Behavior of Shell Effects with the Excitation Energy in Atomic Nuclei

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We study the behavior of shell effects, like pairing correlations and shape deformations, with the excitation energy in atomic nuclei. The analysis is carried out with the finite temperature Hartree-Fock-Bogoliubov method and a finite range density dependent force. For the first time, properties associated with the octupole and hexadecupole deformation and with the superdeformation as a function of the excitation energy are studied. Calculations for the well quadrupole deformed ^{164}Er and ^{162}Dy, superdeformed ^{152}Dy, octupole deformed ^{224}Ra, and spherical ^{118}Sn nuclei are shown. We find, in particular, the level density of superdeformed states to be 4 orders of magnitude smaller than for normal deformed ones.

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It is well known that atomic nuclei can store up to a few hundreds MeV as internal excitation energy. In this situation the nucleus can be described in statistical terms by assigning equal probabilities to all nuclear levels of a given internal energy; see [1] for a recent review. This microcanonical description can be transformed to a more convenient, but approximate, form in which the equilibrated nucleus can be characterized by a certain temperature T (canonical description). One of the most striking features of a heated nucleus is that physical effects like superfluidity or shape deformations are washed out when T increases. In terms of the shell model it can be easily understood since by increasing T one promotes particles from levels below the Fermi surface to levels above it. In the case of pairing correlations, blocking levels amounts to destroying Cooper pairs. In the case of shape deformation, by depopulating the deformation driving levels (intruders) one gets on the average less deformation. Experimental information about nuclear shape changes can be obtained by means of the giant dipole resonance (GDR) built on excited states. Exclusive experiments studying the GDR strength at a given excitation energy (or T) of the nucleus have been carried out in [2–4]. In the finite temperature mean field theory these effects show up as a phase transition at critical T's in the range of 0.5–3.0 MeV. It is clear that, as the nucleus is a finite system, the sharp phase transitions obtained in the mean field approach will be somewhat washed out when statistical fluctuations around the mean field solution are considered. The statistical fluctuations can be treated in the spirit of the Landau theory [5] or from a more fundamental point of view by using path integral techniques like the static path approximation [6,7] or the shell model Monte Carlo [8]. The latter techniques have been applied to a variety of physical situations using separable interactions defined in restricted configuration spaces but not with effective interactions.

Finite temperature Hartree-Fock (FTHF) studies in Refs. [9,10] analyzed shape transitions in finite nuclei. The authors studied spherical nuclei and the quadrupole deformed ^{168}Yb as a function of T using the Skyrme III interaction. For ^{168}Yb they found a phase transition to the spherical shape at $T \approx 2.5$ MeV. The disappearance of superfluidity with T was first studied by Moretto [11] with a microcanonical formalism and by Goodman [12] in the FTHF-Bogoliubov theory (FTHFB) with a schematic interaction. Several authors have also carried out studies on the critical T's for the transition from quadrupole to spherical shape and from the superfluid phase to the normal one using the pairing + quadrupole $(P + Q)$ interaction in a restricted configuration space [13,14]. The main conclusions are that the pairing phase transition takes place at T's around 0.5 MeV and that the transition to a spherical shape takes place at T's around 1.7 MeV in the cases studied at low spin. The last conclusion seems to be in contradiction with the results obtained with the Skyrme III interaction [9] and, as we shall see, with ours. However, when shape fluctuations are considered in the $P + Q$ model [15] the deformations around $T = 1$–2 MeV are closer to the ones obtained, at these temperatures, in the HFB approach with effective forces and large configuration spaces. In the latter case, around these T's, shape fluctuations are less important due to the stiffer energy surfaces.

The purpose of this Letter is to study the behavior of bulk properties of nuclei at zero angular momentum with increasing excitation energy using the finite range density dependent Gogny force [16,17] and a large configuration space. The Gogny force is the only effective interaction which allows completely consistent calculations since it provides both the particle-hole and the particle-particle (pairing) matrix elements. This property makes the Gogny force a good testing ground of pairing properties. In addition, the Gogny force can describe all

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types of shape deformations, as for instance, the reflection asymmetric octupole shape found in some light actinide, superdeformation, or the hexadecupole and higher order components of a given shape. We have carried out FTHFB calculations for nuclei in the rare earth and actinide regions to determine the critical T of the superfluid-normal transition, the shape transition from quadrupole deformed (normal deformed, ND, and superdeformed, SD) to spherical nuclei and the transition from octupole deformed to reflection symmetric shapes. In all cases the behavior of higher order deformation parameters as a function of T is analyzed. The FTHFB equation [12,18] can be derived from the variational principle over the grand canonical potential $\Omega = E - TS - \mu N$, using the HFB partition function, E being the energy, S the entropy, μ the chemical potential, and N the average number of particles in the system. The modifications induced by the use of a density dependent force are the same as in the $T = 0$ case and amount to the introduction of an extra rearrangement potential in the HF field [9]. The FTHFB equation has been solved by expanding the quasiparticle operators in an axially symmetric harmonic oscillator basis containing fourteen shells. The convergence has been checked in selected calculations with 15, 16, and 17 major shells; see also [9]. To avoid eventual continuum contributions (which, as stated in [19], are large for $T > 4.0$ MeV) we shall limit our calculations to $T < 3.0$ MeV. Axially symmetric shapes are the only ones allowed in the calculations, but reflection symmetry is not imposed in order to study the octupole degree of freedom. As a consequence, the center of mass position has to be constrained to be at the origin. The set of parameters used for the Gogny force is the one called D1S set [20]. It has been used over the last 15 years to study a great wealth of low energy nuclear structure phenomena. For the numerical applications we have chosen nuclei typifying the effects we want to illustrate.

In Fig. 1 we show some results for the *well-deformed* nucleus ^{164}Er as a function of T. In panel (a) the excitation energy E^* versus T is displayed. Aside from the irregularity around $T \approx 0.7$ MeV and the smaller one around $T \approx 2.7$ MeV, the behavior is quadratic, as expected in a Fermi gas—$E^* = aT^2$. For $T \leq 1$ MeV, the results are also shown multiplied by 10 for more resolution. In panel (b) the particle-particle correlation energies [$E_{PP} = \frac{1}{2}\mathrm{Tr}(\Delta\kappa)$] for protons and neutrons are displayed. They increase rather abruptly as T grows and become negligible at $T \approx 0.7$ MeV for protons and neutrons; see inset. This behavior *qualitatively* agrees with previous calculations with the $P + Q$ Hamiltonian [13] and other simple model Hamiltonians and indicates that the vanishing of pairing with T is a genuine feature independent of the pairing force used. *Quantitatively*, however, our calculations with finite range forces always have higher transition T's than the schematic pairing forces. In panel (c) we have plotted the β_2, β_4, and β_6 deformation parameters, the β_4 and β_6 deformation parameters have been scaled. They increase

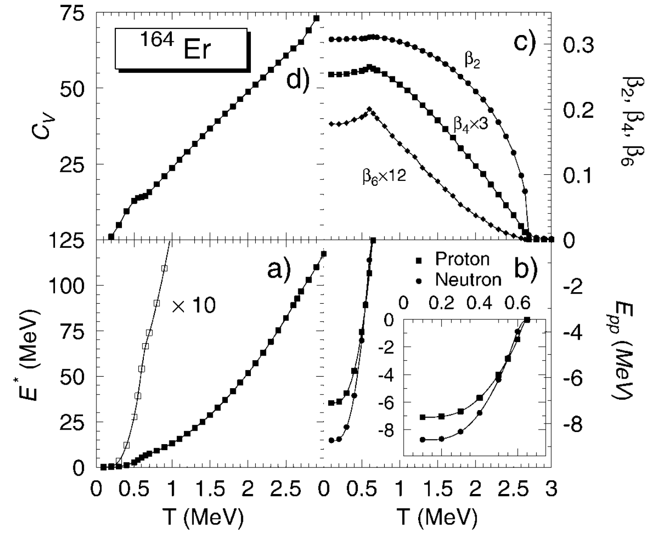

FIG. 1. Excitation energies (a), pairing energies (b), deformation parameters (c), and specific heat (d), as a function of T for the nucleus ^{164}Er.

smoothly at low T up to $T \approx 0.7$ MeV, where they start to decrease. The initial enhancement of the deformation can be related to the weakening of pairing correlations in that range of T. At $T \approx 2.7$ MeV the deformation parameters become zero and the phase transition to the spherical regime takes place. It is interesting to note that the collapse to the spherical shape drives all deformation parameters to zero at the same time and that the critical temperature is larger than the one found with schematic (separable) forces and small configuration spaces. These deformation parameters are the most probable ones; the inclusion of fluctuations will provide the average deformation parameters.

The irregularities caused by phase changes with T are more clearly seen in the specific heat ($C_V = T\partial S/\partial T$) which we have plotted in panel (d). We observe that there are indeed changes in C_V at the T where the transition to the nonsuperfluid phase takes place and at the one where the transition to the spherical phase occurs. The behavior of the specific heat is rather typical: at low T's, where pairing correlations are present, we have a quadratic increase that becomes linear as soon as the transition to the nonsuperfluid phase takes place, for a Fermi gas $C_V = 2aT$ where a is the level density parameter in Bethe's formula. For this nucleus we obtain $a = 12.98$ MeV^{-1} which is consistent with values obtained with the Skyrme interaction [19] for other nuclei.

For a better understanding of the shape transition we have plotted in Fig. 2 the self-consistent HF single particle energies for protons and neutrons as a function of T. We observe how, as T approaches the critical T of 2.7 MeV, the single particle levels bunch together into the spherical levels. The energies of these levels are very close to the corresponding ones obtained by constraining the nucleus to the spherical shape in a HF calculation at $T = 0$. In other words, in the T range considered in this Letter, at high

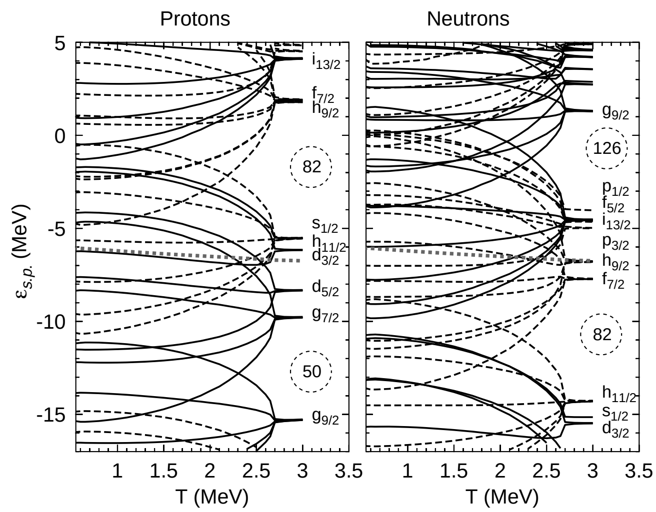

FIG. 2. Self-consistent single particle energies of the nucleus ^{164}Er for protons and neutrons versus T.

T the shell effects which drive deformation disappear but not the ones providing the magic numbers in the spherical shape.

To analyze shape changes including *superdeformation* (SD) we have chosen the nucleus ^{152}Dy which is known to have a SD minimum a few MeV above the normal deformed (ND) ground state. Between the SD minimum and the ND one there is a barrier that prevents the jumping of the SD mean field configuration to the ND one. As we shall see, that barrier disappears as the nucleus is heated and only the ND minimum remains.

In Fig. 3 we show similar results as in Fig. 1 but for ^{152}Dy, dashed lines correspond to values in the SD minimum. In panel (a) the excitation energies of the SD and ND minima (referred to the ground state, i.e., the ND at zero T) versus T, are plotted. At zero T the SD minimum is around 7 MeV above the ground ND state. Therefore, we expect that at a T such that the ND state has an excitation energy larger than 7 MeV the SD minimum must be washed out. That is exactly what we find, at T's above 0.75 MeV (at excitation energies larger than 14 MeV) we do not find any SD solution. In panel (b) we display the pairing energies for both minima. In the SD minimum the proton pairing is rather small and vanishes at $T = 0.55$ MeV, the neutron pairing is zero as expected, since in the SD there is a shell closure in neutrons. In the ND minimum the pairing collapse for protons occurs at $T = 1.0$ MeV and for neutrons at $T = 0.6$ MeV. These effects can be observed in panel (a) in the ND energy curve. In panel (c) the deformation parameters are plotted. We find large values at the SD minimum which keep rather constant up to $T \approx 0.5$ MeV, where they start to decrease up to $T \approx 0.75$ MeV where the SD minimum disappears. The ND deformation parameters (same symbols as for the SD case) are rather small and go to zero at $T \approx 1.3$ MeV. In panel (d) the specific heats for both minima are represented, the SD values have been shifted by 10 units for clarity reasons. In the T region where the SD minimum exists both curves almost coincide. This would not be the case if we had plotted the specific heat versus the excitation energies instead of versus T.

We have also carried out the same kind of calculations for the nucleus ^{224}Ra, which has been predicted [21] to have a permanent *octupole deformation* at $T = 0$. In Fig. 4(c) we can study the T driven phase transition from octupole deformed to a reflection-symmetric shape. For this nucleus we find that all deformation parameters remain more or less constant until the pairing correlations disappear. From this point on they decrease, the octupole parameter in a faster way than the other ones, until they vanish at $T = 1.3$ MeV. For panels (a), (b), and (d) similar comments as to the previous figures do apply.

Level densities (l.d.), $\rho(E^*)$, can be microscopically evaluated in the usual way; see, for example,

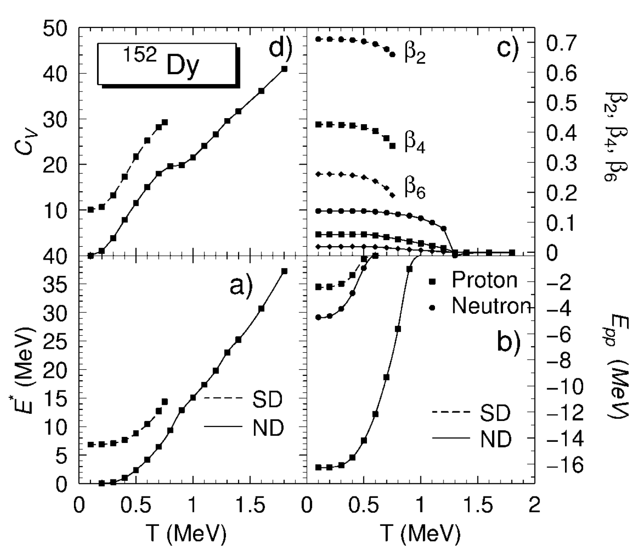

FIG. 3. Same as Fig. 1 for the nucleus ^{152}Dy at the normal and at the superdeformed minimum.

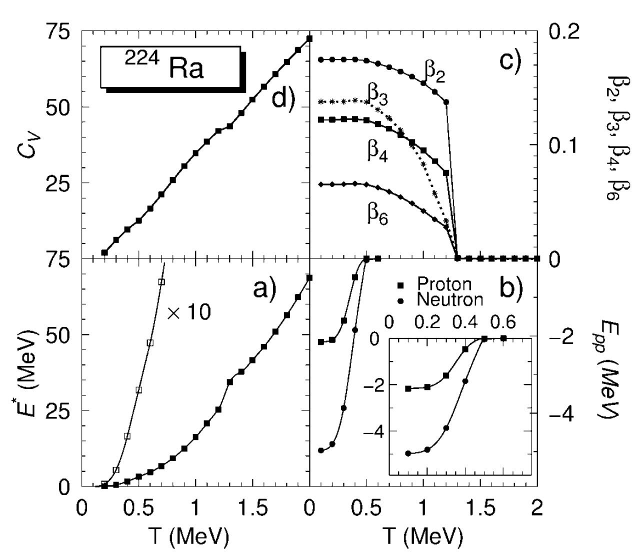

FIG. 4. Same as Fig. 1 for ^{224}Ra.

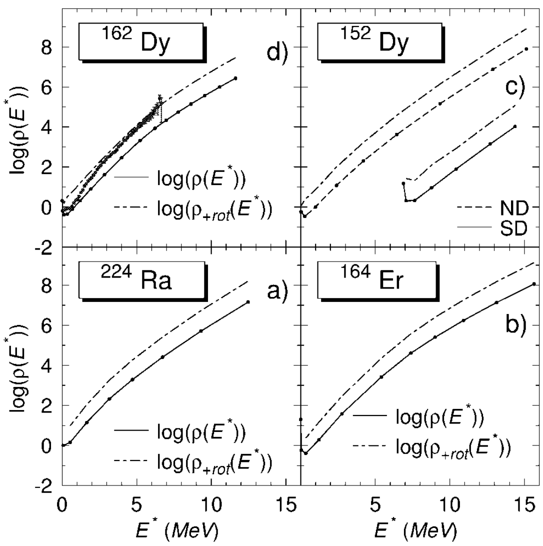

FIG. 5. Level density of the nuclei ^{162}Dy, ^{164}Er, ^{224}Ra, and of the nucleus ^{152}Dy at the normal and at the superdeformed minimum.

Eq. (2B-14) of Ref. [22]. In Fig. 5 we show these quantities for the nuclei ^{224}Ra, ^{164}Er, ^{152}Dy (in the ND and SD wells) and ^{162}Dy plotted versus the excitation energy measured from the ground states. In all cases we observe the overall expected exponential dependence and the well-known abnormal behavior at very small excitation energies of the mean field approximation. For ^{152}Dy it is interesting to see the different l.d. in the ND well and in the SD one, at a given energy the l.d. of ND states is about 4 orders of magnitude larger than the one of SD states. Obviously, these l.d.'s are the multiquasiparticle ones. To calculate the total l.d. the collective states (rotational and vibrational) must be included. To do it microscopically is quite involved. For good rotors, however, the rotational states can be included phenomenologically assuming that each multiquasiparticle state is the head of a band. The l.d. including rotational states are represented in the figure by the dot-dashed lines and increase the l.d. by about 1 order of magnitude. The inclusion of the vibrational levels, which is more complicated, will provide another order of magnitude. To compare with the experiment we have plotted the data of Ref. [23] for ^{162}Dy, which do not provide absolute values. At small excitation energies we do not expect a statistical theory to provide accurate results. Above 3.0 MeV excitation energy, however, our results do agree well with the experimental data.

Finally, we have also performed calculations concerning the pairing phase transition in the *spherical nucleus* ^{118}Sn, magic in protons. As T is increased in this nucleus the neutron pairing energy shows the typical "square root" behavior and dies out at a T of 1 MeV. The high transition T we can correlate to the very strong pairing correlations seen in the ground state of ^{118}Sn at zero T.

In conclusion, for the first time the behavior of shell effects with varying T is studied using the Gogny force. We find that the Gogny force produces free-energy surfaces that are stiffer than those found previously with schematic forces, thus leading to higher critical T's for shape transitions. In all calculated nuclei there is a critical temperature at which all deformation parameters $\beta_2, \beta_3, \beta_4, \ldots$ collapse to zero. The critical temperature for the quenching of the pairing correlations is higher than for separable pairing forces. One must be aware, as shown in theories beyond the FTHFB approximation with schematic forces and small configuration spaces [15,24], that additional correlations will wash out the sharp transitions found. Lastly, the level density for superdeformed states is found to be about 4 orders of magnitude smaller than for normal deformed ones

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