case of the Coulomb potential, the direct calculation of the exchange energy density up to \( h^2 \) order in the ETF approach (local case) leads to

\[
\varepsilon_{\text{Coul,ex}}^{\text{ETF}} = -\frac{3}{4} \left( \frac{3}{\pi} \right)^{1/3} \rho^{4/3} - \frac{7}{432\pi(3\pi^2)^{1/3}} \frac{(\nabla \rho)^2}{\rho^{4/3}},
\]

where \( \rho \) is the proton density. Eq.(42) agrees with the result reported previously in [17].

As a first test of our ETF approach, let us compare the exchange Coulomb energy obtained using eq.(42) with the quantal result as well as the same energy derived through the NV, CB and Slater approximations to the DM. To this end and following ref. [11], we use HO wavefunctions with fixed parameters \( \alpha = 0.752 \text{ fm} \) for \(^4\text{He}\), \( 0.546 \text{ fm} \) for \(^{16}\text{O}\) and \( 0.481 \text{ fm} \) for \(^{40}\text{Ca}\). Table 1 shows the quantal (QM label), NV, CB, Slater (SL label) and ETF results for the exchange Coulomb energy. From this Table it can be seen that the ETF results almost reproduce the quantal values and improve those obtained using the NV, CB and Slater approximations.

### 3.1 Comparison with quantal results

In order to check the quality of our approach in the calculation of HF energies, we present here a restricted variational calculation for uncharged \(^4\text{He}\), \(^{16}\text{O}\) and \(^{40}\text{Ca}\) nuclei using the Brink-Boeker and Gogny forces. To this end we use HO wavefunctions and minimize with respect to the HO parameter \( \alpha = \sqrt{m\omega/\hbar} \).

At this point it should be noted that the semiclassical energy [37] (as well as that calculated in the simplest Slater approach) is free of shell effects if it is obtained using a smooth density [32]. Consequently, the semiclassical results should be compared rather with a HF calculation based on the smoothed Strutinsky density matrix [24] than with the purely quantal HF calculations.
However, a direct comparison with quantal results in the mean field approach is possible if shell effects are added to the semiclassical results (at Slater or ETF levels) according to the Strutinsky energy theorem. One possible way of incorporating shell-effects is based on the Kohn-Sham [24] approximation widely used in atomic physics [17] and discussed for the nuclear case in [25]. Basically the KS approach consists of solving the quantal HF equation using a local effective potential obtained as a functional derivative of the density-dependent exchange-correlation energy. In our restricted variational calculation the Kohn-Sham scheme is applied by minimizing the sum of the quantal kinetic plus direct energies with the semiclassical (Slater or ETF) exchange energy eqs.(39).

The exact quantal energies (corrected from the centre-of-mass motion) are obtained from eq.(36) with the DM evaluated analytically [26] (however, see below for the special case of closed HO shells) together with its corresponding root mean square radius (RMSR) \( <r^2>^{1/2} \). These quantities are displayed in Table 2 with the label QM for the Brink-Boeker and Gogny force. Table 2 also shows the same results obtained using the NV and CB truncations of the quantal DM (labelled NV and CB respectively). The binding energies and RMSR obtained within the KS scheme starting from the semiclassical Slater or ETF exchange energies eq.(39) are also collected in Table 2 with the SL(KS) and ETF(KS) labels. The differences between the KS (Slater and ETF) results and the purely quantal ones show the quality of the semiclassical approach to the exchange energy. From this comparison one can see that the Slater approach is very poor in the case of the Brink-Boeker force, underbinding all of the considered nuclei and giving RMSR larger than the quantal values. However, the result is more satisfactory for the Gogny force. This difference is due to the fact that the non-local effects are larger in the Brink-Boeker force than in the Gogny case. The non-local effects are better accounted for in the ETF(KS) approximation for which agreement with the quantal HF results is good for both effective forces considered in this paper. The ETF results in the KS scheme are similar to those obtained using the NV and CB approximations to the quantal DM for both Brink-Boeker and Gogny interactions.

As has been pointed out in Section 2, the NV and CB truncations of the quantal DM become truncations of the ETF DM if the \( M_2 \) momentum weighted integrals are also computed with the same ETF approach [17]. To check the quality of these approximations to the ETF DM, we
have again computed the binding energies and RMSR using the NV and CB truncations of the ETF DM within the KS scheme. The corresponding results are also collected in Table 2 with the NV(KS) and CB(KS) labels. From the analysis of the KS results it can be seen that the agreement of NV(KS) and CB(KS) with ETF(KS) is similar to the one found comparing the NV and CB results with the QM values. On the other hand, this agreement improves when the non-locality of the effective force is smaller. From Table 2 it can also be seen that the ETF(KS) energies and RMSR agree better with the corresponding quantal results than the NV(KS) and CB(KS) values.

Some time ago another different approximation was presented in the literature [27]. In this approach rather than starting from first principles, a phenomenological density matrix is proposed in which the parameters were determined by imposing the correct local semiclassical kinetic energy density and the projector character of the DM in an integrated form. Using this parametrized DM and the Gogny interaction, the binding energy of $^{16}O$ and $^{40}Ca$ (including the Coulomb energy) are $-128.3\text{MeV}$ and $-337.9\text{MeV}$ respectively. These results can be compared with the ones obtained in our ETF(KS) approach $-122.6\text{MeV}$ and $-335.2\text{MeV}$ and with the fully quantal results $-126.0\text{MeV}$ and $-338.4\text{MeV}$. The results obtained using the ETF(KS) approximation are slightly worse than those obtained with the phenomenological DM discussed previously, but clearly improve the CB results reported in [27], which are $-118.2\text{MeV}$ and $-326.4\text{MeV}$ for $^{16}O$ and $^{40}Ca$ respectively.

3.2 Comparison with Strutinsky results

Let us now discuss the quality of the Slater and ETF energies within the semiclassical framework. In this case they have to be compared with the ones obtained using the Strutinsky averaged method [19]. The starting point for a Strutinsky calculation of the energy using trial HO wavefunctions is the smooth density matrix [28] from which the particle and kinetic energy can also be derived. For an effective nuclear interaction with two Gaussian type form factors (as in the case of the forces studied in this paper) and HO closed shells, the direct and exchange energies can be obtained analytically:

$$E_{\text{dir}} = \sum_{i=1}^{2} \frac{16X_{d,i}}{\sqrt{\pi}} \left( \frac{\alpha^2}{\gamma_i} \right)^{3/2} \sum_{K=0}^{K_{\text{max}}} \sum_{M=0}^{K_{\text{max}}} \bar{n}_K \bar{n}_M \sum_{K_1=0}^{K} \sum_{M_1=0}^{M} L_{K-K_1}^{1/2}(0) L_{M-M_1}^{1/2}(0)$$
\[
\Gamma(K_1 + M_1 + \frac{3}{2}) \frac{(\frac{\alpha^2}{\gamma_i})^{K_1+M_1}}{K_1! M_1!} \left( F\left[-M_1, -K_1, -M_1 - K_1 - \frac{1}{2}, 1 - \frac{\gamma_i^2}{\alpha^2} (1 - \frac{\alpha^2}{\gamma_i})^2\right]\right) \]

(43)

\[
E_{exc} = \frac{2}{\pi} \frac{32}{\gamma_i} \frac{\alpha^2}{\gamma_i^{3/2}} \frac{\Delta K_{max} K_{max} - K K_{max} - K}{K_1 = 0} \frac{\Delta M_{max} M_{max} - K M_{max} - M}{M_1 = 0} \frac{\tilde{n}_K + K_i \tilde{n}_K + M_i}{K!} \frac{\Delta (K_1 + \frac{3}{2})}{K_1! M_1!} \left( 1 - \frac{\alpha^2}{\gamma_i} \right)^{K_1+M_1} \left( F\left[-M_1, -K_1, -M_1 - K_1 - \frac{1}{2}, 1 - \frac{\alpha^4}{\gamma_i^2} (1 - \frac{\alpha^2}{\gamma_i})^2\right]\right), \]

(44)

where \(\gamma_i = 2/\mu_i^2 + \alpha^2\) and \(F\) are the Gauss hypergeometric functions. In eqs.(43-44) \(X_{d,i} = w_i + b_i/2 - h_i/2 - m_i/4\) and \(X_{e,i} = w_i/4 + b_i/2 - h_i/2 - m_i\) are the usual combination of the direct and exchange parameters of the central effective interaction and \(\mu_i\) is the range of each Gaussian form factor.

The Strutinsky occupation numbers that come into in the energy calculation are obtained from a HO spectrum. In this way the smooth energy becomes a function of the HO length \(\alpha\). The Strutinsky energy is obtained by minimizing with respect to \(\alpha\) to simulate the self-consistency \[29\] with the additional constraint that the minimization procedure is performed in the plateau region \[13, 19\]. With a smoothing parameter \(\gamma = 1.25 \hbar \omega\), the HO parameters that minimize the Strutinsky energies of the \(^4\text{He}, ^{16}\text{O}\) and \(^{40}\text{Ca}\) nuclei are \(\alpha = 0.647, 0.550\) and \(0.509 \text{ fm}^{-1}\) respectively using the Brink-Boeker force and \(\alpha = 0.643, 0.567\) and \(0.516 \text{ fm}^{-1}\) in the case of the Gogny interaction. The binding energies and RMSR obtained in this way for uncharged \(^4\text{He}, ^{16}\text{O}\) and \(^{40}\text{Ca}\) nuclei are collected in Table 3 with the label ST. The semiclassical binding energies at Slater and ETF levels are computed starting from the Strutinsky particle density obtained previously in order to drop the shell effects completely \[22\]. These results are shown in Table 3 labelled SL and ETF(a) respectively.

The Strutinsky value represents the energy which varies smoothly with the number of nucleons \(A\). For each nucleus the difference between its quantal value QM reported in Table 2 and the corresponding ST result given in Table 3 is the so-called shell energy. This is a subtle quantity that is not reproduced by SL or ETF approaches up to \(\hbar^2\) order. As has been pointed out in previous literature, if the ETF kinetic energy density functional only contains the \(\hbar^0\) and \(\hbar^2\) contributions, its integral is not able to reproduce the Strutinsky kinetic energy at least in the case of a set of nucleons moving in a HO or Woods-Saxon type external potential. \[22\]. However, if the \(\hbar^4\) contributions are included in the functional, the ETF kinetic energies are in much better agreement with the Strutinsky values \[22, 28\]. In our non-local calculations the
differences found between Strutinsky and ETF (up to $\hbar^2$ order) total energies are roughly similar to those found for the kinetic energy in the case of an external HO potential \cite{28}. This fact suggests including approximately the $\hbar^4$ corrections to ETF by adding to $\tau_{\text{ETF}}$ which enters equations (38) and (39) the $\hbar^4$ contribution in the local potential case:

$$
\tau_4 = \frac{1}{6480}(3\pi^2)^{-2/3}\rho^{1/3}[24\left(\frac{\Delta \rho}{\rho}\right)^2 - 27\frac{\Delta \rho}{\rho}(\nabla \rho)^2 + 8(\nabla \rho)^4].
$$

(45)

From this approximated calculation we find that almost all the correction comes from the kinetic energy term, whereas the exchange part gives only a minor contribution. The total energy when this $\hbar^4$ correction is included perturbatively is shown in Table 3 labelled ETF($\hbar^4$). It can be seen that the Strutinsky binding energies are very well reproduced by this approximate ETF($\hbar^4$) calculation showing again the importance of including $\hbar^4$ corrections in ETF in order to obtain a better description of the shell energies \cite{22,28}.

For finite-range forces the non-local effects contribute to the DM (35) through the gradients and the derivative with respect to $k$ of the inverse effective mass calculated at $k = k_F = (6\pi^2\rho/g)^{1/3}$. To investigate the influence of these non-local corrections to the HF energy, we have again obtained this energy using the DM corresponding to a local potential (11). In this case, the kinetic energy reduces to that corresponding to the local case and the $\hbar^2$ exchange energy is calculated using (39) but with $\tau$ corresponding to the local case. The HF energies calculated in this way are also displayed in Table 2 with the label ETF(b). From these results it can be seen that, in fact, the $\hbar^2$ effective mass corrections to the DM (35) are almost negligible for the Gogny force but they become more important for the Brink-Boeker interaction where the non-local effects are larger.

4 Summary and Outlook

In this paper we have derived, for the first time to our knowledge, the Extended Thomas-Fermi approximation to the one-body density matrix up to $\hbar^2$-order for a non-local single particle Hamiltonian. The $\hbar^2$ contribution can be written in terms of spherical Bessel functions combined with second-order gradients of the local density and the inverse of the effective mass as well as momentum derivatives of the latter computed at the Fermi momentum. This density matrix includes, as particular cases, results reported previously in the literature \cite{17,18} for the local...
We have compared this new semiclassical approximation with former approaches, namely the Negele-Vautherin [9] and Campi-Bouyssy [11] ones. It is found that as in the case of the quantal density matrix, the Extended Thomas-Fermi approximation sums all the momentum weighted integrals [8], but with their quantal values replaced by their semiclassical counterparts. In this respect the Extended Thomas-Fermi approach differs from the Negele-Vautherin and Campi-Bouyssy approximations, which are truncations of the quantal density matrix. It should also be pointed out that if within the Negele-Vautherin and Campi-Bouyssy approaches the quantal momentum weighted integrals are replaced by their semiclassical counterparts, they become truncations of the Extended Thomas-Fermi density matrix.

We have applied this semiclassical approach for deriving the Hartree-Fock energy of a nucleus in the case of effective finite-range interactions. In this case the $\hbar^2$-order Extended Thomas-Fermi kinetic and exchange energies contain, in addition to the second-order gradients of the local density and inverse effective mass, new terms that account for the momentum dependence of the effective mass.

We have checked our Extended Thomas-Fermi approach to the Hartree-Fock energy by performing restricted variational calculations with the Gogny and Brink-Boeker effective forces of the binding energy of $^4He$, $^{16}O$ and $^{40}Ca$ using trial harmonic oscillator local densities. At a quantal level our Extended Thomas-Fermi approach up to $\hbar^2$-order to the exchange energy can be used within the Kohn-Sham scheme to obtain a local approximation to the non-local quantal energy density. It is found that this Kohn-Sham approach gives binding energies and root mean square radii similar to the corresponding results obtained using the Negele-Vautherin and Campi-Bouyssy truncations of the quantal density matrix.

We have also performed restricted variational Strutinsky averaged Hartree-Fock calculations with the same finite-range nuclear interactions. These results are compared with the pure Thomas-Fermi (Slater) and Extended Thomas-Fermi values obtained starting from the Strutinsky kinetic energy and particle densities. The Extended Thomas-Fermi binding energies including only $\hbar^2$-order contributions are not able to reproduce the Strutinsky results and consequently cannot be used for obtaining the shell energies. We have approximately estimated the $\hbar^4$-order contribution to the binding energy and verified that if this correction is taken into
account, the Strutinsky values are practically recovered.

Although the Extended Thomas-Fermi approach applied to a non-local one-body Hamiltonian gives reasonably good results, to improve this semiclassical approximation by adding the full $\hbar^4$-order contributions seems to be in order. Another way of improving the semiclassical results presented here to obtain the smooth part of the energy is by using the Variational Wigner-Kirkwood approach [15] which slightly differs from the Extended Thomas-Fermi approximation presented in this paper. We reserve these extensions of the semiclassical calculations in the non-local case for a future work.

On the other hand, other effective finite-range forces such as M3Y together with the Double Folded Model have been recently applied to compute the real part of the microscopic heavy-ion optical potential. In these calculations, the exchange part is usually obtained using the Negele-Vautherin or Campi-Bouyssy approaches to the density matrix with a semiclassical kinetic energy density [21]. To use the full Extended Thomas-Fermi density matrix to obtain the real part of the heavy-ion optical potential is another promising application of the method developed in this paper and will be presented in a forthcoming publication [30].

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Appendix

The WK density matrix up to $\hbar^2$ order (assuming degeneracy $g$) in coordinate space for a non-local potential is given by the inverse Wigner transform of (31)

$$\tilde{\rho}_{WK}(R, s) = g \int \frac{dk}{(2\pi)^3} \tilde{f}_{WK}(R, k) e^{iks} = \frac{gk^3}{6\pi^2} \frac{3j_1(kFs)}{kFs}$$

$$- \frac{gh^2}{16m\pi^2} \frac{\partial}{\partial \lambda} \int dk k^2 j_0(ks) F_1(R, k) \delta(\lambda - H_W)$$

$$+ \frac{gh^2}{48m\pi^2} \frac{\partial^2}{\partial \lambda^2} \int dk k^2 j_0(ks) F_2(R, k) \delta(\lambda - H_W)$$

that written in terms of the local Fermi momentum $k_F$ with the help of:

$$\delta(\lambda - H_W) = \frac{m}{\hbar^2 k_F f(R, k_F)}$$

and

$$\frac{\partial \lambda}{\partial k_F} = \frac{\hbar^2 k_F}{m} + V_k(R, k_F) = \frac{\hbar^2 k_F f(R, k_F)}{m}$$

reads

$$\tilde{\rho}_{WK}(R, s) = \frac{gk^3}{6\pi^2} \frac{3j_1(kFs)}{kFs} + j_0(kFs) \rho_{2, WK}(R)$$

$$+ \frac{g}{48\pi^2} \frac{\partial j_0(kFs)}{\partial k_F} \left[ \frac{m}{\hbar^2 k_F f(R, k_F)} \frac{d}{dk} \left[ \frac{kF_2}{f(R, k)} \right] + \frac{m}{\hbar^2} \frac{d}{dk} \left[ \frac{F_2}{f(R, k)^2} \right] \right]$$

$$- \frac{3kF_1}{f(R, k)} \Big|_{k=k_F} + \frac{g}{48\pi^2} \frac{\partial^2 j_0(kFs)}{\partial k_F^2} \left[ \frac{m}{\hbar^2 k_F f(R, k_F)} \right]^2 \left[ \frac{kF_2}{f(R, k)} \right] \Big|_{k=k_F},$$

where $\rho_{2, WK}$ is the WK $\hbar^2$-order contribution to the density in the non-local problem given in the Appendix A of [15] and the inverse effective mass $f(R, k)$ is defined as in eq.(34).

In eq.(49) the gradients of the non-local potential $V(R, k)$ appearing in $F_1(R, k), F_2(R, k)$ and their momentum derivatives have to be evaluated at $k = k_F$. To do this one starts from the definition of the Fermi energy:

$$\frac{\hbar^2 k_F^2}{2m} + V(R, k) = \lambda,$$  \hspace{1cm} (50)

where $k_F$ is also a function of $R$. Now taking the gradients of (50), the spatial derivatives of the potential are transformed into gradients of the local Fermi momentum through:

$$(\nabla V)_{k_F} + \frac{\hbar^2 k_F}{m} f(R, k_F) \nabla k_F = 0$$
\[
(\Delta V)_{k_F} + \frac{\hbar^2}{2m}(k_F f(R, k_F)\Delta k_F + f(R, k_F)(\nabla k_F)^2 + 2k_F \nabla f(R, k_F)\nabla k_F + k_F f_k(R, k_F)(\nabla k_F)^2) = 0.
\]

To obtain the ETF DM one proceeds as in the local potential case. First the WK local density up to \(\hbar^2\)-order is inverted to obtain

\[
k_F = k_0 - \frac{2\pi^2}{g k_0^2} \rho_{2, WK}[k_0],
\]

where \(k_0\) is the zeroth order local Fermi momentum given by \(k_0 = (6\pi^2 \rho/g)^{1/3}\) and the gradients of \(V\) that appear in \(\rho_{2, WK}\) have been replaced by gradients of \(k_0\) with the help of eqs. (51 - 52).

Finally, expanding \(k_F\) in the WK DM (49) with the help of (53) one obtains the ETF density matrix written as

\[
\tilde{\rho}_{ETF} = \frac{g k_0^3}{6\pi^2} \frac{3 j_1(k_0 s)}{k_0 s} + \frac{g k_0^2}{144\pi^2} \left[ \left( 7 + 6k_0 \frac{f_k}{f} + 2k_0^2 \frac{f_{kk}}{f} - k_0^2 \frac{f_k^2}{f^2} \right) \frac{(\nabla k_0)^2}{k_0} + (4 + 2k_0 \frac{f_k}{f}) \Delta k_0 \right.
\]

\[
+ (6 - 2k_0 \frac{f_k}{f}) \frac{\nabla f \nabla k_0}{f} + 4k_0 \frac{\nabla f_k \nabla k_0}{f} + 2k_0 \frac{\Delta f}{f} - k_0 \frac{(\nabla f)^2}{f} \right] \frac{d j_0(k_0 s)}{d(k_0 s)}
\]

\[
+ \frac{g k_0^2 s^2}{144\pi^2} \left[ 2 \frac{(\nabla k_0)^2}{k_0} - \Delta k_0 \right] \frac{d^2 j_0(k_0 s)}{d^2(k_0 s)}. \tag{54}
\]

If now the gradients of \(k_0\) are written in terms of gradients of the density using eqs. (8 - 9) one obtains the ETF DM for a non-local potential written as a functional of the local density which is just (35).

The HF energy of an uncharged and spin-saturated nucleus in the ETF approximation can be obtained by replacing the quantal integrand in (36) by its corresponding ETF approximation. The ETF kinetic energy density can be derived from the ETF DM using [13]

\[
\tau_{ETF}(R) = \left( \frac{1}{4} \Delta_R - \Delta_s \right) \tilde{\rho}_{ETF}(R, s)|_{s=0}
\]

from where eq. (38) is easily obtained.

The direct energy is obtained using the the diagonal part of the DM that in the ETF approach reduces simply to the local density \(\rho\).
The exchange potential is given by $V_{ex}(R, s) = v(s)\tilde{\rho}(R, s)$ and, consequently, the ETF exchange energy will be

$$
\varepsilon_{ex}^{ETF}(R, s) = \frac{1}{2} \int ds V_{ex}^{ETF}(R, s) \tilde{\rho}_{ETF}(R, s)
$$

$$
= \frac{1}{2} \int ds v(s) \left[ \tilde{\rho}_{ETF,0}^2(R, s) + 2\tilde{\rho}_{ETF,0}(R, s)\tilde{\rho}_{ETF,2}(R, s) \right]
$$

$$
= \frac{1}{2} \rho^2(R) \int ds v(s) \frac{9j_0^2(k_F s)}{(k_F s)^2} + \frac{1}{2} \int ds V_{ex,0}^{ETF}(R, s) \tilde{\rho}_{ETF,2}(R, s). \quad (56)
$$

The integral over $s$ in the $h^2$ contribution to the ETF exchange energy can be performed analytically taking into account the fact that in Wigner space the $h^0$ ETF exchange potential (Slater) can also be written as

$$
V_{ex,0}^{ETF}(R, k) = \int ds V_{ex,0}^{ETF}(R, s) e^{-iks} = \int ds v(s) \tilde{\rho}_0(R, s)j_0(ks) \quad (57)
$$

if the exchange potential is spherically symmetric in $k$.

The $k$ derivatives calculated at $k = k_0$ are easily obtained starting from (57):

$$
V_{ex,0,k}(R, k_0) = \int ds v(s) \tilde{\rho}_0(R, s) s \frac{dj_0(ks)}{d(ks)} = \frac{\hbar^2 k(f - 1)}{m} \bigg|_{k = k_0} \quad (58)
$$

$$
V_{ex,0,kk}(R, k_0) = \int ds v(s) \tilde{\rho}_0(R, s) s^2 \frac{d^2j_0(ks)}{d(ks)^2} = \frac{\hbar^2 (f + k f_k - 1)}{m} \bigg|_{k = k_0}. \quad (59)
$$

With the help of eqs. (58) and (59) the integral over $s$ of the $h^2$ part of (56) can be done obtaining

$$
\varepsilon_{ex,2}(R) = \frac{\hbar^2 k_0^2}{36m\pi^2} \left\{ (f - 1) \left[ (9 + 6k_0 \frac{f_k}{f} + 2k_0^2 \frac{f_k}{f} - k_0^2 \frac{f_k^2}{f^2}) \left( \nabla k_0 \right)^2 + (3 + 2k_0 \frac{f_k}{f}) \Delta k_0 \right. \right.
$$

$$
+ \left. (6 - 2k_0 \frac{f_k}{f}) \frac{\nabla f \nabla k_0}{f} + 4k_0 \frac{\nabla f_k \nabla k_0}{f} + 2k_0 \frac{\Delta f}{f} - k_0 \frac{(\nabla f)^2}{f} \right] \right. \right.
$$

$$
\left. + \left. k_0 f_k \left[ 2 \left( \frac{(\nabla k_0)^2}{k_0} - \Delta k_0 \right) \right] \right\}. \quad (60)
$$

Using this equation and replacing the gradients of $k_0$ by gradients of $\rho$ with the help of (38-39) together with the ETF kinetic energy density given by (38), the $h^2$ contribution to the exchange energy in the ETF approximation can be recast in the form given in eq. (39).
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FIGURE CAPTIONS

Figure 1. Ratio of off-diagonal to diagonal quantal density matrix $\rho(\mathbf{R} + s/2, \mathbf{R} - s/2)/\rho(\mathbf{R})$ for $^{40}\text{Ca}$ as a function of the interparticle distance $s$ for some values of the centre-of-mass distance $R$ (in fm). The different curves appearing in the Figure are explained in the text.

Figure 2. Ratio of off-diagonal to diagonal semiclassical density matrix $\rho(\mathbf{R} + s/2, \mathbf{R} - s/2)/\rho(\mathbf{R})$ for $^{40}\text{Ca}$ as a function of the interparticle distance $s$ for some values of the centre-of-mass distance $R$ (in fm). The different curves appearing in the Figure are explained in the text.
TABLE CAPTIONS

Table 1. Extended Thomas-Fermi (ETF) Coulomb exchange energies for $^4$He, $^{16}$O and $^{40}$Ca compared with the quantal (QM), Slater (SL), Negele-Vautherin (NV) and Campi-Bouyssy (CB) values reported in ref. [11].

Table 2. Total quantal binding energies and root mean square radius for $^4$He, $^{16}$O and $^{40}$Ca obtained quantally (QM) and using the different approximations described in the text.

Table 3. Total binding energies and root mean square radius for $^4$He, $^{16}$O and $^{40}$Ca obtained from the Strutinsky averaged method (ST) and with the different Extended Thomas-Fermi approaches described in the text.
## TABLE I

|         | $^4He$ | $^{16}O$ | $^{40}Ca$ |
|---------|--------|----------|----------|
| QM      | -0.86  | -2.98    | -7.46    |
| NV      | -0.47  | -2.31    | -6.42    |
| CB      | -0.78  | -2.75    | -7.03    |
| SL      | -0.74  | -2.75    | -7.05    |
| ETF     | -0.82  | -2.89    | -7.31    |

## TABLE II

|         | $^4He$  | $^{16}O$  | $^{40}Ca$  |
|---------|---------|-----------|------------|
|         | $E < r^2 >^{1/2}$ | $E < r^2 >^{1/2}$ | $E < r^2 >^{1/2}$ |
|         | (MeV)   | (fm)      | (MeV)      | (fm)  | (MeV)      | (fm)  |
| QM      | -28.24  | 1.72      | -106.62    | 2.65  | -323.98    | 3.36  |
| NV      | -23.69  | 1.86      | -100.32    | 2.71  | -313.49    | 3.40  |
| CB      | -25.61  | 1.80      | -101.96    | 2.70  | -315.22    | 3.39  |
| NV(KS)  | -21.75  | 1.89      | -97.55     | 2.73  | -309.42    | 3.41  |
| CB(KS)  | -22.39  | 1.87      | -98.27     | 2.72  | -310.10    | 3.40  |
| SL(KS)  | -17.51  | 2.00      | -87.85     | 2.79  | -291.78    | 3.45  |
| ETF(KS) | -23.78  | 1.82      | -101.61    | 2.69  | -317.11    | 3.38  |

|         | $^4He$  | $^{16}O$  | $^{40}Ca$  |
|---------|---------|-----------|------------|
|         | $E < r^2 >^{1/2}$ | $E < r^2 >^{1/2}$ | $E < r^2 >^{1/2}$ |
|         | (MeV)   | (fm)      | (MeV)      | (fm)  | (MeV)      | (fm)  |
| QM      | -29.66  | 1.88      | -138.07    | 2.63  | -406.47    | 3.34  |
| NV      | -28.53  | 1.91      | -135.72    | 2.65  | -402.68    | 3.36  |
| CB      | -29.04  | 1.90      | -136.31    | 2.64  | -403.22    | 3.36  |
| NV(KS)  | -27.41  | 1.93      | -133.65    | 2.65  | -399.57    | 3.36  |
| CB(KS)  | -27.53  | 1.93      | -133.80    | 2.65  | -399.62    | 3.36  |
| SL(KS)  | -25.80  | 1.96      | -129.49    | 2.67  | -392.33    | 3.37  |
| ETF(KS) | -29.05  | 1.91      | -135.38    | 2.64  | -402.66    | 3.35  |
|       | $^4\text{He}$ | $^{16}\text{O}$ | $^{40}\text{Ca}$ |
|-------|--------------|----------------|-----------------|
|       | $E$ (MeV)    | $<r^2>^{1/2}$ (fm) | $E$ (MeV) | $<r^2>^{1/2}$ (fm) | $E$ (MeV) | $<r^2>^{1/2}$ (fm) |
| ST    | -16.71       | 1.94           | -89.15        | 2.75           | -296.79   | 3.42         |
| SL    | -22.77       | 1.94           | -97.73        | 2.75           | -307.94   | 3.42         |
| ETF(a)| -22.51       | 1.94           | -98.06        | 2.75           | -310.51   | 3.42         |
| ETF(b)| -21.71       | 1.94           | -96.20        | 2.75           | -307.03   | 3.42         |
| ETF($\bar{h}^4$)| -17.64  | 1.94       | -90.19        | 2.75           | -298.71   | 3.42         |

|       | $^4\text{He}$ | $^{16}\text{O}$ | $^{40}\text{Ca}$ |
|-------|--------------|----------------|-----------------|
|       | $E$ (MeV)    | $<r^2>^{1/2}$ (fm) | $E$ (MeV) | $<r^2>^{1/2}$ (fm) | $E$ (MeV) | $<r^2>^{1/2}$ (fm) |
| ST    | -22.95       | 1.95           | -125.14        | 2.67           | -386.44   | 3.37         |
| SL    | -31.85       | 1.95           | -140.59        | 2.67           | -409.45   | 3.37         |
| ETF(a)| -27.78       | 1.95           | -133.39        | 2.67           | -398.18   | 3.37         |
| ETF(b)| -27.60       | 1.95           | -132.85        | 2.67           | -397.22   | 3.37         |
| ETF($\bar{h}^4$)| -23.67  | 1.95       | -125.30        | 2.67           | -386.07   | 3.37         |
