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RESEARCH ARTICLE

Shape transitions and fluctuations of hot rotating ^{197}TI nucleus

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Abstract

The shape transitions of nuclei at high excitation energy and the role of thermal fluctuations on the shape parameters is examined. Landau theory of phase transitions is used to determine the shape evolution with temperature and spin. The constants in the Landau expression for free energy are obtained by the free energy surfaces calculated using the finite temperature version of the cranked Nilsson - Strutinsky shell correction method. Paring is not included in the study. We report that the ground state of the considered ^{197}Tl nucleus is prolate. At high spin the nucleus persist in the same shape with much elongation. But at high temperature and spin a spherical to prolate shape transition leading to triaxial is obtained. It is seen that with thermal fluctuations the averaged shapes for the above nuclei at different temperatures and spins are mostly triaxial which are quite different from the most probable prolate or oblate shapes.

Keywords

High spin states of nuclei

Structural transitions

Thermal fluctuations

Landau theory of phase transitions

Cranked Nillsson - Strutinsky method

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Introduction

The study of shape transitions of hot rotating nuclei at high excitation energy is a topic of current interest in nuclear structure studies. Growing experimental information is presently becoming available on the shapes and properties of hot rotating nuclei which are formed in heavy ion fusion reactions where transfer of energy and angular momentum of the relative motion excites the compound nucleus. The properties of hot rotating nuclei are usually studied by observing the particle and γ- decay patterns of the compound nucleus. Hot and rotating nuclei are expected to exhibit a rich variety of different shapes. One of the main prospects of using recently developed multi detector arrays is the more accurate study of shape transitions in hot rotating nuclei. To study the shapes of hot rotating nuclei, mean field theories such as the microscopic Hartree-Fock Bogoliubov cranking theory [1-3] and macroscopic Landau theory [4-6] have to be used. Apart from these, the more appropriate Mottelson – Nilsson [7] and Nilsson – Strutinsky [8-9] approaches can also be used for studying hot rotating nuclei. Mean field theories ignore statistical fluctuations in the order parameters. For a nucleus with finite number of particles, thermal

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fluctuations can be large [10]. They can produce an average value for the order parameters which is qualitatively different from the equilibrium or mean field value [9,11-13]. Theoretically, for finite temperature one should also consider thermal fluctuations. The purpose of this work is to study the shape evolutions in ^{197}Tl nucleus as a function of spin and temperature. In the first phase of this work, the cranked Nilsson Strutinsky method with fixed spin approximation [9] is used to obtain the shape and deformation for the considered nuclei. Then Landau theory of shape transitions is used to study the shape variations due to thermal fluctuations. The outline of the paper is as follows: in section 2, we describe the theoretical framework for obtaining shape evolutions. The third section deals with the Landau theory of shape transitions and the effect of thermal fluctuations on shape parameters. section 4 describes the results obtained along with a detailed discussion. Finally, the paper ends with the conclusions drawn from the study.

Theoretical Framework

Shape of excited Nuclei by mean field method

The cranked Nilsson - Strutinsky method in the rotating frame with cylindrical representation is used for obtaining potential energy surfaces for thallium nucleus. In this method the nucleons move in a cranked Nilsson potential with the deformation determined by β and γ. The cranking is performed around one of the principal axes, the z- axis and the cranking frequency is given by ω. The shell energy calculations for non-rotating case (I=0) assumes a single particle field

$$H^0 = \sum_i h^0 \quad (1)$$

where h^0 is the triaxial Nilsson Hamiltonian given by

$$h_i^0 = \frac{p^2}{2m} + \frac{1}{2} m \sum_{k=1}^{3} \omega_k^2 x_k^2 - \kappa \hbar \overset{0}{\omega}_0 [2l.s + \mu(l^2 - 2\langle l^2 \rangle)] \quad (2)$$

The oscillator frequencies ω_i are given by the Hill Wheeler parameterization as [14]

$$\omega_i = \omega_0 \exp\left[-\sqrt{\frac{5}{4\pi}}\beta \cos\left(\gamma + \frac{2}{3}\pi j\right)\right] \quad (3)$$

with the constraint of constant volume for equipotentials

$$\omega_x \omega_y \omega_z = \overset{0}{\omega}_0^3 = \text{constant}, \quad (4)$$

The oscillator frequencies are chosen separately for protons and neutrons as

$$\hbar\omega_0 = (41MeV) A^{-\frac{1}{3}}\left(1 + \frac{1}{3}\frac{N-Z}{A}\right) \quad \text{for protons}$$

$$\hbar\omega_0 = (41MeV) A^{-\frac{1}{3}}\left(1 - \frac{1}{3}\frac{N-Z}{A}\right) \quad \text{for neutrons} \quad (5)$$

For the Nilsson parameters κ and μ, the following values are chosen [15] separately for protons and neutrons:

Protons		Neutrons	
κ	μ	κ	μ
0.070	0.390	0.073	0.290

In the expression for h_i^0 (Eqn. 2), the term $\langle l^2 \rangle$ has been doubled to obtain better agreement between the Strutinsky-smoothed moment of inertia and the rigid rotor value(here within 10%). Accordingly, the parameter D has been re-determined with the help of single-particle levels in the given mass region. The Hamiltonian (2) is diagonalized in cylindrical representation up to N=11 major shells.

For the rotating case $(I \neq 0)$, the Hamiltonian becomes

$$H^\omega = \sum_i h_i^\omega , \quad (6)$$

where

$$h_i^\omega = h_i^0 - \omega j_z , \quad (7)$$

if it is assumed that the rotation takes place around the Z-axis.

The single particle energy e_i^ω and the wave function ϕ_i^ω are given by

$$h_i^\omega \phi_i^\omega = e_i^\omega \phi_i^\omega \quad (8)$$

The spin projections are obtained as

$$\langle m_i \rangle = \langle \phi_i^\omega | j_z | \phi_i^\omega \rangle \quad (9)$$

The total shell energy is given by

$$E_{sp} = \sum_i \langle \phi_i^\omega | h_i^0 | \phi_i^\omega \rangle = \sum_i \langle e_i \rangle , \quad (10)$$

where

$$e_i^\omega = \langle e_i \rangle - \hbar\omega \langle m_i \rangle \quad (11)$$

Thus the total spin and shell energy for the unsmoothened single particle level distribution is given by

$$I = \sum_i \langle m_i \rangle \quad (12)$$

$$E_{sp} = \sum_i e_i^\omega + \hbar\omega I \quad (13)$$

Since the difficulties encountered in the evaluation of total energy for large deformations through the summation of single particle energies for I=0 case may be present for I≠0 case also [16], we use the Strutinsky shell correction method adopted to I≠0 case by suitably tuning the angular velocities to yield fixed spins.

For the Strutinsky smeared single particle level distribution Eqs. (12) and (13) transform into

$$\tilde{I} = \sum_i \langle \tilde{m}_i \rangle \quad (14)$$

And $$\tilde{E}_{sp} = \sum_i^N \tilde{e}_i^{\omega} + \hbar\omega\tilde{I} \quad (15)$$

The total energy in cranked Nilsson Strutinsky prescription is thus given by

$$E_T(T,I;\beta,\gamma) = E(T,I;\beta,\gamma) - TS - \tilde{E}_{sp}(T,I;\beta,\gamma) + E_{RLDM} \quad (16)$$

where the rotating liquid drop energy at constant spin

$$E_{RLDM} = E_{LDM} - \frac{1}{2} J_{rig}\omega^2 + \hbar\omega\tilde{I} \quad (17)$$

the second term on the right hand side being the rotational energy. Here the liquid drop energy E_{LDM} is given by the sum of Coulomb and surface energies and J_{rig}, the rigid body moment of inertia defined by β and γ including the surface diffuseness correction.

The calculations are carried out by varying ω values in steps of $0.025\omega_0$ from $\omega = 0.0$ to $\omega = 0.3\omega_0$, ω_0 being the oscillator frequency for tuning to fixed spins. γ is varied from -180^0 to -120^0 in steps of -10^0, $\gamma=-180^0$ corresponding to noncollective oblate and $\gamma=-120^0$ corresponding to collective prolate. In a collective rotation, the rotation axis is perpendicular to the symmetry axis. For a non-collective rotation, the rotation axis combines with the symmetry axis. β values are varied from 0.0 to 0.6 in steps of 0.1.

For calculating the single particle energies the cranked Nilsson triaxial model is used with Hill-Wheeler parameterization for the frequencies so as to deal with very large deformations. It is to be stated that pairing is not taken into account in these calculations. Thermal fluctuations are not taken into account in the first calculations.

Effect of thermal fluctuations using Landau Theory of Phase Transitions

For finite temperatures, one should also consider the thermal fluctuations which create shapes different from the most probable shape obtained by minimizing the free energy F = E - TS. These shape fluctuations can significantly alter the properties of hot rotating nuclei. According to this theory, the free energy at $\omega = 0$ can be written to fourth order in β as

$$F(T,\omega=0,\beta,\gamma) = Fo(T) + A(T)\beta^2 - B(T)\beta^3\cos 3\gamma + C(T)\beta^4 \quad (18)$$

where the coefficients Fo, A, B and C depend on the temperature T and β and γ are the usual intrinsic deformation parameters.

The free energy which depends on β and γ will also depend on the orientation angles relative to the rotation axis ω for the rotating case $\omega \neq 0$.

Extending Eqn. (18) to the rotating case with ω parallel to Z axis,

$$F(T,\omega,\beta,\gamma) = F(T,\omega=0;\beta,\gamma) - \frac{1}{2} J_{zz}(\beta,\gamma,T)\omega \quad (19)$$

For fixed spin this can be Legendre transformed as

$$F(T,I;\beta,\gamma) = F(T,I=0;\beta,\gamma) + \frac{I^2}{2J_{zz}(\beta,\gamma,T)} \quad (20)$$

where

$$J_{zz} = J_0(T) - 2R(T)\beta\cos\gamma + 2J_1(T)\beta^2 + 2D(T)\beta^2\sin^2\gamma \quad (21)$$

with J, R and D suitably defined to absorb various numerical constants. The R term has the leading shape dependence of the rigid-body moment of inertia, while the D term alone would represent the leading shape dependence of the irrotational moment of inertia. For ω dependent terms in eqn. (19), as in reference [17,18], the rigid-body moment of inertia is assumed, setting

$$J_0 = \frac{2}{5} m A R_0^2, \quad R = \left[\frac{5}{16\pi}\right]^{1/2} J_0 \quad \text{and} \quad (22)$$

$$D = J_1 = 0$$

In this study, the Landau constants A(T), B(T) and C(T) are evaluated by least square fitting with the ω = 0 free energy surfaces obtained by Strutinsky method. This method has the advantage that the accuracy of the fitting can be checked by the resulting error bars.

In the Strutinsky prescription, the free energy is computed as

$$F(T,I;\beta,\gamma) = E(T,I;\beta,\gamma) - TS - \tilde{E} + E_{RLDM} \quad (23)$$

Here, S is the total entropy of the fermion gas and is given by

$$S = -\sum_{i=1}^{\infty}[f_i \ln f_i + (1-f_i)\ln(1-f_i)] \quad (24)$$

Expressed in terms of Fermi-Dirac occupation numbers

$$f_i = \frac{1}{1+\exp[\frac{(e_i^{\omega}-\lambda)}{T}]} \quad (25)$$

The chemical potential □ □ with the constraint $\sum_{i=1}^{\infty} f_i = N$, where N is the total number of particles.

$$E_{RLDM} = E_{LDM} - \frac{1}{2}J_{rig}\omega^2 + \hbar\omega\tilde{I} \quad (26)$$

Here the liquid drop energy E_{LDM} is given by the sum of Coulomb and surface energies, J_{rig} the rigid body moment of inertia defined by β and γ including the surface diffuseness correction, and $\tilde{I}$ is the Strutinsky smoothed spin.

Thermal fluctuations and their effect on the shape parameters

For a nucleus with finite number of particles and at moderately high temperatures, thermal fluctuations produce an average shape, which is qualitatively different from equilibrium shapes predicted by mean field theories. These shape fluctuations can significantly alter the properties of hot rotating nuclei. The probability of finding the nucleus in a state with deformation $\alpha_{2\mu}$ is characterized by the free energy $F(\alpha_{2\mu}; I,T)$ is,

$$\mathrm{P}(\alpha_{2\mu};I,T) \propto e^{-F(\alpha_{2\mu};I,T)/T} \quad (27)$$

with $$F(\alpha_{2\mu};I,T) = E(\alpha_{2\mu};I,T) - TS$$

Using classical statistics, therefore, the ensemble average of an observable X which is deformation – dependent, is given by an average over all possible shapes.

$$\overline{X}(I,T) = \frac{\int X(\alpha_{2\mu};I,T)e^{-F(\alpha_{2\mu};I,T)/T}D[\alpha_{2\mu}]}{\int D[\alpha_{2\mu}]e^{-F(\alpha_{2\mu};I,T)/T}} \quad (28)$$

where $D[\alpha_{2\mu}]$ is the volume element in the deformation space. Using equation (28), the ensemble average of β is,

$$\overline{\beta} = \langle\beta\rangle = \frac{\int \beta\mathrm{P}(\beta,\gamma)\beta^4\left|\sin 3\gamma\right| d\beta d\gamma}{\int \mathrm{P}(\beta,\gamma)\beta^4\left|\sin 3\gamma\right| d\beta d\gamma} \quad (29)$$

Similarly the ensemble average of γ is

$$\overline{\gamma} = \langle\gamma\rangle = \frac{\int \gamma\mathrm{P}(\beta,\gamma)\beta^4\left|\sin 3\gamma\right| d\beta d\gamma}{\int \mathrm{P}(\beta,\gamma)\beta^4\left|\sin 3\gamma\right| d\beta d\gamma} \quad (30)$$

where $\beta^4\left|\sin 3\gamma\right| d\beta d\gamma$ is the volume element as given in the Bohr rotation – vibration model.

Equation (27) shows that when the temperature is zero, there are no thermal shape fluctuations. Then the averaged shape is identical to the most probable shape. But at finite temperature, the averaged shape may be different from the most potable shape.

Results and Discussion

The aim of this work is to study the shape evolutions in hot rotating ^{197}Tl nucleus using cranked Nilsson Strutinsky method including the most important thermal fluctuations. The first step in the study of shape evolutions in hot rotating medium mass nuclei is to use the cranked Nilsson - Strutinsky method. The second step is to study the shape evolutions and the effect of thermal fluctuations on shape transitions using Landau theory in the considered nuclei. We performed calculations taking γ = -120^0 to -180^0 in steps of –10^0 and the deformation parameter β is varied from 0.0 to 0.6 in steps of 0.1 and spin I = 0 to 50$\hbar$ for different temperatures. The resulting free energy surfaces are then least square fitted with those of Landau theory to extract the respective Landau constants. Then the averaged values of β and γ are evaluated by using equation (28) to obtain the shape variations with thermal fluctuations.

Shape evolutions using cranked Nilsson – Strutinsky method

In order to carryout an depth study of shape transitions in hot rotating ^{197}Tl nucleus we have used the cranked Nilsson – Strutinsky method. Thermal fluctuations are not included in these first calculations. In the calculations performed here to generate the potential energy surfaces, the spin is varied from I = 0 to 50 ħ at different temperatures such as T = 0.0 MeV, T = 0.5 MeV, T = 1.5 MeV, T = 2.0 MeV and T = 2.5 MeV. The Hill - Wheeler expressions for the frequencies have been used in the cranked Nilsson model in order to take care of large deformations involved in the calculations. Calculations have been done for neutron and proton levels separately by choosing the appropriate constants κ and μ applicable for this region [15]. The energy levels are generated up to N = 11 shells which is found to be sufficient for these calculations.

Figures 1 to 6 show the shape transitions with spin (*) obtained at temperatures T = 0.0 MeV, T = 0.5 MeV, T = 1.0 MeV, T = 1.5 MeV, T = 2.0 MeV and T = 2.5 MeV respectively for ^{197}Tl. It is noted from **Fig 1** that ^{197}Tl nucleus is prolate in shape at its ground state (T = 0.0 MeV and I = 0 ħ) with deformation β = 0.1. The nucleus stays in the prolate shape on further increase of spin with deformation increases as a function of spin. As spin increases the nuclei undergo a shape transition to triaxial (near oblate) shape at I = 40 ħ and then to oblate at I = 50 ħ. At temperature T = 0.5 MeV **Fig 2**, the ^{197}Tl nucleus takes a shape transition from spherical to prolate on increasing spin. It stays in the oblate shape on further increase of spin and the deformation reaches 0.3 at spin I = 50 ħ. Almost the same trend is obtained for temperature T = 1.0 MeV **Fig 3**. At temperature T = 1.5 MeV **Fig 4**, the nuclei undergo spherical to prolate transition with deformation increases as a function of spin and this happens up to spin I = 40 ħ. At I = 50 ħ there occurs a shape transition leading to triaxial (near oblate) shape. At temperature T = 2.0 MeV **Fig 5** the shape changes from oblate to prolate and then to clear triaxial shape. At higher temperature T = 2.5 MeV **Fig 6**, a same type of spherical to prolate transition is obtained as a function of spin. At this temperature and at high spin of about I = 40 ħ, a more elongated form of ellipsoidal configuration with β = 0.3 is obtained. On further increase of spin an antistretching effect is obtained as a function of spin. It is noted from the above figures that the shape of ^{197}Tl nucleus is prolate in its ground state and at high temperature and spin, it undergo a spherical to prolate and then to triaxial transition which is in confirmity with the experimental observation.

Effect of thermal fluctuations on shape parameters using Landau Method

For the study of shape evolutions in medium mass nuclei at moderate temperatures, it is necessary to include thermal fluctuations which may create shapes different from the most probable shape obtained by cranked Nilsson Strutinsky method. In the second step we have studied the effect of thermal fluctuations on shape evolutions of ^{197}Tl using the Landau theory of shape transitions. The Landau constants A(T), B(T) and C(T) are evaluated by least square fitting with the ω=0 free energy surfaces obtained by using the cranked Nilsson-Strutinsky method. In this, the expansion of the Landau free energy is done up to fourth power of β. In the calculations performed here, to generate ω=0 free energy surface, the spin is varied from I = 0 ħ to 50 ħ in steps of 10 ħ at temperatures T = 0.0 MeV, T = 0.5 MeV, T = 1.0 MeV, T = 1.5 MeV, T = 2.0 MeV and T = 2.5 MeV.

In the potential energy calculation the deformation parameters β and γ are varied in the range β = 0.0 to 0.6 with $\Delta\beta$ = 0.1 and γ = -180^o to –120^o with $\Delta\gamma$ = -10^o. Since the considered nuclei fall in the mass region A=190, calculations have been done for neutron and proton levels separately by choosing the appropriate constants κ and μ applicable for the region considered.

In Table 1 we give the results of A(T), B(T) and C(T) at various temperatures obtained by using Landau method for ^{197}Tl. In this study, this is done by using the extrema fitting method. The variations of τ, B/C and B^4/C^3 with temperature for the nuclei ^{197}Tl obtained by using Strutinsky method is given in figures 3.7 to 3.9, from which the Landau constants can be extracted. It is noted from these figures that the variations in the Landau parameters are mild at high temperatures. In figures 3.2 to 3.6 we present also the shape evolutions with spin obtained for temperatures T = 0.5 MeV, T = 1.0 MeV, T = 1.5 MeV, T = 2.0 MeV and 2.5 MeV respectively for ^{197}Tl with thermal fluctuations using Strutinsky method (•). The shape evolutions obtained with spin at different temperatures without thermal fluctuations (*) using Strutinsky method as described is also presented for comparison. It is noted from figures 3.2 to 3.6 that when thermal fluctuations are not included, a sharp shape transition from spherical to prolate (*) is obtained as a function of spin. But when thermal fluctuations are included, these sharp shape transitions turn into triaxial shapes (•) with γ fascinating in between –140^0 and –160^0 which is clearly seen. It becomes clear from these figures that the sharp spherical and oblate/prolate shapes are washed out when thermal fluctuations are incorporated.

Summary and Conclusion

To conclude, in this work we have made an attempt to study the shape evolutions in hot rotating ^{197}Tl nuclei using cranked Nilsson – Strutinsky method. In the ground state the considered ^{197}Tl nuclei is found to be prolate. At high spin the nucleus persist in the same shape with much elongation. But at high temperature and spin a spherical to prolate shape transition leading to triaxial is obtained. Any study involving hot rotating nuclei should incorporate thermal fluctuations in its fold. With this view we have used the Landau theory of shape transitions with free energy expansion up to fourth power of β to include thermal fluctuations. The sharp shape transitions obtained by Strutinsky method, turn into triaxial shapes when thermal fluctuations are included. Most of our predictions are well matching with the available experimental results applicable to the considered nuclear region. It should be interesting to see experimentally whether such phase transitions and large deformations can be detected in this heavy nuclei through giant dipole resonance (GDR) built on excited states.

Table 1 Landau constants for ^{197}Tl obtained by Strutinsky method using Least square fit (extrema fitting method).

T(MeV)	A(T)	B(T)	C(T)
0.5	81.7302 $\pm 8.2302 \times 10^{-2}$	-5.7178 $\pm 2.4394 \times 10^{-1}$	-17.3757 $\pm 1.3918 \times 10^{-2}$
1.0	83.4815 $\pm 6.9218 \times 10^{-2}$	-5.4214 $\pm 2.0516 \times 10^{-1}$	-17.6373 $\pm 1.1705 \times 10^{-2}$
1.5	80.5684 $\pm 3.7702 \times 10^{-2}$	-4.391 $\pm 1.1175 \times 10^{-1}$	-11.3385 $\pm 6.3757 \times 10^{-3}$
2.0	76.6544 $\pm 1.6581 \times 10^{-2}$	-4.1246 $\pm 4.9145 \times 10^{-2}$	-4.9452 $\pm 2.8039 \times 10^{-3}$
2.5	75.6593 $\pm 5.9801 \times 10^{-3}$	-3.7696 $\pm 1.7725 \times 10^{-2}$	-1.690 $\pm 1.0113 \times 10^{-3}$

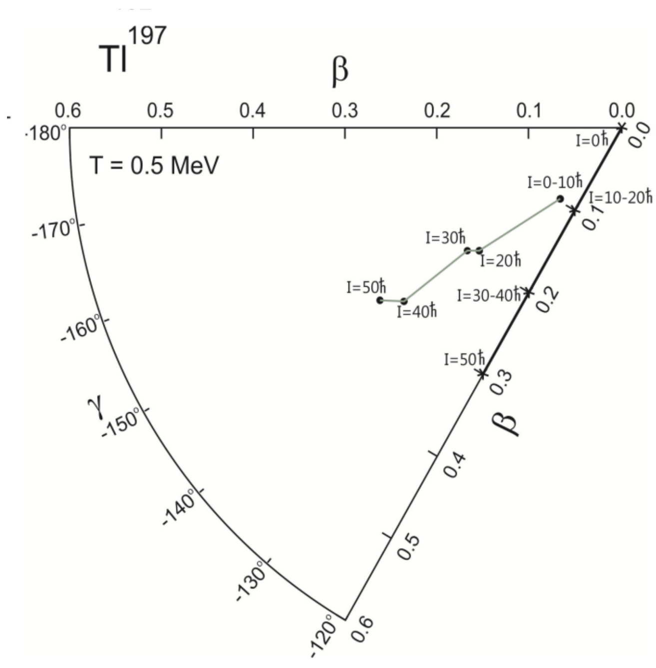
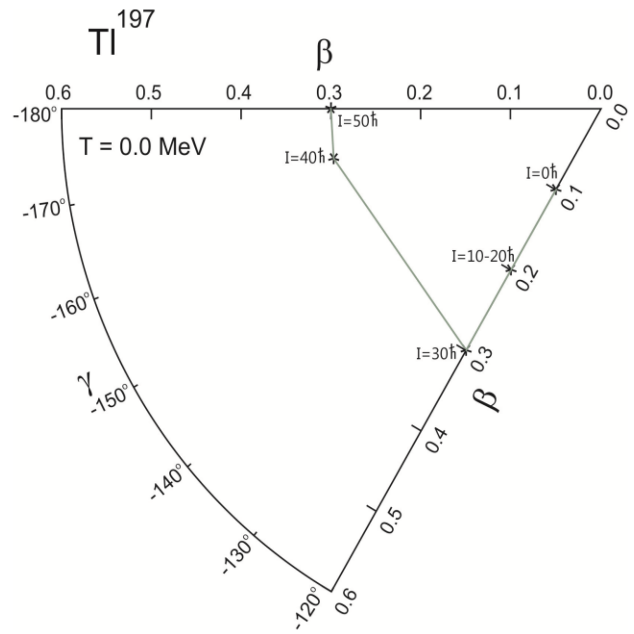


Fig 2 Shape evolutions in ^{197}Tl obtained as a function of spin at temperature T = 0.5 MeV with (•) and without (*) thermal fluctuations.



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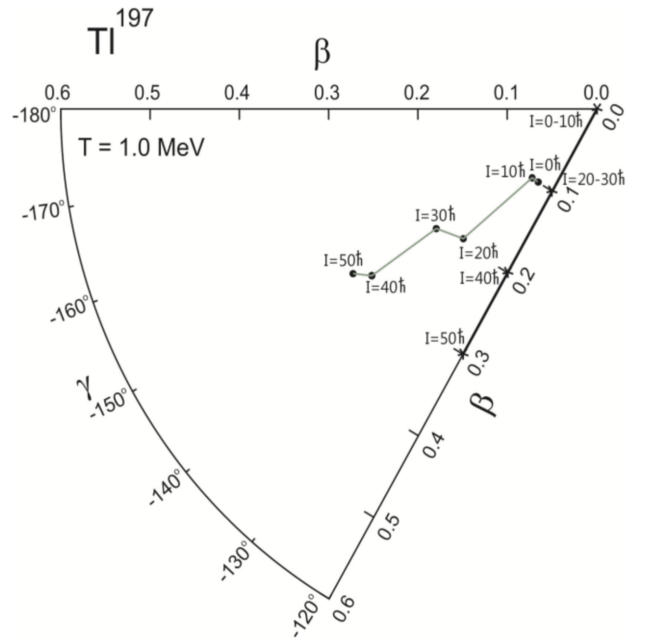

Fig 3 Shape evolutions in ^{197}Tl obtained as a function of spin at temperature T = 1.0 MeV with (•) and without (*) thermal fluctuations.

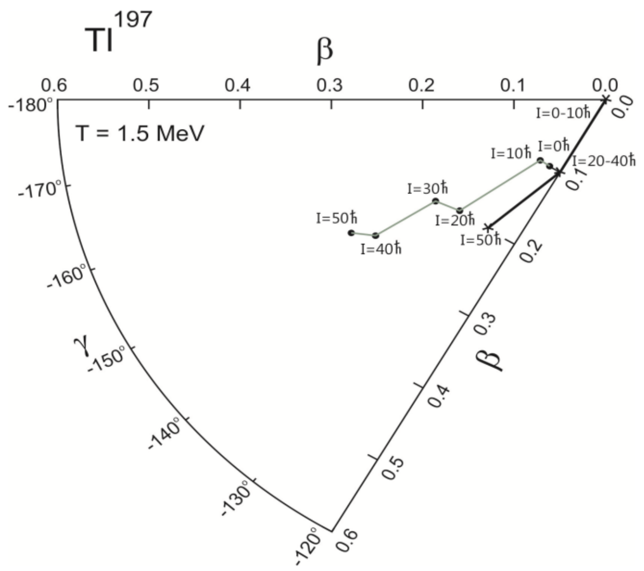

Fig 4 Shape evolutions in ^{197}Tl obtained as a function of spin at temperature T = 1.5 MeV with (•) and without (*) thermal fluctuations.

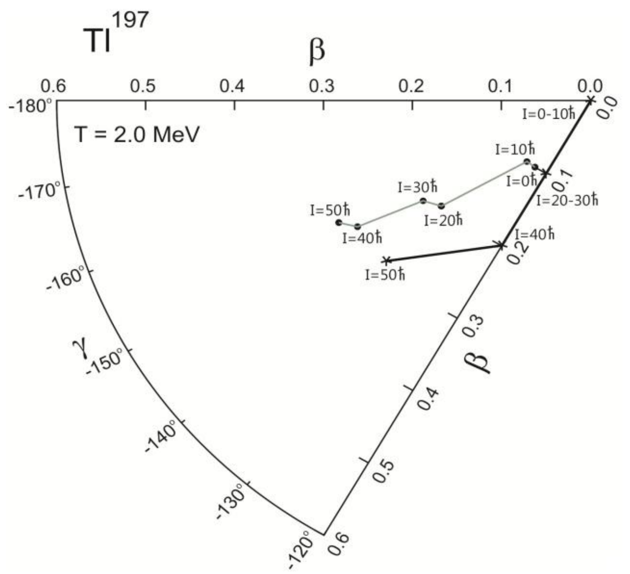

Fig 5 Shape evolutions in ^{197}Tl obtained as a function of spin at temperature T = 2.0 MeV with (•) and without (*) thermal fluctuations.

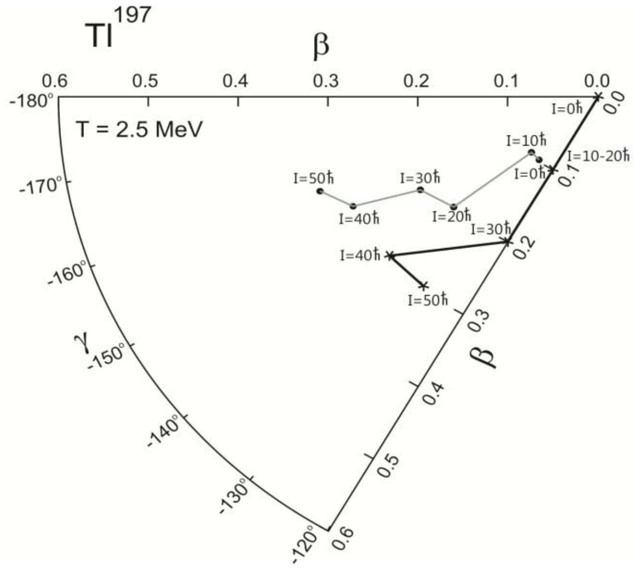

Fig 6 Shape evolutions in ^{197}Tl obtained as a function of spin at temperature T = 2.5 MeV with (•) and without (*) thermal fluctuations

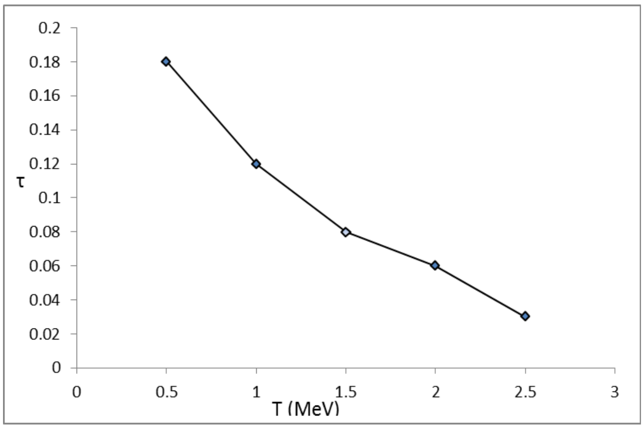

Fig 7 Variation of τ with temperature for ^{197}Tl using ω=0 free energy surfaces obtained by the Strutinsky method.

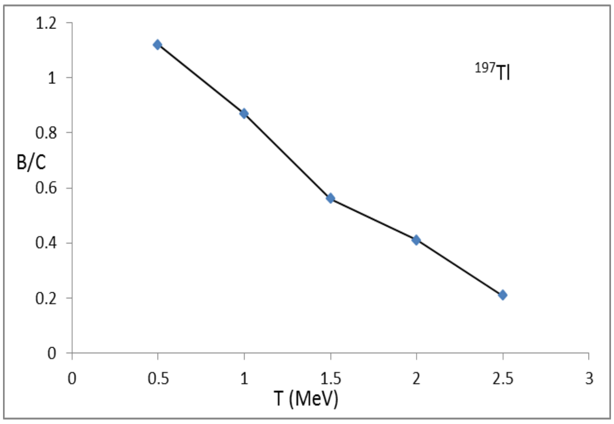

Fig 8 Variation of B/C with temperature for ^{197}Tl using ω=0 free energy surfaces obtained by the Strutinsky method.

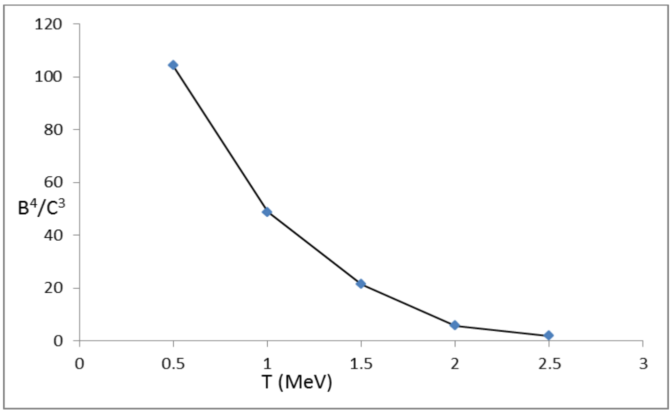

Fig 9 Variation of B^4/C^3 with temperature for ^{197}Tl using ω=0 free energy surfaces obtained by the Strutinsky method.

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