

THE EXTENDED THOMAS-FERMI MODEL AT FINITE TEMPERATURE

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Résumé - Le modèle ETF est généralisé à des températures finies pour un système de Fermions avec une masse effective variable. Pour la première fois, la fonctionnelle $\tau[\rho]$ correspondante est présentée elle contient tous les termes de l'ordre \hbar^2 d'une façon consistente.

Abstract - We generalize the ETF model to finite temperature for a system of Fermions with variable effective mass. For the first time we present the corresponding functional $\tau[\rho]$ which contains consistently all terms of order \hbar^2 .

The kinetic energy density functional $\tau_{\text{ETF}}[\rho]$, derived within the extended Thomas-Fermi (ETF) model /1,2,3/ has been widely used in several branches of physics /4/ and recently also been successfully applied in density variational calculations for average nuclear ground-state properties and deformation energies /5,6/. Its generalization to excited nuclear systems at temperatures $T > 0$, which are of growing interest both in heavy ion /7/ and astrophysics /8,9/, has so far only been realized in approximate ways. Either one used just the pure TF approximation /8,10/ or the low-temperature expansion /11,12/, or an ad hoc combination /13,14/ of the TF functional plus the gradient correction terms known from the $T = 0$ case.

In the present note we shall derive the functionals for the kinetic energy density $\tau[\rho]$ and the entropy density $\sigma[\rho]$ appropriate to the $T > 0$ case, consistently up to second order in \hbar^2 . For the sake of a simpler presentation, we restrict ourselves first to the case of a purely local potential $V(\vec{r})$ and discuss nonlocalities at the end.

We start from the well-known expressions for the entropy, the intrinsic and the free (Helmholtz) energy of a system on noninteracting Fermions in an external potential:

$$S = \int d^3r \sigma(\vec{r}) = -\sum_i [n_i \ln n_i + (1-n_i) \ln (1-n_i)], \quad (1)$$

$$E = \int d^3r \mathcal{E}(\vec{r}) = \sum_i \varepsilon_i n_i, \quad (2)$$

$$F = \int d^3r \mathcal{F}(\vec{r}) = E - TS, \quad (3)$$

where ε_i are the single particle (s.p.) energies and n_i the Fermi occupation numbers

$$n_i = \left[1 + \exp\left(\frac{\lambda - \varepsilon_i}{T}\right) \right]^{-1} \quad (4)$$

with the chemical potential λ . (We use $k \equiv 1$ and express the temperature T in units of MeV.) We also write in the usual way the spatial density $\rho(\vec{r})$ and the kinetic energy densities $\tau(\vec{r})$ and $\tau^*(\vec{r})$ in terms of the s.p. wavefunctions $\varphi_i(\vec{r})$:

$$\rho(\vec{r}) = \sum_i |\varphi_i(\vec{r})|^2 n_i, \quad (5)$$

$$\tau(\vec{r}) = \sum_i |\vec{\nabla} \psi_i(\vec{r})|^2 n_i, \quad (6)$$

$$\tau_*(\vec{r}) = -\sum_i \psi_i^*(\vec{r}) \Delta \psi_i(\vec{r}) n_i. \quad (7)$$

For systems with time reversal symmetry, the densities τ and τ_* are connected by

$$\tau(\vec{r}) = \tau_*(\vec{r}) + \frac{1}{2} \Delta \rho(\vec{r}). \quad (8)$$

Semiclassical approximations to the above quantities can most easily be obtained using the Bloch density $C(\vec{r}, \beta)$ which is related to the density $\rho(\vec{r})$ by an inverse Laplace transform:

$$\rho(\vec{r}) = \mathcal{L}_\lambda^{-1} \left[\frac{1}{\beta} C(\vec{r}, \beta) \right] = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{\lambda \beta} \frac{1}{\beta} C(\vec{r}, \beta) d\beta. \quad (c > 0) \quad (9)$$

Knowing that the transition from the $T = 0$ to the $T > 0$ case can be made by folding the $T = 0$ spectral density with the function $f_T(E) / 15/$:

$$f_T(E) = \frac{1}{4T} \text{Cosh}^{-2}(E/2T), \quad (10)$$

it is easy to realize that the Bloch density at $T > 0$ is given by

$$C(\vec{r}, \beta) = C_0(\vec{r}, \beta) \cdot \tilde{f}_T(\beta), \quad (11)$$

where $C_0(\vec{r}, \beta)$ is the Bloch density at $T = 0$ *

$$C_0(\vec{r}, \beta) = \sum_i |\psi_i(\vec{r})|^2 e^{-\beta \epsilon_i} \quad (12)$$

and $\tilde{f}_T(\beta)$ is the (two-sided!) Laplace transform of $f_T(E)$ eq. (10):

$$\tilde{f}_T(\beta) = \int_{-\infty}^{+\infty} e^{-\beta E} f_T(E) dE = \frac{\pi \beta T}{\sin(\pi \beta T)}. \quad (13)$$

Using simple rules of Laplace transforms, one finds the following expressions for the above defined densities:

$$\mathcal{F}(\vec{r}) = \lambda \rho(\vec{r}) - \mathcal{L}_\lambda^{-1} \left[\frac{1}{\beta^2} C(\vec{r}, \beta) \right], \quad (14)$$

$$\sigma(\vec{r}) = \frac{\partial}{\partial T} \mathcal{L}_\lambda^{-1} \left[\frac{1}{\beta^2} C(\vec{r}, \beta) \right], \quad (15)$$

$$\frac{\hbar^2}{2m} \tau_*(\vec{r}) = -\rho(\vec{r}) V(\vec{r}) - \mathcal{L}_\lambda^{-1} \left[\frac{1}{\beta} \tilde{f}_T(\beta) \frac{\partial}{\partial \beta} C_0(\vec{r}, \beta) \right]. \quad (16)$$

So far, all equations are exact, i.e. they contain the quantum-mechanical shell effects. We now replace the "cold" Bloch density $C_0(\vec{r}, \beta)$ by the one obtained in the Wigner-Kirkwood expansion /16/ up to second order in \hbar :

$$C_0^{WK}(\vec{r}, \beta) = C_{TF}(\vec{r}, \beta) \left\{ 1 + \frac{\hbar^2}{12m} \left[\frac{1}{2} \beta^2 (\vec{\nabla} V)^2 - \beta^2 \Delta V \right] \right\}, \quad (17)$$

*) Note that β is only a mathematical parameter here and does not have the meaning of an inverse temperature!

where the TF approximation has the form *)

$$G_{TF}(\vec{r}, \beta) = \frac{1}{4} \left(\frac{2m}{\pi \hbar^2} \right)^{3/2} \beta^{-3/2} e^{-\beta V(\vec{r})} \quad (18)$$

The inverse Laplace transforms can now be done analytically and yield the following densities

$$\rho(\vec{r}) = A_T \left\{ J_{3/2}(\eta) + \frac{1}{24} \frac{\hbar^2}{2m} \left[T^{-2} \Delta V J_{-3/2}(\eta) + \frac{3}{4} T^{-3} (\vec{\nabla} V)^2 J_{-5/2}(\eta) \right] \right\}, \quad (19)$$

$$\begin{aligned} \mathcal{F}(\vec{r}) = \lambda \rho(\vec{r}) - A_T \left\{ \frac{2}{3} T J_{3/2}(\eta) - \right. \\ \left. - \frac{1}{12} \frac{\hbar^2}{2m} \left[T^{-1} \Delta V J_{-1/2}(\eta) + \frac{1}{4} T^{-2} (\vec{\nabla} V)^2 J_{-3/2}(\eta) \right] \right\}, \quad (20) \end{aligned}$$

$$\begin{aligned} \frac{\hbar^2}{2m} \tau_x(\vec{r}) = A_T \left\{ T J_{3/2}(\eta) + \right. \\ \left. + \frac{1}{24} \frac{\hbar^2}{2m} \left[T^{-1} \Delta V J_{-1/2}(\eta) + \frac{3}{4} T^{-2} (\vec{\nabla} V)^2 J_{-3/2}(\eta) \right] \right\}, \quad (21) \end{aligned}$$

$$\begin{aligned} \sigma(\vec{r}) = -\eta \rho(\vec{r}) + A_T \left\{ \frac{5}{3} J_{3/2}(\eta) + \right. \\ \left. + \frac{1}{24} \frac{\hbar^2}{2m} \left[-T^{-2} \Delta V J_{-1/2}(\eta) + \frac{1}{4} T^{-3} (\vec{\nabla} V)^2 J_{-3/2}(\eta) \right] \right\} \quad (22) \end{aligned}$$

with

$$A_T = \frac{1}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} T^{3/2}. \quad (23)$$

The quantity η is given by

$$\eta = \frac{\lambda - V(\vec{r})}{T} \quad (24)$$

and $J_p(\eta)$ are the so-called Fermi integrals. For $p > -1$ they are defined by

$$J_p(\eta) = \int_0^{\infty} \frac{x^p}{1 + \exp(x - \eta)} dx \quad (p > -1) \quad (25)$$

For $p \leq -1$, the integral (25) does not exist. However we can extend the definition of $J_p(\eta)$ to $p < -1$ by the recurrence relation

*) All formulae hold for one kind of Fermions; a spin factor of 2 is included.

$$J_p(\eta) = \frac{1}{p+1} \frac{d}{d\eta} J_{p+1}(\eta), \quad (26)$$

which leads to well-behaved, continuous functions $J_p(\eta)$ for all values of p . Note that we do not encounter here the turning point problem which is well known in the $T = 0$ case: all the densities eqs. (19) - (22) are continuous and finite everywhere in space. Only in the limit $T \rightarrow 0$ will the semiclassical corrections with $J_p(\eta)$ for $p < -1$ diverge at the classical turning points given by $\eta = 0$. The functionals which we shall derive are thus rigorously defined in all space.

As in the $T = 0$ case, we now seek to eliminate the potential V (i.e. η) and its derivatives from the above equations, being consistent to order \hbar^2 relative to the TF terms. To this purpose we write

$$\rho = \rho_0 + \rho_2 = A_T J_{1/2}(\eta) + \rho_2. \quad (27)$$

We now solve eq. (27) for η writing

$$A_T J_{1/2}(\eta) = \rho - \rho_2 = A_T J_{1/2}(\eta_0 + \eta_2), \quad (28)$$

where η_0 is defined by inverting the equation

$$\rho = A_T J_{1/2}(\eta_0). \quad (29)$$

The fact that ρ_2 , which is of order \hbar^2 relative to ρ_0 , contains η does not disturb us: since η_2 will be of order \hbar^2 relative to η_0 , we can replace η by η_0 everywhere in ρ_2 of eq. (19), hereby neglecting only terms of order \hbar^2 . Expanding eq. (28) we find

$$\eta_2 = - \frac{2 \rho_2(\eta_0)}{J_{1/2}(\eta_0) \cdot A_T}. \quad (30)$$

The next step is to express the derivatives of the potential by those of the density, which is easily done after deriving twice the equation (29). The result is

$$A_T T^{-1} (\vec{\nabla} V)^2 = \frac{4 J_{1/2}(\eta_0)}{J_{1/2}^2(\eta_0)} \frac{(\vec{\nabla} \rho)^2}{\rho}, \quad (31)$$

$$A_T T^{-1} \Delta V = - \frac{2}{J_{1/2}(\eta_0)} \left[\Delta \rho + \frac{J_{1/2}(\eta_0) J_{3/2}(\eta_0)}{J_{1/2}^2(\eta_0)} \frac{(\vec{\nabla} \rho)^2}{\rho} \right]. \quad (32)$$

It is now just a matter of some algebra to expand eqs. (19) - (22) around η_0 , to collect all gradient terms and express them in terms of ρ using eqs. (31), (32). This leads us to the "ETF" functionals

$$\tau_{\text{ETF}}[\rho] = \tau_{\text{TF}}[\rho] + \tau_2[\rho], \quad (33)$$

$$\sigma_{\text{ETF}}[\rho] = \sigma_{\text{TF}}[\rho] + \sigma_2[\rho], \quad (34)$$

where the TF terms have the well-known form /10/

$$\frac{\hbar^2}{2m} \tau_{\text{TF}}[\rho] = A_T T J_{3/2}(\eta_0), \quad (35)$$

$$\sigma_{\text{TF}}[\rho] = -\eta_0 \rho + \frac{5}{3} A_T J_{3/2}(\eta_0), \quad (36)$$

and n_0 is given by solving eq. (29). Since only the integrals of the above densities are of final interest, we give below the expressions for the gradient corrections which one obtains after some suitable partial integrations. (The case of a variable effective mass, where integrals over τ_0 occur, will be discussed below.) These expressions are

$$\tau_2[\rho] = [\zeta(\eta_0) - \nu(\eta_0)] \frac{(\bar{\nabla}\rho)^2}{\rho} = \gamma(\eta_0) \frac{(\bar{\nabla}\rho)^2}{\rho}, \quad (37)$$

$$\sigma_2[\rho] = -\frac{1}{T} \frac{\hbar^2}{2m} \nu(\eta_0) \frac{(\bar{\nabla}\rho)^2}{\rho} \quad (38)$$

Hereby we have used the abbreviations

$$\zeta(\eta_0) = -\frac{J_{1/2}(\eta_0) J_{-3/2}(\eta_0)}{12 J_{-1/2}^2(\eta_0)}, \quad (39)$$

$$\nu(\eta_0) = \frac{3}{2} \zeta(\eta_0) - 36 [\zeta(\eta_0)]^2 + \frac{3}{8} \frac{J_{1/2}^2(\eta_0) J_{-5/2}(\eta_0)}{J_{-1/2}^3(\eta_0)} \quad (40)$$

$\tau_2[\rho]$ is similar to the Weizsäcker term, but with a n_0 -dependent (i.e. density dependent) coefficient. If one is only interested in the total free energy, one may use the following expressions

$$\mathcal{F}_{\text{TETF}}[\rho] = \mathcal{F}_{\text{TF}}[\rho] + \mathcal{F}_2[\rho], \quad (41)$$

$$\mathcal{F}_{\text{TF}}[\rho] = V\rho + T\eta_0\rho - \frac{2}{3}A_T T J_{3/2}(\eta_0), \quad (42)$$

$$\mathcal{F}_2[\rho] = \frac{\hbar^2}{2m} \zeta(\eta_0) \frac{(\bar{\nabla}\rho)^2}{\rho}. \quad (43)$$

We found that the function $\zeta(\eta_0)$ eq. (39) can be approximated to within less than 3 % for all values of η_0 by the expression

$$\zeta(\eta_0) \approx \frac{1}{36} \left[1 + \frac{2}{(1+e^{\eta_0})^{1/2}} \right]. \quad (44)$$

It is now interesting to study the limit $T \rightarrow 0$ of the above expressions. For that we have to distinguish two regions. Inside the classically allowed region, $\lambda > V(\vec{r})$ and thus η_0 will go to $+\infty$. We then can use the following asymptotic expansion of the $J_p(\eta_0)$ /17/

$$J_p(\eta_0) \approx \frac{1}{p+1} \eta_0^{p+1} \left[1 + p(p+1) \frac{\pi^2}{6} \eta_0^{-2} + \mathcal{O}(\eta_0^{-4}) \right]. \quad (45)$$

We find that in this case

$$\left. \begin{aligned} \zeta(\eta_0) &\xrightarrow{T \rightarrow 0} \frac{1}{36}, \\ \nu(\eta_0) &\xrightarrow{T \rightarrow 0} 0 \text{ as } T^2. \end{aligned} \right\} (\eta_0 > 0) \quad (46)$$

$$\left. \begin{aligned} \zeta(\eta_0) &\xrightarrow{T \rightarrow 0} \frac{1}{12}, \\ \nu(\eta_0) &\xrightarrow{T \rightarrow 0} 0 \text{ as } e^{\lambda/T} \quad (\lambda < 0). \end{aligned} \right\} (\eta_0 < 0) \quad (47)$$

We thus recover the well-known (corrected) Weizsäcker coefficient in $\tau_2[\rho]$. The result eq. (47) also is not surprising, since the entropy has to go to zero like T . Outside the classically allowed region, η_0 goes to $-\infty$ and we can use the asymptotic series for negative η_0 /17/

$$J_p(\eta_0) = \Gamma(p+1) \sum_{k=1}^{\infty} (-1)^{k-1} \frac{1}{k^{p+1}} e^{k\eta_0}. \quad (\eta_0 < 0) \quad (48)$$

In the limit $T \rightarrow 0$ we find herewith the result

$$\left. \begin{aligned} \zeta(\eta_0) &\xrightarrow{T \rightarrow 0} \frac{1}{12}, \\ \nu(\eta_0) &\xrightarrow{T \rightarrow 0} 0 \text{ as } e^{\lambda/T} \quad (\lambda < 0). \end{aligned} \right\} (\eta_0 < 0) \quad (49)$$

$$\left. \begin{aligned} \zeta(\eta_0) &\xrightarrow{T \rightarrow 0} \frac{1}{12}, \\ \nu(\eta_0) &\xrightarrow{T \rightarrow 0} 0 \text{ as } e^{\lambda/T} \quad (\lambda < 0). \end{aligned} \right\} (\eta_0 < 0) \quad (50)$$

Thus, $\sigma_2[\rho]$ goes to zero in all space, as it should. The coefficient in τ_2 is found to be different outside the classically allowed region from that inside by a factor of 3.

Note that in all derivations of $\tau_2[\rho]$ at $T = 0$ /1-3/, the classically forbidden region was not accessible; the functional derived in the classically allowed region was simply assumed to hold over all space by analytical continuation. From the above we now know that the form of the Weizsäcker correction τ_2 is also correct in the outside region, but the coefficient jumps at the turning point and is thus not analytical:

$$\tau_2[\rho] = \frac{(\bar{v}_p)^2}{p} \left[\frac{1}{36} \Theta(\lambda - \nu) + \frac{1}{12} \Theta(\nu - \lambda) \right]. \quad (T = 0) \quad (51)$$

If the functional eq. (51) is used to derive an Euler type variational equation (where V will be a functional of ρ , too), this discontinuity will have consequences which will be discussed elsewhere. For the present we note that in those applications where the energy is calculated from eq. (51) with a parametrized density ρ , it has very little influence whether one uses $1/36$ or the correct coefficient $1/12$ in the outside region, since in all realistic cases the turning point lies rather far in the tail of the density. (Typically, ρ is reduced to a few per milles of its central value at the turning point, see also fig. 1.) We have checked that the difference amounts to less than 1 MeV out of a total kinetic energy of several thousand MeV in medium and heavy nuclei.

For any finite temperature T , the functionals $\tau_2[\rho]$ eq. (37) and $\sigma_2[\rho]$ eq. (38) are well-behaved with analytical coefficients which can be readily computed. They depend explicitly on the temperature through the relation $\eta_0(\rho)$ eq. (29). As an illustration, we show in fig. 1 the coefficients $\nu(\eta_0)$ and $\gamma(\eta_0) = \zeta(\eta_0) - \nu(\eta_0)$ along with the density $\rho(r)$ as functions of the radius r at two temperatures, $T = 1$ and 4 MeV. (The parameters of $\rho(r)$ correspond to those found selfconsistently for the $N = 146$ neutrons in a spherical calculation for the nucleus ^{240}Pu with a realistic force.)

The case of a variable effective mass, as it is encountered in context with Skyrme type effective nucleon-nucleon interactions /18/, is dealt with exactly as above, except that some more algebra is required. We shall just quote the results here. Starting from the Hamiltonian

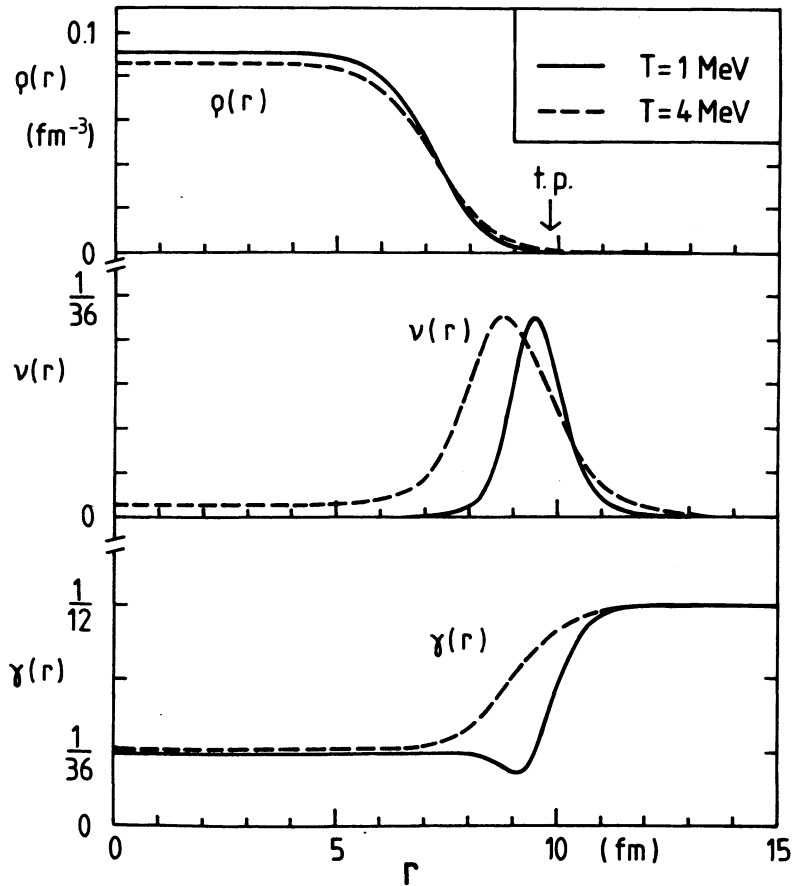


Fig. 1 - Density $\rho(r)$ and the coefficients γ and v of the gradient corrections eq. (37) and $\tau_2[\rho]$ eq. (38), plotted versus radius r at two temperatures: $T = 1$ MeV and $T = 4$ MeV. The arrow above the tail of the density indicates the location of the classical turning point (t.p.).

$$\hat{H} = -\frac{\hbar^2}{2m} \vec{\nabla} \cdot f(\vec{r}) \vec{\nabla} + V(\vec{r}), \quad (52)$$

we obtain the same TF expressions as above except that the mass m must be replaced everywhere by

$$m^*(\vec{r}) = m f^{-1}(\vec{r}). \quad (53)$$

The gradient corrections become, after suitable partial integrations:

$$f\tau_2[\rho] = \gamma(\eta_0) f \frac{(\vec{\nabla}\rho)^2}{\rho} + \delta(\eta_0) \rho \frac{(\vec{\nabla}f)^2}{f} + \frac{5}{12} f \Delta\rho + 3\zeta(\eta_0) \vec{\nabla}\rho \cdot \vec{\nabla}f, \quad (54)$$

$$T\sigma_2[\rho] = -\frac{\hbar^2}{2m} v(\eta_0) \left[f \frac{(\vec{\nabla}\rho)^2}{\rho} - \frac{9}{4} \rho \frac{(\vec{\nabla}f)^2}{f} \right], \quad (55)$$

where

$$\delta(\eta_0) = \frac{1}{4} \left[v(\eta_0) + 9\zeta(\eta_0) - \frac{7}{12} \right]. \quad (56)$$

The simplest form of the free energy density correction is

$$\begin{aligned} \mathcal{F}_2[\rho] = \frac{\hbar^2}{2m} \left\{ \zeta(\eta_0) f \frac{(\vec{\nabla}\rho)^2}{\rho} + \left[\frac{9}{4}\zeta(\eta_0) - \frac{7}{48} \right] \rho \frac{(\vec{\nabla}f)^2}{f} + \right. \\ \left. + \left[3\zeta(\eta_0) - \frac{5}{12} \right] \vec{\nabla}\rho \cdot \vec{\nabla}f \right\}. \end{aligned} \quad (57)$$

Note that when computing the total (free) energy with a Skyrme force, the integral over $f[\rho]$ contains not only the kinetic energy, but automatically also that part of the potential energy which contains τ_0 . (In this case, the term $V\rho$ in eq. (42) has to be replaced by the complete Skyrme potential energy density minus the τ_0 terms.)

It is readily seen that inside the classically allowed region, the coefficients of $f\tau_2$ eq. (54) reduce to the ones known in the $T = 0$ limit /2/. Including also a spin-orbit potential of the form

$$\hat{H}_{so} = -i \vec{W}(\vec{r}) \cdot (\vec{\nabla} \times \vec{\sigma}) \quad (58)$$

in the Hamiltonian, we found that one recovers the same form of the semiclassical corrections up to order \hbar^2 as in the $T = 0$ case /2/. Explicitly, we get for the spin-orbit density (see ref. /18/ for the definition)

$$\vec{j}[\rho] = -\vec{W} \frac{2m}{\hbar^2} \frac{1}{f} \rho \quad (59)$$

and for the spin-orbit contribution to the kinetic energy density

$$\tau_2^{so}[\rho] = \frac{1}{2} (\vec{W})^2 \left(\frac{2m}{\hbar^2} \right)^2 \frac{1}{f^2} \rho, \quad (60)$$

so that the total spin-orbit contribution to the energy density is (up to second order)

$$E_{so}[\rho] = -\frac{1}{2} (\vec{W})^2 \frac{2m}{\hbar^2} \frac{1}{f} \rho. \quad (61)$$

(See refs. /2,3/ for the detailed treatment of the spin-orbit and effective mass contributions in the $T = 0$ case.)

In a recent publication /14/ we have studied an approximation where the exact TF expressions at $T > 0$ were used together with the gradient correction terms $\tau_2[\rho]$ and $\tau_4[\rho]$ known from the $T = 0$ case /3/ (strictly valid only inside the classically allowed region). We found this approximate functional to give a fairly good reproduction of the results found in Hartree-Fock calculations at $T > 0$. It failed, however, in succeeding attempts to calculate fission barriers. This is mainly due to the fact that no correction $\sigma_2[\rho]$ to the entropy was included. (Its form could of course not be guessed from the $T = 0$ case.) This correction, and the correct coefficients of all gradient terms, turn out to be crucial for calculations of

deformation energies ^{*}).

We have used the above TETF functionals, including the "cold" correction $\tau_4[\rho]$, to compute the fission barrier of ^{240}Pu using the SkM* /6,19/ at various temperatures. For the details of the variational ETF calculations with parametrized trial densities, we refer to refs. /5,6/. Fig. 2 shows the results. The free deformation energy is plotted versus the elongation parameter c ; it is normalized to zero at sphericity ($c = 1.0$) for each temperature. We note that up to $T \approx 1$ MeV, the deformation energy does not change appreciably. The barrier disappears at $T \approx 4.5$ MeV.

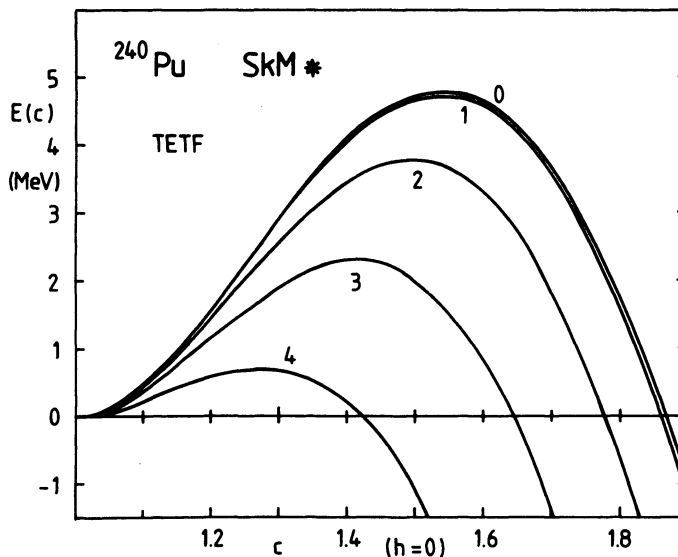


Fig. 2 - Fission barriers for ^{240}Pu obtained from a variational calculation using the TETF functionals eqs. (54) - (57) and the Skyrme force SkM* /19/. c is the elongation parameter (half diameter along symmetry axis in units of spherical radius). See ref. /6/ for the definition of deformed diffuse densities. The numbers indicate the temperature (in MeV).

This "critical temperature" is appreciably higher than what has been estimated before using the low- T expansion /11,12/. This expansion is only valid if $T \ll (\lambda - V)$, which however is never the case in the outer part of the nuclear surface, even at small temperatures. The fact that this approximation leads to a too strong decrease of the surface energy with increasing temperature has already been noted /14/. In Fig. 3 we plot the barrier height E_f (relative to the spherical minimum) versus temperature T .

The dashed line is the result of a corresponding calculation with the low- T -expanded functional, in which the only temperature dependent contribution is a term proportional to $\rho^{1/3} T^2$ (see e.g. refs. /6,13/). We see that it leads, indeed, to a drastic overestimation of the finite-temperature effect on the fission barrier height. The variation found with the present TETF functionals seems to be in accordance with the estimates based on HF calculations by Sauer et al. /20/, although an exact comparison cannot be made since a different Skyrme force has been used by these authors.

^{*}) That approximate functionals can work well for spherical systems but fail for deformation energies, is known also in the $T = 0$ case /6/.

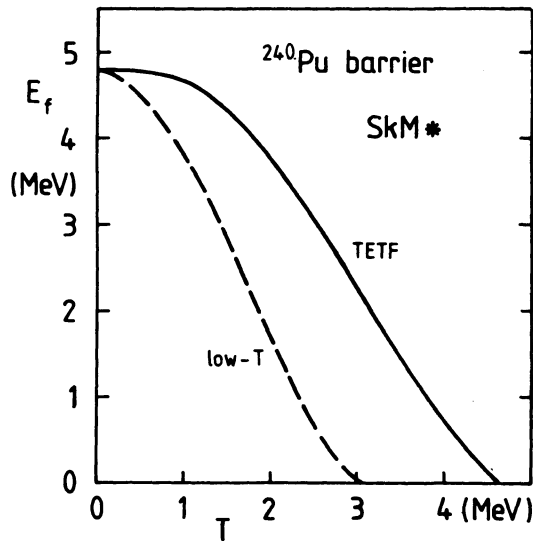


Fig.3 - Barrier height of ^{240}Pu versus temperature T . Solid line: TETF results from figure 2. Dashed line: corresponding result obtained with the low-temperature expanded functionals.

In summary, we have derived for the first time the TETF-functionals $\tau[\rho]$ and $\sigma[\rho]$ appropriate to the finite temperature case up to second order terms, including also the effects of a variable effective mass. The consistent treatment of all 4th order corrections will be hopelessly complicated, but the present results in which the "cold" correction $\tau_4[\rho]$ was used (and $\sigma_4[\rho]$ was neglected) seem encouraging. It will be the object of further studies to test these functionals against HF and other model results.

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