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Temperature and angular momentum dependence of the quadrupole deformation in sd-shell

P A GANAI[1,*], J A SHEIKH[1], I MAQBOOL[1] and R P SINGH[2]
[1]Department of Physics, University of Kashmir, Srinagar 190 006, India
[2]Inter-University Accelerator Centre, New Delhi 110 067, India
*Corresponding author. E-mail: prince_ganai@yahoo.co.uk

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Abstract. Temperature and angular momentum dependence of the quadrupole deformation is studied in the middle of the sd-shell for ^{28}Si and ^{27}Si isotopes using the spherical shell model approach. The shell model calculations have been performed using the standard universal sd-shell (USD) interaction and the canonical partition function constructed from the calculated eigensolutions. It is shown that the extracted average quadrupole moments show a transitional behaviour as a function of temperature and the infered transitional temperature is shown to vary with angular momentum. The quadrupole deformation of the individual eigenstate is also analysed.

Keywords. Spherical shell model; USD interaction; canonical partition function; quadrupole deformation.

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The study of phase transition in quantum many-body systems is one of the frontier research topics in physics. Phase transitions are observed in both macroscopic as well as small quantum many-body systems. In macroscopic systems, for instance, a metallic superconductor, the linear dimension of the system is quite large and the transition from one phase to the other occurs at one point [1]. For small systems, the fluctuations play a very central role and the existence of the discontinuity in the heat capacity critically depends on the number of constituent particles in the system. This has been demonstrated in small metallic grains in which discontinuity is observed with large number of electrons in the grain. However, as the number of electrons in the grain approaches around 100, the discontinuity or the peak structure in the heat capacity disappears [2–5].

Phase transitions have also been studied extensively in atomic nuclei using the Hartree–Fock–Bogoliubov (HFB) method. The HFB theory predicts phase transition as a function of rotational frequency (angular momentum) and temperature (excitation energy). The shape transition as a function of rotational frequency has been well studied in most of the regions of the nuclear chart. In particular, in the rare-earth region the examples of the shape transition are documented in the textbooks [6,7]. Most of the nuclei in this region are prolate deformed with the rotational axis perpendicular to the symmetry axis at low spins and it is known that this shape changes to oblate non-collective at higher angular momenta in many nuclei in this region. For instance, in ^{160}Yb, the shape is prolate for spins up to $40\hbar$ and above this spin value the shape becomes oblate non-collective. The phase transition has also been investigated using the finite temperature HFB approach [8,9] and Landau theory [10]. The main conclusion from these studies is that nuclei which are deformed at low temperatures exhibit a shape transition to spherical shape as the temperature of the system is raised. The critical temperature at which this shape transition occurs has a maximum value for isotopes between magic numbers and in rare-earth nuclei this maximum temperature is about 1.85 MeV [10].

It is known that the phase transition obtained in the above studies critically depends on the inclusion of the quantal and statistical fluctuations [8,11]. In the absence of the fluctuations, the phase transition is sharp first order and when some aspects of the fluctuations are considered, the phase transition is smoothed out. These studies have been mostly performed for heavier nuclei using the grand canonical ensemble. The situation is very different for lighter mass nuclei as it is possible to perform the exact shell model calculations and the canonical partition function can be constructed. The canonical partition function will incorporate fluctuations accurately. The purpose of the present work is to investigate the shape transition in the sd-shell using the canonical partition function constructed from the spherical shell model eigenstates. In a recent work, we have used this approach to study the pairing correlations [12].

The spherical shell model calculations have been performed for ^{28}Si and ^{27}Si using the recently developed shell model program [12,13]. The shell model Hamiltonian, generally, contains single-particle and two-body parts and in the second quantized notation is written as

$$\hat{H} = \hat{h}_{sp} + \hat{V}_2, \tag{1}$$

where

$$\hat{h}_{sp} = \sum_{rs} \epsilon_{rs}\, c_r^\dagger\, c_s, \tag{2}$$

and

$$\begin{aligned}\hat{V}_2 &= \frac{1}{4}\sum_{rstu} \langle rs|v_a|tu\rangle c_r^\dagger c_s^\dagger c_u c_t \\ &= \sum_{rstu\Gamma} \frac{\sqrt{(2\Gamma+1)}}{\sqrt{(1+\delta_{rs})(1+\delta_{tu})}} \langle rs|v_a|tu\rangle_\Gamma \\ &\quad \times (A_\Gamma^\dagger(rs) \times \tilde{A}_\Gamma(tu))_0, \end{aligned} \tag{3}$$

where ϵ_{rs} are the single-particle energies of the spherical shell model states, which are diagonal except in the radial quantum numbers and $\langle rs|v|tu\rangle$ are the two-body interaction matrix elements and in the present work are chosen to be those of 'USD'. The two-particle coupled operator in eq. (3) is given by $A_\Gamma^\dagger(rs) = (c_r^\dagger c_s^\dagger)_\Gamma$ and $\tilde{A}_{\Gamma M_\Gamma} = (-1)^{\Gamma - M_\Gamma} A_{\Gamma - M_\Gamma}$. The labels $r, s, ...$ in the above equations denote the quantum numbers of angular momentum and isospin of the single-particle states. 'Γ' quantum number labels both angular momentum and isospin of the two-particle coupled state. The above notation is the same as that used in [14].

In the present work, the statistical averages have been calculated using the canonical ensemble approach since the exact solutions have well-defined particle number. The average value of a physical quantity F in canonical ensemble is given by [15,16]

$$\langle\langle F \rangle\rangle = \sum_i F_i \mathrm{e}^{-E_i/T}/Z, \tag{4}$$

where

$$Z = \sum_i \mathrm{e}^{-E_i/T}, \quad \hat{H}|i\rangle = E_i|i\rangle, \quad F_i = \langle i|\hat{F}|i\rangle. \tag{5}$$

The statistical averages have been evaluated from the lowest 1000 eigenstates, obtained from the diagonalization of the shell model Hamiltonian, eq. (1), for each angular momentum. For a few cases, we have also calculated the averages with 1500 eigenstates and results were similar to those with 1000 eigenstates.

The average quadrupole moment of the shell model states has been calculated from the expectation value of the operator

$$\hat{Q} = e_p \hat{Q}_p + e_n \hat{Q}_n, \tag{6}$$

where the quadrupole operator is given by

$$\hat{Q}_{p(n)} = \sqrt{16\pi/5} \sum_{rs} \langle r||r^2 Y_2||s\rangle (a_r^\dagger \times \tilde{a}_s)^2. \tag{7}$$

The effective charges $e_p = 1.5$ and $e_n = 0.5$ have been used and the harmonic oscillator length parameter has been calculated with $\hbar\omega = 45A^{-1/3} - 25A^{-2/3}$ [17].

The shell model calculations have been performed in the middle of the sd-shell for ^{28}Si and ^{27}Si with the USD interaction [18]. The results for ^{28}Si and ^{27}Si are presented in figure 1 with the left side depicting the average quadrupole moment for ^{28}Si and the right side the results for ^{27}Si. For ^{28}Si at low temperature, the average quadrupole moment has a constant value of about 20 efm^2 up to temperature, $T = 1.2$ MeV and above this temperature the quadrupole moment drops. For higher temperatures, the quadrupole moment is noted to approach zero, indicating that shape transition from deformed to spherical shape has occurred. It is noted that the drop in the quadrupole moment is spread from $T = 1$ to 4 MeV and it is not possible to determine the exact phase transitional point. In the grand canonical mean-field calculations, the phase transition occurs at one point. In the present canonical study, the phase transition is smeared out due to the fluctuations present. The transitional point in quadrupole moment can be approximately inferred as the middle of two points – one at which the drop begins and the other point where the constant behaviour is again observed. These two temperature points for $I = 2$ in figure 1 are 1 MeV and 4 MeV and, therefore, the transitional point is inferred as $T = 2.5$ MeV. It is to be noted that positive quadrupole moment in figure 1 corresponds to the oblate shape for the ground-state band of ^{28}Si using the standard relationship between the laboratory and intrinsic quadrupole moments [19].

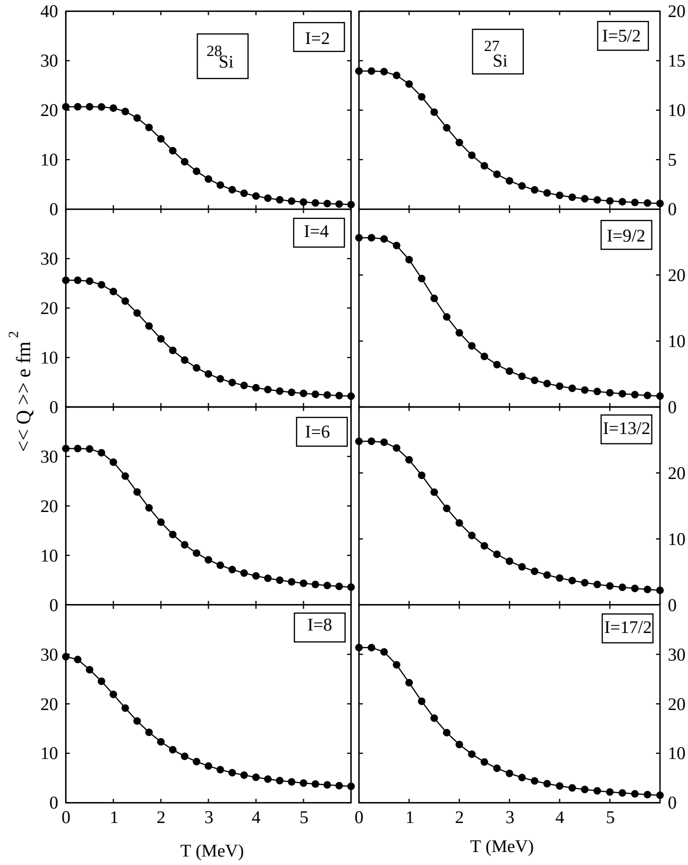

Figure 1. Quadrupole moments are plotted as a function of temperature for various angular momentum states. The left panel depicts the results for ^{28}Si and the right panel for ^{27}Si.

For lighter mass sd-shell nuclei, the question of phase transition has been quite controversial. The mean-field HFB calculations predict the phase transition, evident from the peak structure obtained in the heat capacity [20] at temperature, $T = 2.1$ MeV and the vanishing of the quadrupole moment. The quadrupole moment has a finite value at low temperatures and then depicts a transition at $T = 2.1$ MeV. The canonical shell model calculations, however, depicted a different behaviour. The canonical heat capacity does show a peak structure as in the grand canonical mean-field analysis, but the calculated quadrupole moments did not vanish. The analysis in these investigations were performed mostly for ^{24}Mg and all the angular momentum states were used to construct the canonical partition function [21,22]. In the present study of ^{28,27}Si, the number of eigenstates for each angular momentum are quite large and the partition function for each angular momentum can be independently constructed.

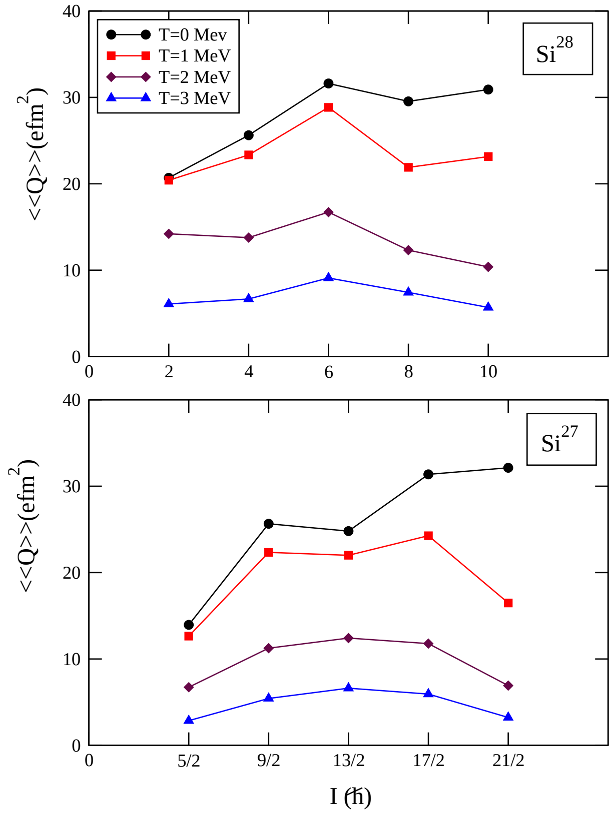

Figure 2. Angular momentum dependence of the quadrupole deformation for temperatures 0, 1, 2 and 3 MeV is plotted for the two studied isotopes of ^{28}Si and ^{27}Si.

It is evident from figure 1 that the quadrupole moments show a transitional behaviour for each calculated angular momentum ensemble. The interesting observation from figure 1 is that the drop in the quadrupole moment is shifted to lower temperatures with increasing angular momentum. For $I = 4$, the drop in quadrupole moment is noted to start at $T = 0.8$ MeV and the transitional point is inferred to be $T = 2.3$ MeV. For $I = 6$, the drop in the quadrupole moment occurs at a slightly lower temperature as compared to $I = 4$ and for $I = 8$ the drop starts at a very low temperature. We have also analysed the temperature behaviour of angular momentum, $I = 1$, 3, 5 and 7 ensembles and for these ensembles the quadrupole moments depict a very irregular dependence on temperature. This would explain the reason that the quadrupole moments in the earlier study did not depict a transitional behaviour as these quantities were averaged over all angular momentum ensembles. Further, results of the present work are in agreement with the mean-field results which predict the transitional behaviour for both quadrupole moment as well as the heat capacity [21]. Although these mean-field calculations were performed for ^{24}Mg, it is expected that these results should be similar for ^{28}Si.

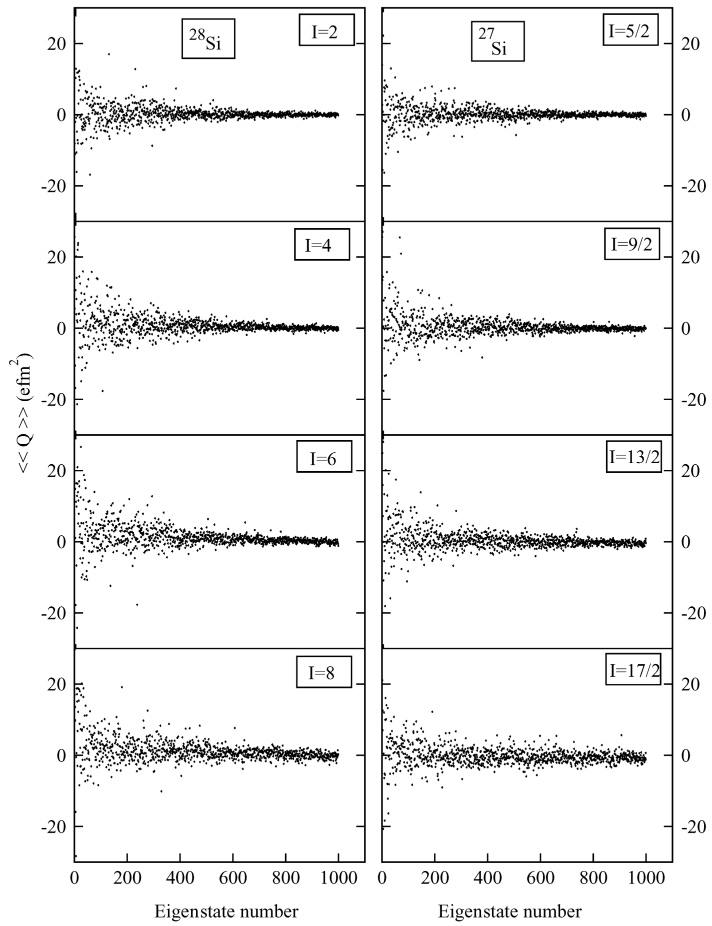

Figure 3. Quadrupole moments are shown for the first 1000 individual eigenstates of the two studied isotopes of ^{28}Si and ^{27}Si.

The results for ^{27}Si, presented on the right side in figure 1, for the angular momentum $I = 5/2$, $9/2$, $13/2$ and $17/2$ ensembles, show that the drop in the quadrupole moment has a similar behaviour as that of the even–even system, ^{28}Si. The transitional point in the quadrupole moment is inferred to be approximately $T = 2.25$ MeV for $I = 5/2$. For $I = 9/2$, this transitional point is slightly lowered and occurs at $T = 2$ MeV. For $I = 13/2$ and $17/2$, the transition also occurs at about $T = 2$ MeV.

In figure 1, quadrupole deformations have been plotted as a function of temperature for a fixed value of angular momentum. It is also quite instructive to show the angular momentum dependence of the quadrupole moment for a fixed value of temperature. In figure 2, angular momentum dependence of the quadrupole deformation for temperatures 0, 1, 2 and 3 MeV is plotted. It is observed from the figure that as the temperature is raised, the quadrupole deformations of higher angular momentum states tends to drop. A clear trend of quadrupole moments dropping with increasing temperature for larger angular momentum ensembles is evident from figure 2.

The advantage in the shell model study is that the analysis can be performed for each individual state [23]. In figure 3, the quadrupole moments are shown for each individual eigenstate and have been plotted for the first 1000 states for both the studied nuclei. The quadrupole moment for the low-lying states are randomly distributed from large positive to negative deformations. However, with increasing eigenstate number, it is evident that the quadrupole moments converge to the spherical shape. In particular, for $I = 2$ and $5/2$, most of the states at higher excitation energy have zero quadrupole moment. The fluctuations from zero quadrupole moment increases with increasing spin and is due to the reason that the dimensionality of the basis states becomes progressively smaller with spin.

In conclusion, temperature and angular momentum dependence of the quadrupole deformation has been studied in the middle of the sd-shell. It is quite evident from the present study that collective states for the studied nuclei, ^{28}Si and ^{27}Si, depict a transitional behaviour from large oblate deformation to spherical shape. This transition is evident from both canonical ensemble study and the quadrupole moments of the individual states.

Finally, we would like to mention that the results of the present work are questionable due to restricted sd-shell configuration space for $T \gtrsim 2.5$ MeV. For higher temperatures, it is expected that the fp-shell will be populated. However, the inclusion of fp shell configuration space is almost impossible in the present context as one needs to evaluate at least 1000 to 1500 eigenstates for each angular momentum to have proper statistical description. The shell model Monte Carlo (SMMC) approach [24] is a possible solution to include the fp-shell and we intend to look into this problem in the near future.

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