Extended Thomas-Fermi Model at Finite Temperature

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We derive for the first time second-order gradient corrections to the Thomas-Fermi kinetic-energy and entropy density functionals for a fermion system at finite temperature. Density variational calculations for a heated nucleus with a Skyrme interaction lead to excellent agreement with results of Hartree-Fock calculations.

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The gradient expansion of the kinetic-energy density functional obtained in the extended Thomas-Fermi (ETF) model[1] has found applications in many branches of physics.[2] For fermions moving in a local potential $V(\vec{r})$ at zero temperatures, it reads

$$\tau[\rho]=\kappa\rho^{5/3}+\tfrac{1}{36}(\nabla\rho)^2/\rho-\tfrac{1}{6}\Delta\rho+\tau_4[\rho], \quad (1)$$

where $\kappa=\frac{3}{5}(3\pi^2)^{2/3}$ (including a spin factor 2), and $\tau_4[\rho]$ contains up to fourth derivatives of the density ρ.[1,3,4] The expansion (1) does not allow reproduction of shell effects; it is, however, well suited for systems where the shell effects play an insignificant role or where they can be added perturbatively at the end of a variational calculation.[5] In the context of nuclear physics, it has been shown that the inclusion of the fourth-order gradient terms $\tau_4[\rho]$ is indispensible in order to yield both correct energies[4] and density profiles in variational calculations.[6] The expansion (1) is an asymptotic one. The sixth- and higher-order gradient terms diverge for densities which fall exponentially to zero, and must therefore be left out. A problem lies in the fact that all gradient corrections can only be calculated *inside* the classically allowed region defined by $\lambda > V(\vec{r})$ (λ is the Fermi energy). At the classical turning points and beyond, the semiclassical $\hbar$ expansion[1,7] of the densities $\rho(\vec{r})$ and $\tau(\vec{r})$ is not defined and the functional $\tau[\rho]$ cannot be determined. It has so far been *assumed* to be the same as inside the classically allowed region, invoking analytical continuation. (See Ref. 4 for a detailed discussion.) As I shall show below, that assumption is wrong, although this has only little effect on the results in practical applications.

In this Letter I shall present the functionals $\tau[\rho]$ and $\sigma[\rho]$—the latter giving the entropy density—for a system of fermions at finite temperature derived consistently up to second-order gradients of ρ. The limit of zero temperature then allows us to examine the validity of the functional equation (1).

Let us briefly sketch the derivation. At finite temperature, the densities $\tau(\vec{r})$, $\rho(\vec{r})$, and $\sigma(\vec{r})$ are defined by

$$\rho(\vec{r})=\sum_\nu|\phi_\nu(\vec{r})|^2 n_\nu,$$
$$\tau(\vec{r})=-\sum_\nu\phi_\nu^*(\vec{r})\Delta\phi_\nu(\vec{r})\,n_\nu,$$
$$S=\int d^3r\,\sigma(\vec{r})$$
$$=-\sum_\nu[n_\nu\ln n_\nu+(1-n_\nu)\ln(1-n_\nu)],$$

where ϵ_ν and $\phi_\nu(\vec{r})$ are the eigenenergies and eigenfunctions of the chosen potential $V(\vec{r})$. S is the entropy and $n_\nu=\{1+\exp(\lambda-\epsilon_\nu)/T\}^{-1}$ are the Fermi occupation numbers. (We put $k\equiv 1$ and measure T in energy units.) The Fermi energy λ is fixed by the particle number $N=\sum_\nu n_\nu$. We also define a free-energy density $F(\vec{r})$ by

$$F=E-TS=\sum_\nu\epsilon_\nu n_\nu-TS=\int d^3r\,\mathcal{F}(\vec{r}).$$

The Bloch density $C(\vec{r},\beta)$ is related to $\rho(\vec{r})$ by an inverse Laplace transform:

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

It can be shown[6] to factorize in the form $C(\vec{r},\beta)=C_0(\vec{r},\beta)f_T(\beta)$, where C_0 is the Bloch density at $T=0$, i.e.,

$$C_0(\vec{r},\beta)=\sum_\nu|\phi_\nu(\vec{r})|^2\exp(-\beta\epsilon_\nu),$$

and $f_T(\beta)=\pi\beta T/\sin(\pi\beta T)$ is the (two-sided) Laplace transform of the function with which one has to fold

the $T=0$ spectral density to pass to the $T>0$ case.[5] Using simple rules of Laplace transforms one finds the relations

$$\mathcal{F}(\vec{r})=\lambda\rho(\vec{r})-\mathcal{L}_{\lambda}^{-1}[C(\vec{r},\beta)/\beta^2],\quad \sigma(\vec{r})=-(\partial/\partial T)\mathcal{F}(\vec{r})=(\partial/\partial T)\mathcal{L}_{\lambda}^{-1}[C(\vec{r},\beta)/\beta^2],$$

$$(\hbar^2/2m)\tau(\vec{r})=-\rho(\vec{r})V(\vec{r})+\mathcal{F}(\vec{r})+T\sigma(\vec{r}).$$

These equations are exact if the exact $C_0(\vec{r},\beta)$ is used. We now replace C_0 by its Wigner-Kirkwood expansion[7] up to order $\hbar^2$:

$$C_0^{\mathrm{WK}}(\vec{r},\beta)=\frac{1}{4}\left(\frac{2m}{\pi\hbar^2\beta}\right)^{3/2}e^{-\beta V(\vec{r})}\left\{1+\frac{\hbar^2}{12m}[\tfrac{1}{2}\beta^3(\nabla V)^2-\beta^2\Delta V]\right\}.$$

After the Laplace inversion in (2) we find for the density[6]

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

where

$$A_T=(2\pi^2)^{-1}(2m/\hbar^2)^{3/2}T^{3/2},\quad \eta=[\lambda-V(\vec{r})]/T,$$

and $J_p(\eta)$ are generalizations of the so-called Fermi integrals,[8] defined for $p>-1$ by

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

For $p<-1$, where this integral does not exist, we define $J_p(\eta)$ by the relation

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

which leads to well-behaved functions $J_p(\eta)$ for all values of p used here. Thus at $T>0$, the density $\rho(\vec{r})$ given by (3) is continuous and finite in all space and we do not meet the turning-point problem known from the $T=0$ case. Analogous expressions are found for $\mathcal{F}(\vec{r})$, $\sigma(\vec{r})$, and $\tau(\vec{r})$; they are explicitly given elsewhere.[6,9] With some algebra one can eliminate ΔV and $(\nabla V)^2$ from these expressions and from Eq. (3) consistently up to order $\hbar^2$. As a result we find the temperature-dependent extended Thomas-Fermi (TETF) functionals (for the detailed derivation, see Ref. 9)

$$\tau_{\mathrm{TETF}}[\rho]=(2m/\hbar^2)A_TTJ_{3/2}(\tilde{\eta})+\gamma(\tilde{\eta})(\nabla\rho)^2/\rho-\tfrac{1}{6}\Delta\rho,\tag{4}$$

$$\sigma_{\mathrm{TETF}}[\rho]=\tfrac{5}{3}A_TJ_{3/2}(\tilde{\eta})-\tilde{\eta}\rho-T^{-1}(\hbar^2/2m)\nu(\tilde{\eta})(\nabla\rho)^2/\rho.\tag{5}$$

Here $\tilde{\eta}(\rho,T)$ is an explicit function of ρ and T, given by $\rho=A_TJ_{1/2}(\tilde{\eta})$. The coefficients γ and ν in Eqs. (4) and (5) are universal functions of $\tilde{\eta}$ given by $\gamma(\tilde{\eta})=\zeta(\tilde{\eta})-\nu(\tilde{\eta})$ and

$$\nu(\tilde{\eta})=\tfrac{3}{2}\zeta(\tilde{\eta})-36[\zeta(\tilde{\eta})]^2+\tfrac{3}{8}J_{1/2}^2(\tilde{\eta})J_{-5/2}(\tilde{\eta})/J_{-1/2}^3(\tilde{\eta}),\quad \zeta(\tilde{\eta})=-\tfrac{1}{12}J_{1/2}(\tilde{\eta})J_{-3/2}(\tilde{\eta})/J_{-1/2}^2(\tilde{\eta}).$$

The leading-order terms in (4), (5) are the familiar Thomas-Fermi expressions.[10] The gradient terms have the same form as in the $T=0$ case but with density- and temperature-dependent coefficients. It is interesting to study their limits for $T\to 0$. Using known asymptotic expansions[8] of the $J_p(\tilde{\eta})$, we find that $\nu(\tilde{\eta})$ always goes to zero faster than T, so that the entropy density vanishes as it should. $\zeta(\tilde{\eta})$ and $\gamma(\tilde{\eta})$ go to the value $\frac{1}{36}$ *inside* the classically allowed region (i.e., for $\tilde{\eta}\to+\infty$) and to $\frac{1}{12}$ *outside* (i.e., for $\tilde{\eta}\to-\infty$). Thus, the functional $\tau[\rho]$ is *not analytic* at $T=0$; the coefficient of the Weizsäcker correction jumps from $\frac{1}{36}$ to $\frac{1}{12}$ as one crosses the classical turning point. This discontinuity has consequences for the Euler-type variational equation which will be discussed elsewhere. For the present we note that if the ener-

gy is calculated from parametrized trial densities,[6] it has very little influence whether one uses $\frac{1}{36}$ or $\frac{1}{12}$ in the outside region, since in realistic cases the turning point lies rather far out in the tail of the density. We have checked that for systems with $N \gtrsim 100$, the difference amounts to less than $\sim 10^{-4}$ of the total kinetic energy.

The functionals in Eqs. (4) and (5) are valid for any system of fermions moving in a local average (external or self-consistent) potential at finite temperature, except that they do not account for possible shell effects. They might be useful in different fields of physics. As a first application to nuclear physics, we have performed density variation calculations for the thermal properties of the nucleus ^{208}Pb. We employed the effective Skyrme nucleon-nucleon interaction SIII which was used earlier in Hartree-Fock (HF) calculations[11] at $T > 0$. For this case we have to include corrections to Eqs. (4) and (5) due to the variable effective nucleon masses and the spin-orbit potentials; they can also be derived consistently up to second-order gradient terms.[9] The fourth-order gradient corrections, which it would be hopeless to derive by hand in the $T > 0$ case, were treated approximately just by use of $\tau_4[\rho]$ as known from the $T = 0$ case.[6] The variational calculations were performed as described in Ref. 6 with trial nucleon densities of Fermi-function type, determining their parameters by a minimization of the total free energy. The results are compared to the old HF results[11] in Figs. 1 and 2.

In Fig. 1 we show the neutron and proton rms radii for ^{208}Pb as functions of the excitation energy $E^* = E(T) - E(0)$ obtained in both approaches. The agreement is seen to be excellent; the TETF results reproduce the HF ones within less than 0.2% for all excitations shown here. (One cannot extend this range of excitation energy without taking into account the formation of an external nucleon gas due to nucleon evaporation.[10])

An important quantity for an excited nucleus is its entropy. According to the Fermi-gas theory,[12] it depends on the excitation energy asymptotically like $S \simeq 2[a_0(E^* + \Delta E)]^{1/2}$ (for $E^* >> |\Delta E|$), where ΔE is the ground-state ($T = 0$) shell correction and $a_0 = \pi \tilde{g}(\lambda)/6$ is the usual level density parameter. [$\tilde{g}(\lambda)$ is the average single-particle level density of the cold system.] We define an "effective level density parameter" a_{eff} by

$$a_{\text{eff}} = \tfrac{1}{4} dS^2/dE^* \simeq S/2T; \tag{6}$$

the latter asymptotic equality is found from the relation[12] $E^* \simeq a_0 T^2 - \Delta E$. Figure 2 shows a_{eff} vs E^*, again calculated for ^{208}Pb in the two approaches. The semiclassical curve is seen to coincide perfectly with the HF curve above $E^* \approx 100$ MeV corresponding to $T \approx 2.5$ MeV for this nucleus. The difference at smaller E^* is due to the shell effects contained in the HF result. Both quantities approach asymptotically the value a_0. [The slight de-

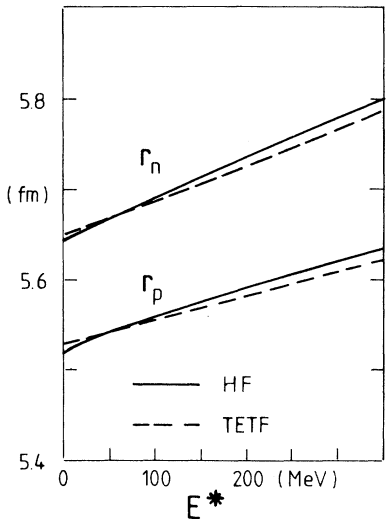

FIG. 1. Root mean square radii of the neutron and proton distributions in ^{208}Pb, plotted vs excitation energy E^*. Solid lines: HF results (Ref. 11). Dashed lines: results of density variational calculations using the present TEFT functionals. (Note the large scale for the radii!)

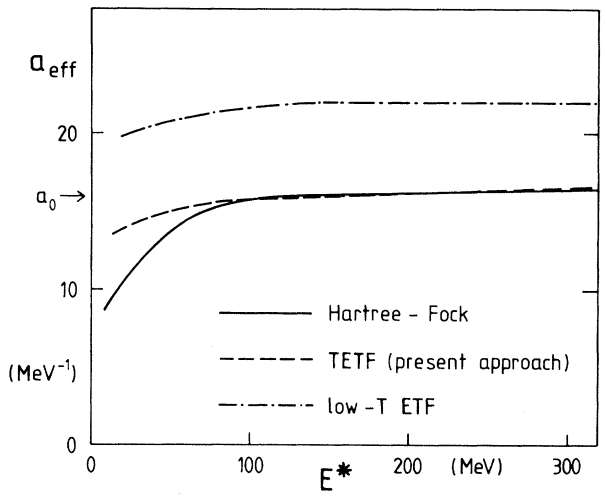

FIG. 2. Effective level density parameter a_{eff}, Eq. (6), for ^{208}Pb vs excitation energy E^*. Solid and dashed lines as in Fig. 1. Dash-dotted line: density variational results obtained in the low-temperature approximation.

viation at large E^* is due to the fact that $\tilde{g}(\lambda)$ is not constant as assumed in the Fermi-gas model.] Also shown in Fig. 2 is the result obtained in the so-called "low-temperature" approximation. The latter is found in the limit $T \ll \lambda - V$, i.e., by expanding Eqs. (4) and (5) for $\tilde{\eta} \gg 1$. This limit is, however, not fulfilled in the nuclear surface, even at low temperatures. The bad result seen in Fig. 2 is therefore not surprising.

We have recently studied[13] an approximation in which the correct TF functionals for $T > 0$ were used and the "cold" gradient corrections $\tau_2[\rho]$ and $\tau_4[\rho]$ were added.[14] Although reasonable results were obtained for ^{208}Pb, a discrepancy of $\sim 7\%$ from the HF result of a_{eff} remained. This error can be traced back to the lack in that approach[13] of a gradient correction to $\sigma[\rho]$. Its contribution to the entropy S is found here always to be negative and to decrease in absolute value from ~ 10 at $T \approx 1$ MeV to ~ 6 at $T \approx 5$ MeV. Its relative smallness (except at very low T) seems to justify our present neglect of the fourth-order corrections to $\sigma[\rho]$. The gradient term in (5) turns out to be crucial in the semiclassical calculation of fission barriers.[6,9]

In summary we have derived for the first time the second-order corrections to the density functionals $\tau[\rho]$ and $\sigma[\rho]$ with their correct temperature-dependent coefficients. Different from the $T=0$ case, these gradient terms are rigorously defined and analytical everywhere in space. In density variational calculations for a finite nucleus we obtain excellent agreement with HF results, in particular at temperatures ($T \gtrsim 2.5$ MeV) where there are no more shell effects; the inclusion of the gradient corrections is decisive in obtaining this good agreement. The variation TETF method with trial nucleon densities is thus an excellent substitute for the much more costly microscopic HF method. Its advantages will be particularly gratifying in the calculation of the equation of state of hot nuclear matter with mixed gaseous and liquid (condensed) phases such as plays an essential role in the collapse of massive stars.[15] The problem of correctly treating the continuum, which one meets in HF calculations, is completely circumvented in the variational TETF method dealing only with local densities. Applications in this direction and calculations of temperature-dependent liquid-drop model parameters[13] using the new functionals are in progress.

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