Temperature induced shell effects in deformed nuclei
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Abstract

The thermal evolution of the shell correction energy is investigated for deformed nuclei using Strutinsky prescription in a self-consistent relativistic mean-field framework. For temperature independent single-particle states corresponding to either spherical or deformed nuclear shapes, the shell correction energy $\Delta_{sc}$ steadily washes out with temperature. However, for states pertaining to the self-consistent thermally evolving shapes of deformed nuclei, the dual role played by the single-particle occupancies in diluting the fluctuation effects from the single-particle spectra and in driving the system towards a smaller deformation is crucial in determining $\Delta_{sc}$ at moderate temperatures. In rare earth nuclei, it is found that $\Delta_{ac}$ builds up strongly around the shape transition temperature; for lighter deformed nuclei like $^{64}$Zn and $^{66}$Zn, this is relatively less prominent.

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In the backdrop of the nuclear mass formula, the shell-correction energy calculated in the microscopic-macroscopic approach of Strutinsky \[1\] plays an extremely important role in properly understanding the ground state masses of atomic nuclei, their equilibrium deformation, double-hump barrier of fissioning nuclei etc. The shell correction energy is evaluated through smoothening of the fluctuations in the single-particle level structure; these fluctuations depend among others on the intrinsic deformation of the nuclear system. With increasing excitation or temperature, occupancies of orbitals tend to wash away the fluctuations arising from the set of single-particle states; it is then found that the shell energy melts away \[2\] with temperature at \(T_{\text{shell}} \sim \hbar \omega_0 / \pi\) (\(\hbar \omega_0 \sim 41A^{-1/3}\)). This is typically \(\sim 2.5\) MeV for rare-earth nuclei. This has however been investigated for a fixed set of single-particle levels corresponding to a fixed intrinsic deformation.

Nuclei, deformed in their ground states undergo phase transition to spherical shapes with increase in temperature \[3\]. For rare-earth nuclei, these temperatures \(T_p\) are typically between \(1 - 2\) MeV. In their ground states, the \(m\)–states emanating from a given \(j\)–shell near the Fermi surface of these nuclei are preferentially occupied driving the system towards a stable deformation. As the nuclei are heated up, these occupancies tend to equalize which tries to restore the spherical symmetry. The different \(m\)–states from a given orbital then become bunched and the single-particle level structure becomes more nonuniform at the spherical shape \((\beta_2 = 0)\). If one calculates the shell correction energy at \(T = 0\) with the deformed ground state level spectrum and the spectrum obtained by constraining the system at \(\beta_2 = 0\), one would always find that the shell correction energy at \(\beta_2 = 0\) would be larger in magnitude. With increasing temperature, the deformation of the nuclei reduces and the occupancies of the single-particle states in the vicinity of the Fermi surface tend to become uniform. The uniform occupancy across the Fermi surface would reduce the shell correction whereas the decrease of deformation enhances the shell correction. In a self-consistent tuning-in of the deformation with temperature, the temperature dependence of the shell correction energy would then be governed by the dual role played by the thermal evolution of the single-particle occupancies, i.e., the interplay between their tendency for a drive towards sphericity and their tendency for the washing out of the shell corrections. For example, if \(T_p\) is considerably less than \(T_{\text{shell}}\), one may find a sharp building-up of the shell correction energy with temperature in the vicinity of \(T_p\). The aim of this note is to investigate in detail this delicate interplay for a few selected nuclei in the relativistic mean field (RMF) theory. For our study, we have chosen isotopes of \(^{64}\text{Sm}\) and \(^{66}\text{Sm}\) in the rare-earth region and two lighter nuclei \(^{64}\text{Zn}\) and \(^{66}\text{Zn}\). In passing, it may be mentioned that Egido \textit{et al} \[5\] have recently pointed out that at relatively high temperature, the shell-effects which drive deformation disappear but not the ones providing magic numbers in spherical nuclei.

The details of the Lagrangian density and the corresponding field equations used for calculating the thermal evolution of the deformation and single-particle levels are given in Refs. \[6\]. In the present calculation, we employ the NL3 parameter set \[8\]. To include the effect of pairing, the occupancies have been modified in the framework of BCS approximation \[7\]. The single-particle states are calculated using spherical oscillator basis with twelve shells. The values of the chemical potential and the pairing gap at a given temperature are calculated using all the single-particle states up to \(2\hbar \omega_0\) (the model space) above the Fermi surface without assuming any core. With increase of the basis space to twenty shells and the model space to \(3\hbar \omega_0\), the changes in the results are insignificant. The continuum
corrections are not taken into account in the temperature range explored ($T \leq 3$ MeV) where it has earlier been found to be quite small. Once the set of single-particle states are obtained in the RMF theory, the shell corrections are evaluated in the standard Strutinsky prescription. The shell correction energy $\Delta_{sc}$ is calculated as

$$\Delta_{sc} = \sum_i n(\epsilon_i, \lambda, T)\epsilon_i - \int \tilde{g}(\epsilon)en(\epsilon, \tilde{\lambda}, T)d\epsilon.$$

In eq. (1), the sum runs over all the single-particle states with energy $\epsilon_i$ in the model space. The function $n$ is the occupancy and $\tilde{g}(\epsilon)$ is the smoothened density of single-particle states. The chemical potentials $\lambda$ and $\tilde{\lambda}$ are obtained for the discrete and the smoothened single-particle states, respectively. Results for $\Delta_{sc}$ calculated in this method taking a fixed set of temperature independent single particle levels are found to be in consonance with those obtained by Bohr and Mottelson using a different prescription.

In Fig. 1, in the top panel, the changing deformation as a function of temperature for the nuclei $^{148}Sm$ and $^{150}Sm$ are displayed. In the bottom panel, the thermal evolution of the neutron single-particle level spectrum of the nucleus $^{150}Sm$ is also shown. The qualitative features of the evolving proton single-particle spectrum for $^{150}Sm$ or the neutron/proton spectra for the nucleus $^{148}Sm$ are similar and are therefore not displayed here. At $T = 0$, the preferential occupation of the $m-$orbitals near the Fermi surface stemming from the $j-$state forces the system towards a static ground state deformation. As the system heats up, the occupancies of different $m-$states evolve in a self-consistent manner and drive the single-particle potential towards a more spherically symmetric one which in turn reorganizes the single-particle orbitals. This reorganization becomes very fast at the shape transition temperature $T_p$ leading to a sudden collapse of the deformation. This is evident from both the panels of Fig. 1.

The thermal evolution of $\Delta_{sc}$ is shown for $^{150}Sm$ in the top panel of Fig. 2. This nucleus is deformed in its ground state with $\beta_2 = 0.19$. With the set of single-particle energy states fixed corresponding to this ground state, the calculated $\Delta_{sc}$ is shown as the dotted line. The dashed-dot line refers to $\Delta_{sc}$ calculated with the set of single-particle states corresponding to the spherical configuration of this nucleus as obtained at the shape transition temperature $T_p$. It may be mentioned that for a fixed spherical shape, the single-particle states are practically independent of temperature below $T \sim 4$ MeV and therefore these set of states have been used for the calculation of $\Delta_{sc}$ (dashed-dot line). In a fully self-consistent calculation, as expected, $\Delta_{sc}$ (solid line) coincides at $T = 0$ with the dotted curve and merges with the dashed-dot curve at and beyond the transition temperature $T_p$. The transition temperature so calculated for this nucleus and for other nuclei are in agreement with those calculated recently also in the RMF framework by Gambhir et al. As the temperature approaches $T_p$, there is a sudden drop in deformation (see Fig. 1), with an abrupt enhancement of $\sim 3$ MeV in $\Delta_{sc}$. Beyond this temperature, the nucleus is spherical and $\Delta_{sc}$ decreases monotonically. A nucleus in a spherical equilibrium configuration in its ground state can not have a positive shell correction energy. Strikingly, here we find that though the shape becomes spherical at and beyond $T_p$, the shell correction energy is positive (more on this is discussed later). In the bottom panel of Fig. 2, the self-consistent thermal evolution of $\Delta_{sc}$ for the nuclei $^{148}Sm$, $^{152}Dy$ and $^{154}Dy$ are shown. They exhibit the same kind of structure as in the case of $^{150}Sm$. 

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The self-consistent thermal evolution of the shell correction energy is also studied for two deformed lighter nuclei, namely, $^{64}\text{Zn}$ and $^{66}\text{Zn}$. In Fig. 3, the temperature evolution of deformation (top panel) and the shell correction energy $\Delta_{sc}$ (bottom panel) are displayed for these two systems. It is found that the collapse of the deformation is a little smoother for these two nuclei compared to the isotopes of $\text{Sm}$ and $\text{Dy}$ studied. A broad but less prominent bump in $\Delta_{sc}$ around the transition temperature is also seen. As pointed out earlier, the thermal evolution of $\Delta_{sc}$ depends on two competing mechanisms, i.e., the smoothening of the fluctuation effects of the single-particle spectra around the Fermi surface and the bunching of different $m$-states with increasing temperature. The counter-balance of these two effects determines the details of the structure in the temperature dependence of $\Delta_{sc}$ for deformed nuclei. This is reflected in Fig. 2 as well as in Fig. 3.

Since spherical nuclei in ground state have negative shell corrections, the positive shell correction energy for the systems turned spherical at or beyond the shape transition temperature at first glance may look counter-intuitive. This, however, can be understood from an examination of the level density of the single-particle states in the vicinity of the Fermi surface within the smearing width taken to be $\sim 1.2\hbar\omega_0$. We are dealing with open-shell deformed nuclei with temperature induced spherical shapes that have different single-particle structure near the Fermi surface as compared to those in the regular spherical (i.e. closed-shell) nuclei. Thus, one need not expect the same behaviour of the shell corrections though the systems are spherical in both cases. In Fig. 4, the results for the shell correction energy $\Delta_{sc}$ for neutrons and protons are given separately for systems $^{150}\text{Sm}$ (top panel) and $^{64}\text{Zn}$ (bottom panel). It is found that $\Delta_{sc}$ remains positive for protons and negative for neutrons in case of $^{150}\text{Sm}$ and the situation is reversed for $^{64}\text{Zn}$. The number of neutrons in $^{150}\text{Sm}$ is closer to a magic number (N=82) whereas the number of protons correspond to a mid-shell. This explains the sign of the shell corrections for neutrons and protons; the total shell correction is the sum of these two. For $^{64}\text{Zn}$, the sign of the proton and neutron shell correction is reversed; here the proton number as compared to the number of neutrons is closer to the magic number 28.

That the shell correction energy dissolves with increasing temperature for a fixed set of single-particle levels is well-known. For deformed nuclei, because of the self-consistent reorganization of the single-particle field, we now find that there is a strong build-up of the shell correction energy at the shape transition temperature. This is a manifestation of the delicate interplay between the self-consistent evolution of the single-particle states with temperature and their occupancies. In phenomenological analyses of the temperature dependence of the level density of deformed nuclei, the temperature induced shell correction would have a role to play. The temperature dependent shell effects are generally included using a single wave fluctuation of the level density $[2][3]$ that corresponds to a fixed set of single particle states; as is seen, for a proper evaluation of the level density for deformed systems the reorganisation of the single particle spectra with temperature need to be considered.

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Figure Captions

Fig. 1 (a) The evolution of the deformation $\beta_2$ as a function of temperature for $^{148}\text{Sm}$ and $^{150}\text{Sm}$. (b) The thermally evolving single-particle neutron spectrum for $^{150}\text{Sm}$.

Fig. 2 (a) The shell-correction energy for $^{150}\text{Sm}$ is shown for different choices of single-particle states (see text). (b) The self-consistent evolution of $\Delta_{sc}$ as a function of temperature for the nuclei $^{148}\text{Sm}$, $^{152}\text{Dy}$ and $^{154}\text{Dy}$.

Fig. 3 (a) Same as Fig. 2a for the nuclei $^{64}\text{Zn}$ and $^{66}\text{Zn}$. (b) Same as Fig. 3b for the systems $^{64}\text{Zn}$ and $^{66}\text{Zn}$.

Fig. 4 The neutron and proton contributions to the total shell-correction energy for the systems $^{150}\text{Sm}$ and $^{64}\text{Zn}$. 
Fig. 1
Fig. 3
Fig. 4

Proton
Neutron

$^{150}$Sm

$^{64}$Zn

$\Delta_{sc}$ (MeV)

T (MeV)