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HOT NUCLEI IN A SEMICLASSICAL MEAN-FIELD DESCRIPTION

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Recent results of density variational calculations for hot nuclear systems are reported. The question of the maximum temperature of a free, hot compound nucleus is addressed. A consistent set of temperature-dependent liquid drop parameters for the free energy of a nucleus is given.

1. INTRODUCTION: SEMICLASSICAL MEAN-FIELD THEORY

The properties of hot nuclear systems are of actual interest both in heavy ion physics[1] and in astrophysics[2]. We shall discuss some of them here in a mean-field approach, making use of effective nucleon-nucleon interactions of the Skyrme-type[3]. This approach, which is very successful in describing nuclear ground-state properties[4], must be re-examined by a rigorous ab initio manybody treatment[5,6] for systems at finite temperature T. Recent Brückner calculations[6] at $T > 0$ seem to justify for the first time the use of an effective interaction with 'frozen' parameters (i.e. those determined from fits to ground-state properties at $T = 0$) in Hartree-Fock (HF)[7-9] or related calculations [10,11], at least up to temperatures $\sim$ 10 MeV. It also appears [6,12] that correlation effects which increase the level density at low excitations tend to disappear with increasing temperature, thus favouring the simple HF or mean-field approximation.

Early HF calculations at $T > 0$ have already shown[7,8] that another effect of the 'heating' of the Pauli principle is that shell effects rapidly disappear. At temperatures $T \gtrsim 2.5$ MeV, finite nuclei no longer exhibit quantal structures such as the shell effects in their binding energies, and behave like classical systems. Therefore, a semiclassical description is evidently appropriate, such as the density variational approach which was recently developed not only for hot nuclei[13,14] but also for the description of average nuclear ground-state properties[10]. Its essential ingredient is the local density functional for the free energy F of a system of non-interacting Fermions at $T > 0$ which can be gained[13,14] from a semiclassical expansion of the density matrix in powers of $\hbar$, leading to the so-called extended Thomas-Fermi (ETF) model (see e.g. ref. 10 for an outlay of this model). With this functional, the free energy can be expressed in terms of the local one-body density $\rho(\vec{r})$ alone:

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$$F = E - TS = \int d^3r\ f[\rho(\vec{r})], \tag{1}$$

where the functional $f[\rho]$ has the general form

$$f[\rho] = f_\infty(\rho) + \beta(\rho)(\vec{\nabla}\rho)^2 + \gamma(\rho)\Delta\rho + \ldots \tag{2}$$

The term $f_\infty(\rho)$ gives the exact free energy of an infinite system with constant density ρ; the next two terms are second-order and the dots stand for higher-order gradient corrections[14] which are important for inhomogeneous, finite size systems. Note that the coefficients $\beta(\rho)$ and $\gamma(\rho)$, as well as those of the higher-order corrections, are uniquely determined for a given effective interaction. It has been explicitly shown[14,15] that eq. (1), including the ETF functional with gradient corrections up to 4th order, exactly reproduces the quantum-mechanical (HF) free energy and entropy of a nucleus for $T \gtrsim 2.5$MeV, where the shell effects have disappeared.

We shall in the following report briefly on two applications of the approach sketched above: in sect. 2 we raise the question of the maximum temperature which an isolated, hot nucleus can sustain, and in sect. 3 we give, as a more practical result, a set of temperature-dependent liquid drop model (LDM) parameters, derived consistently from a realistic Skyrme force.

2. HOW HOT CAN NUCLEI BECOME?

We try to answer this question within the static meanfield framework. The answer depends on the physical circumstances for which we have in mind two scenarios. The first is that of a collapsing massive star on its way to become (or not become, see ref. 2) a supernova. Here, finite temperatures and pressures exist, so that - at least locally in a given 'shell' of the star - condensed nuclei may exist in thermal equilibrium with a gas mixture of nucleons and leptons. The second situation is that of a hot compound nucleus formed in a heavy ion collision, where no external pressure is present to establish an equilibrium; this is at best a metastable situation.

In either case we try to find the density distribution from the variational ansatz

$$\delta/\delta\rho(\vec{r}) \int d^3r\{f[\rho(\vec{r})] - \lambda\rho(\vec{r}) + P_o\} = 0. \tag{3}$$

λ is the Lagrange multiplier for conserving the number A of nucleons, and P_o is the external pressure. Eq. (3) together with eq. (2) leads to the following Euler-Lagrange equation:

$$\delta f[\rho]/\delta\rho = f'_\infty(\rho) + 2[\gamma'(\rho) - \beta(\rho)]\Delta\rho + [\gamma''(\rho) - \beta'(\rho)](\vec{\nabla}\rho)^2 + \ldots = \lambda. \tag{4}$$

(Primes denote derivatives with respect to ρ. For simplicity, we only assume here one kind of nucleons. In a realistic case, one will use two Lagrange multipliers λ_p, λ_n and obtain two coupled equations for neutron and proton densities ρ_n and ρ_p, respectively.) The boundary conditions will be discussed separately in the two different scenarios.

1.1 Equilibrium case with external pressure $P_o \neq 0$

We consider an isolated nucleus, embedded in an infinite nucleon gas at finite pressure P_o. In the limit where the nucleus is very large, we have thermal equilibrium of a condensed (liquid) phase with density ρ_o and a gas phase with density ρ_g; these limiting densities far away from the nucleus' surface are given by

$$f'_\infty(\rho_o) = f'_\infty(\rho_g) = \lambda; \tag{5}$$

pressure equilibrium implies

$$P(\rho_o) = \lambda\rho_o - f_\infty(\rho_o) = P(\rho_g) = \lambda\rho_g - f_\infty(\rho_g) = P_o. \tag{6}$$

The four eqs. (5,6) are solved simultaneously by the familiar Maxwell construction; at each fixed temperature T they fix the 4 quantities λ, P_o, ρ_o and ρ_g. The maximum temperature for which a solution can be found is the critical temperature T_c of the gas/liquid phase transition. For realistic forces with an infinite matter incompressibility (at T = 0) $K_\infty \simeq 200 - 250$ MeV one gets $T_c \simeq 14$-16 MeV.

In finite nuclei, ρ_o, λ and T_c are modified by: 1) compression effects due to the finiteness of K_∞, tending to increase ρ_o; 2) Coulomb repulsion of the protons, tending to destabilize the nucleus and to decrease ρ_o, and 3) further asymmetry effects as soon as $\rho_n \neq \rho_p$ due to the Pauli principle. Bonche et al.[9] performed HF calculations in a Wigner-Seitz approximation, using a subtraction procedure which is equivalent to including a pressure $P_o \neq 0$ in eq. (3). They found a maximum temperature $T_m \simeq 8$-10 MeV for ^{208}Pb (depending on the interaction), beyond which the nucleus ceases to be bound. The same procedure was also used in density variational calculations with ETF functionals, leading to identical results[11].

1.2 Metastable case with $P_o = 0$

When a hot compound nucleus is formed in a heavy ion collision, there is no external gas providing the pressure necessary to form a thermodynamical equilibrium. In fact, such a nucleus is unstable and decays by nucleon evaporation (or other channels: fission, γ-decay, fragmentation, ...). However, if its lifetime is long enough, it may be treated as a metastable system, very much like a superheated classical liquid drop at vanishing external pressure[16].

The Euler equation (4) has been studied for the metastable case ($P_o = 0$) in the semi-infinite limit by Stocker and Burzlaff[1]. In the condensed region (i.e. far inside a very large nucleus) the density goes to a constant $\tilde{\rho}_o$ given by the saturation condition at T > 0:

$$f'_\infty(\tilde{\rho}_o) = f_\infty(\tilde{\rho}_o)/\tilde{\rho}_o = \lambda . \qquad (7)$$

Outside the surface, the density does not go to a constant value, but has a minimum at a finite distance R_o: $\rho(R_o) = \tilde{\rho}_g$, $\rho'(R_o) = 0$; further one finds[17]

$$f_\infty(\tilde{\rho}_g) = \lambda\tilde{\rho}_g . \qquad (8)$$

The maximum temperature T_m, for which a solution of eqs. (4,7,8) can be found, is typically $\sim$ 3-4 MeV lower than the critical temperature T_c of the equilibrium case.

For describing finite, metastable nuclei, we propose the following modified variational procedure[18]: The (spherical) nucleus is put into an infinite box with radius R_o; eq. (3) (with $P_o = 0$) is modified to

$$\delta \int_o^{R_o} 4\pi\, r^2 dr\, \{f[\rho(r)] - \lambda\rho(r)\} = 0, \qquad (9)$$

thus including R_o in the variation. Varying $\rho(r)$ with fixed R_o leads again to eq. (4); variation of R_o gives the additional boundary condition

$$f[\tilde{\rho}_g] = \lambda\tilde{\rho}_g . \qquad (10)$$

In addition, we have the boundary conditions

$$\rho'(r = 0) = \rho'(R_o) = 0. \qquad (11)$$

The particle number is given by

$$A = 4\pi \int_o^{R_o} r^2 dr\, \rho(r). \qquad (12)$$

In the limit $A \to \infty$, this procedure yields the old result of ref. 17.

The numerical solution of eqs. (4,10-12) is in progress. Preliminary results of variational calculations with parametrized trial densities[19] yield a limiting temperature of ^{208}Pb of $T_m \simeq 5 - 5.5$ MeV, hereby using the Skyrme SkM* force[10,20]. This corresponds to a limiting excitation energy per particle of $E^*/A \sim 3$-4 MeV. Although the experimental situation is far from conclusive, some hints for limiting values of E^*/A of this order may have been observed[1].

Binding energies and entropies were found[19] to depend very little on the exterior density $\tilde{\rho}_g$ up to $T \lesssim 4$ MeV, thus validating older results[10] of calculations where $\tilde{\rho}_g$ was put to zero in the trial densities. There the fission barrier of ^{240}Pu was found to vanish at $T \simeq 4 - 4.5$ MeV, due to the decreasing surface tension of the hot nucleus (see sect. 3 below).

From the variational results of $\tilde{\rho}_g$ and R_o one can calculate the pressure of the nucleus' surface on the walls of the box, and thus estimate the evaporation rate. We find[18,19] that $\tau_{ev} \lesssim 10^{-23}$ sec for $T \gtrsim 5$ MeV. Thus, a mean field no longer exists at $T \gtrsim 5$ MeV, since the evaporation channel is completely open.

In conclusion, we do not expect isolated compound nuclei to exist beyond temperatures $T \simeq 4$-5 MeV due to their immediate decay by evaporation and, for $A \gtrsim 240$, by fission.

3. TEMPERATURE DEPENDENCE OF LDM PARAMETERS

In many applications it is convenient to estimate average binding energies using a semi-empirical mass formula. For ground-state masses, the LDM and its refinement, the droplet model[21], have become rather popular. For heated nuclear systems we have to know the temperature dependence of the LDM (or droplet model) parameters. The density variational method described above serves as an ideal tool to derive these parameters consistently from a given effective interaction [10]. We write the free energy in the form

$$F = F_{sym} + F_{asym} + F_{coul} \ . \tag{13}$$

The liquid-drop type expansion of the symmetric part (for N = Z) is

$$F_{sym}(A) = a_v A + a_s A^{2/3} + a_c A^{1/3} + a_o \ . \tag{14}$$

It was shown recently[22,23] that eq. (14) reproduces the exact variational ETF total energies (or HF energies for $2.5 \lesssim T \lesssim 5$ MeV) within less than 1 MeV, even for nuclei as light as $A \gtrsim 10$. Hereby, the presence of the curvature energy coefficient a_c, amounting to $\sim 10 - 13$ MeV for all realistic interactions (and including the socalled compression energy[21] of $\sim -(2\text{-}3)$MeV), and of the constant term a_o (typically $\sim -(8\text{-}12)$MeV) are of great importance.

For the asymmetry energy, the droplet model[21] expression

$$F_{asym} = JAI^2/[1 + (9J/4Q)A^{-1/3}], \tag{15}$$

where $I = (N-Z)/A$, J is the volume asymmetry energy and Q the surface stiffness parameter, has been nicely verified by the ETF density variational calculations[10,23] for $|I| \lesssim 0.3$. Note that, as emphasized from the beginning[21], the Taylor expansion of eq. (15) in powers of $A^{-1/3}$ is not justified since, typically, $(9J/4Q) \gtrsim 2$.

The approximation

$$F_{coul} = c_1 Z^2/A^{1/3} + c_2 Z^2/A \qquad (16)$$

was found[23] to reproduce within < 1 MeV the Coulomb energies (including exchange) for nuclei with $6 \lesssim A \lesssim 240$.

The systematic determination of the parameters in F_{sym} and F_{asym} from semi-infinite nuclear matter calculations has been described in ref. 21 and, for the ETF density functional approach with Skyrme forces, in ref. 10. The temperature dependence of the a_i in eq. (14) was discussed both for the equilibrium[10,14] and the metastable situation[18,19]. The difference was shown to be negligible for $T \lesssim 4$ MeV. In this domain, a quadratic approximation of the form[8]

$$a_i(T) = a_i(0) - T^2/\varepsilon_i \quad (T \text{ in MeV}) \qquad (17)$$

has been found to be accurately fulfilled[23].

In table 1 we present the set of parameters $a_i(0)$ and ε_i, according to eq. (17), determined from density variational ETF calculations[10,19,23]. We hereby used the interaction SkM* which yields excellent fits of ground-state properties[10,20] (energies, radii, fission barrier of ^{204}Pu) and giant resonance energies[24,25] for nuclei not too far off the β stability line. These parameters, using eqs. (13-17), should reproduce the total free energies of nuclei with $10 \lesssim A \lesssim 300$ for $0 \lesssim T \lesssim 4$ MeV within ∿ 1-2 MeV, irrespectively of the presence of an external nucleon gas.

Table 1

LD and droplet model parameters (all in units of MeV) determined selfconsistently from the SkM* interaction. See eqs. (13) to (17) for the definitions.

	a_v	a_s	a_c	a_o	J	Q	c_1	c_2
$a_i(0)$	-15.776	17.22	10.24	-8.0	30.03	35.4	0.737	-1.28
ε_i	18.88	10.5	18.0	10.2	32.05	2.2	1'778.0	59.3

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