SURFACE PROPERTIES OF HOT THERMALLY FISSILE NUCLEI

International School of Nuclear Physics (40th course)
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September 18, 2018

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Plan of the talk:

- Introduction
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  - Neutron rich thermally fissile nuclei
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- Formalism
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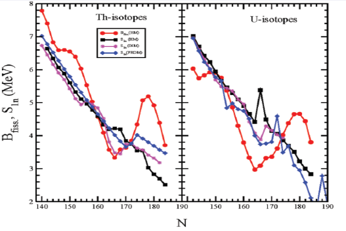
Introduction: Thermally fissile nuclei

- Thermally fissile nuclei have the tendency to undergo fission even when a zero energy neutron (at room temperature) hit them.
- In nature, ^{233,235}U and ^{239}Pu have the thermally fissile characteristics. Out of these, ^{235}U is naturally available with the isotopic fraction of abundance $\sim$ 0.7%.
- ^{233}U and ^{239}Pu are formed by ^{232}Th and ^{238}U, respectively, through neutron absorption and subsequent $\beta-$ decay processes.
- One of the applications of thermally fissile nuclei is to use them in controlled energy production.
- Because of the limited availability of these nuclei, we concern whether any other heavier isotopes possessing thermally fissile properties could exist or can be synthesized in a laboratory.

Introduction: Neutron-rich thermally fissile nuclei

- It is important to mention that Satpathy *et.al.*, have found some neutron-rich Thorium and Uranium isotopes, showing the thermally fissile behavior [1].
- They have made the prediction on the basis of neutron separation energy (S_n) and fission barrier height (B_{fiss}) and found that neutron rich isotopes of Uranium with neutron number $N = 154 - 172$ exhibit the thermally fissile nature.



- These predicted neutron-rich thermally fissile nuclei, having an excess of neutrons, can produce more energy than that of naturally available thermally fissile nuclei.

[1] Pramana Journal of Physics **70**, 87 (2008).

Introduction: Way of fissioning

- In a fission process, the naturally available thermally fissile nuclei ^{233,235}U and ^{239}Pu absorb a slow neutron and make the compound nuclei ^{234,236}U and ^{240}Pu, respectively. These compound nuclei are further fissioned into fragments and emit neutrons.
- The neutron rich thermally fissile nuclei undergo multi-fragmentation fission; an exotic decay mode where along with fragments some prompt scission neutrons are emitted from the neck [1].
- Such properties will have important implications in stellar evolution involving r-process nucleosynthesis.
- The exotic fission process is directly connected with the neutron multiplicity of the surface region.
- Due to the importance of thermally fissile nuclei, it would be worthy to study their bulk and surface properties.

Introduction: Surface properties

Symmetry energy

- Symmetry energy is the energy cost in converting asymmetric nuclear matter to symmetric one.
- The isospin asymmetry in nuclear matter arises due to the differences in densities and masses of protons and neutrons.
- Nuclear symmetry energy plays its crucial role in different areas of nuclear physics, for example, in structure of ground state nuclei, dynamics of heavy-ion reactions, and the structure, dynamics, and composition of neutron stars [2].

[2] J. Phys. G: Nucl. Part. phys. **45**, 075102 (2018) and the referneces therein,

Introduction: Surface properties

- Experimentally, symmetry energy is not a direct measurable quantity. It is extracted from the observables related to it.
- It has been found that neutron skin thickness of ^{208}Pb is correlated to symmetry energy, L-coefficient, and the size of the neutron star [3].
- Even the precise measurement of neutron skin thickness is difficult, yet it is a sensitive probe of the nuclear symmetry energy.
- Along with the symmetry energy, we have also calculated the neutron pressure, curvature coefficient, neutron skin thickness, and the deformation parameters of ^{234,236}U, ^{240}Pu, and ^{250}U at finite temperature.
- The symmetry energy, neutron pressure, and curvature coefficient of the nuclei are calculated from the corresponding quantities of nuclear matter by using the local density approximation.

[3] Phys. Rev. Lett. **85**, 5296 (2000).

Introduction: Why at finite temperature?

- S. J. Lee *et.al.*, showed that the surface symmetry energy term is more sensitive to temperature than the volume energy term [4].
- The dependence of symmetry energy on density and temperature have a crucial role in understanding various phenomena in heavy ion collision, supernovae explosions, the liquid-gas phase transition of asymmetric nuclear matter, and mapping the location of neutron drip line in the nuclear landscape [5].
- The probability of fission fragments and hence the fission yield change at finite temperature [6].

[4] Phys. Rev. C **82**, 064319 (2010).
[5] Phys. Rep. **410**, 335 (2005).
[6] Phys. rev. C **95**, 064613 (2017).

Formalism:

Temperature Dependent Relativistic Mean Field Model (TRMF)

RMF is one of the microscopic model which successfully predict ground state properties of nuclei like binding energy, deformation parameter, charge radius *etc*.. In this model, nucleon are considered to move in the mean field of residual nucleon. They interact through the exchange of meson. The RMF Lagrangian density is given as:

$$
\begin{aligned}
\mathcal{L}(r) \;=\;& \bar{\varphi}(r)\left(i\gamma^{\mu}\partial_{\mu} - M + g_s\sigma - g_{\omega}\gamma^{\mu}\omega_{\mu} - g_{\rho}\gamma^{\mu}\tau\vec{\rho}_{\mu} - e\gamma^{\mu}\frac{1+\tau_3}{2}A_{\mu}\right)\varphi(r) \\
&+\frac{1}{2}\left(\partial^{\mu}\sigma\partial_{\mu}\sigma - m_s^2\sigma^2\right) - \frac{1}{4}V^{\mu\upsilon}V_{\mu\upsilon} + \frac{1}{2}m_{\omega}^2\omega^{\mu}\omega_{\mu} \\
&-\frac{1}{4}\vec{R}^{\mu\upsilon}\vec{R}_{\mu\upsilon} + \frac{1}{2}m_{\rho}^2\vec{\rho}^{\mu}\vec{\rho}_{\mu} - \frac{1}{4}F^{\mu\upsilon}F_{\mu\upsilon} \\
&-m_s^2\sigma^2\left(\frac{k_3}{3!}\frac{g_s\sigma}{M} + \frac{k_4}{4!}\frac{g_s^2\sigma^2}{M^2}\right) + \frac{1}{4!}\zeta_0 g_{\omega}^2(\omega^{\mu}\omega_{\mu})^2 \\
&-\Lambda_{\omega}g_{\omega}^2g_{\rho}^2(\omega^{\mu}\omega_{\mu})(\vec{\rho}^{\mu}\vec{\rho}_{\mu}) \qquad (1)
\end{aligned}
$$

By using variational principle and applying mean field approximation, equations of motion for nucleonic and mesonic fields are obtained. Redefining fields as $\Phi = g_s\sigma$, $W = g_\omega\omega^0$, $R = g_\rho\vec{\rho}^0$ and $A = eA^0$, the Dirac equation corresponds to the above Lagrangian density is

$$\Big\{ -i\alpha\cdot\nabla + \beta[M - \Phi(r)] + W(r) + \frac{1}{2}\tau_3 R(r) + \frac{1+\tau_3}{2}A(r)\Big\}\varphi_i(r) = \varepsilon_i\,\varphi_i(r) \tag{2}$$

The equations of motion for Φ, W, R and A fields are given as

$$-\Delta\Phi(r) + m_s^2\Phi(r) = g_s^2\rho_s(r) - \frac{m_s^2}{M}\Phi^2(r)\left(\frac{\kappa_3}{2} + \frac{\kappa_4}{3!}\frac{\Phi(r)}{M}\right) \tag{3}$$

$$-\Delta W(r) + m_\omega^2 W(r) = g_\omega^2\rho(r) - \frac{1}{3!}\zeta_0 W^3(r) - 2\,\Lambda_\omega R^2(r)W(r) \tag{4}$$

$$-\Delta R(r) + m_\rho^2 R(r) = \frac{1}{2}g_\rho^2\rho_3(r) - 2\,\Lambda_\omega R(r)W^2(r) \tag{5}$$

$$-\Delta A(r) = e^2\rho_{\rm p}(r) \tag{6}$$

where the baryon, scalar, isovector and proton densities are

$$\rho(r) = \sum_i n_i \varphi_i^\dagger(r)\varphi_i(r) = \rho_p(r) + \rho_n(r) \quad (7)$$

$$\rho_s(r) = \sum_i n_i \varphi_i^\dagger(r)\beta\varphi_i(r) = \rho_{sp}(r) + \rho_{sn}(r) \quad (8)$$

$$\rho_3(r) = \sum_i n_i \varphi_i^\dagger(r)\tau_3\varphi_i(r) = \rho_p(r) - \rho_n(r) \quad (9)$$

$$\rho_{\mathrm{p}}(r) = \sum_i n_i \varphi_i^\dagger(r)\left(\frac{1+\tau_3}{2}\right)\varphi_i(r) \quad (10)$$

Formalism: TRMF...

The energy densities for nucleonic and mesonic fields corresponding to the above Lagrangian density are

$$\mathcal{E}_{nucl.}(r) = \sum_i \varphi_i^{\dagger}(r)\Big\{ -i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta\,[M-\Phi(r)] + W(r) + \frac{1}{2}\tau_3 R(r) + \frac{1+\tau_3}{2}A(r)\Big\}\varphi_i(r) \quad (11)$$

and

$$\mathcal{E}_{mes.}(r) = \frac{1}{2g_s^2}\left[(\boldsymbol{\nabla}\phi(r))^2 + m_s^2\phi^2(r)\right] + \left(\frac{\kappa_3}{3!}\frac{\Phi(r)}{M} + \frac{\kappa_4}{4!}\frac{\Phi^2(r)}{M^2}\right)\frac{m_s^2}{g_s^2}\Phi^2(r) - \frac{1}{2g_\omega^2}\left[(\boldsymbol{\nabla}W(r))^2 + m_\omega^2 W^2(r)\right] - \frac{1}{2g_\rho^2}\left[(\boldsymbol{\nabla}R(r))^2 + m_\rho^2 R^2(r)\right] - \frac{\zeta_0}{4!}\frac{1}{g_\omega^2}W^4(r) - \Lambda_\omega R^2(r)\cdot W^2(r) \quad (12)$$

Formalism: TRMF...

The total energy is given by

$$E(T) = \sum_i \epsilon_i n_i + E_{mes.} + E_{pair} + E_{c.m.} \quad (13)$$

with

$$E_{pair} = -G\left[\sum_{i>0} u_i v_i\right]^2 \quad (14)$$

$$E_{c.m.} = -\frac{3}{4} \times 41 A^{-1/3} \quad (15)$$

The temperature introduced through the partial occupancies which is given as,

$$n_i = v_i^2 = \frac{1}{2}\left[1 - \frac{\epsilon_i - \lambda}{\tilde{\epsilon}_i}[1 - 2f(\tilde{\epsilon}_i, T)]\right] \quad (16)$$

with

$$f(\tilde{\epsilon}_i, T) = \frac{1}{(1 + exp[\tilde{\epsilon}_i / T])} \quad and$$

$$\tilde{\epsilon}_i = \sqrt{(\epsilon_i - \lambda)^2 + \triangle^2} \quad (17)$$

Formalism: Temperature dependent equation of state and nuclear matter properties

Energy density

$$
\begin{aligned}
\mathcal{E}(T) &= \frac{2}{(2\pi)^3}\int d^3k\,\epsilon_i^*(k)(f_{i+}+f_{i-}) + \rho W + \frac{m_s^2\Phi^2}{g_s^2}\left(\frac{1}{2}+\frac{\kappa_3}{3!}\frac{\Phi}{M}+\frac{\kappa_4}{4!}\frac{\Phi^2}{M^2}\right) \\
&\quad -\frac{1}{2}m_\omega^2\frac{W^2}{g_\omega^2}-\frac{1}{4!}\frac{\zeta_0 W^4}{g_\omega^2}+\frac{1}{2}\rho_3 R-\frac{1}{2}\frac{m_\rho^2}{g_\rho^2}R^2-\Lambda_\omega(R^2\times W^2) \qquad (18)
\end{aligned}
$$

Pressure

$$
\begin{aligned}
P(T) &= \frac{2}{3(2\pi)^3}\int d^3k\,\frac{k^2}{\epsilon_i^*(k)}(f_{i+}+f_{i-}) - \frac{m_s^2\Phi^2}{g_s^2}\left(\frac{1}{2}+\frac{\kappa_3}{3!}\frac{\Phi}{M}+\frac{\kappa_4}{4!}\frac{\Phi^2}{M^2}\right) \\
&\quad +\frac{1}{2}m_\omega^2\frac{W^2}{g_\omega^2}+\frac{1}{4!}\frac{\zeta_0 W^4}{g_\omega^2}+\frac{1}{2}\frac{m_\rho^2}{g_\rho^2}R^2+\Lambda_\omega(R^2\times W^2) \qquad (19)
\end{aligned}
$$

Formalism: Temperature dependent equation of state and nuclear matter properties

with the equilibrium distribution functions defined as

$$f_{i_\pm} = \frac{1}{1 + exp[(\epsilon_i^* \mp \nu_i)/T}, \qquad (20)$$

where $\epsilon_i^* = (k^2 + M_i^{*2})^{1/2}$ $(i = p, n)$, $M_{p,n}^* = M_{p,n} - \Phi$, k is the momentum of nucleon, and the nucleon effective chemical potential

$$\nu_i = \mu_i - W - \frac{1}{2}\tau_3 R; , \qquad (21)$$

where τ_3 is the third component of isospin operator.

Formalism: Temperature dependent equation of state and nuclear matter properties

The binding energy per nucleon $\mathcal{E}/A$=$e(\rho,\alpha)$ (where ρ is the baryon density) can be expanded by Taylor series expansion method in terms of isospin asymmetry parameter α $\left(= \frac{\rho_n-\rho_p}{\rho_n+\rho_p}\right)$:

$$e^{NM}(\rho,\alpha) = \frac{\mathcal{E}}{\rho_B} - M = e^{NM}(\rho,\alpha=0) + S^{NM}(\rho)\alpha^2 + \mathcal{O}^{NM}(\alpha^4), \quad (22)$$

where $e(\rho,\alpha=0)$ is the energy density of the symmetric nuclear matter (SNM) and $S(\rho)$, is the symmetry energy of a system, which is defined below.

$$S^{NM}(\rho) = \frac{1}{2}\left[\frac{\partial^2 e^{NM}(\rho,\alpha)}{\partial\alpha^2}\right]_{\alpha=0}. \quad (23)$$

Formalism: Temperature dependent equation of state and nuclear matter properties

Near the saturation density ρ_0, the symmetry energy can be expanded through the Taylor series as:

$$S^{NM}(\rho) = J^{NM} + L^{NM}\mathcal{Y} + \frac{1}{2}K_{sym}^{NM}\mathcal{Y}^2 + \mathcal{O}^{NM}[\mathcal{Y}^3], \tag{24}$$

where $J^{NM} = S^{NM}(\rho_0)$ is the symmetry energy at saturation and $\mathcal{Y} = \frac{\rho-\rho_0}{3\rho_0}$. The coefficients $L^{NM}(\rho_0)$, and $K_{sym}^{NM}(\rho_0)$ are defined as:

$$L^{NM} = 3\rho \frac{\partial S^{NM}(\rho)}{\partial \rho}\bigg|_{\rho=\rho_0} = \frac{3P^{NM}}{\rho}\bigg|_{\rho=\rho_0}, \tag{25}$$

$$K_{sym}^{NM} = 9\rho^2 \frac{\partial^2 S^{NM}(\rho)}{\partial \rho^2}\bigg|_{\rho=\rho_0}, \tag{26}$$

Here, L^{NM}, P^{NM}, and K_{sym}^{NM} represent the slope parameter, pressure and curvature of symmetric nuclear matter at the saturation density, respectively.

Formalism: Local density approximation (LDA)

In LDA, the symmetry energy coefficient is given by [7]

$$S(T)\left(\frac{N-Z}{A}\right)^2 = \frac{1}{A}\int \rho(r) S^{NM}[\rho(r), T]\left[\frac{\rho_n(r)-\rho_p(r)}{\rho(r)}\right]^2 d\mathbf{r}, \qquad (27)$$

where, $S^{NM}[\rho(r), T]$ is the symmetry energy of infinite symmetric nuclear matter at finite temperature (T) and at the local density $\rho(r)$ of a nucleus. Similarly, we can find the pressure and curvature coefficient.

[7] Phys. Rev. C **76**, 041602(R), (2007).

Parameters used:

Table: The table for parameter sets. The nucleon mass M taken as 939.0 MeV. All the coupling constants are dimensionless, except k_3 which is in fm^{-1}.

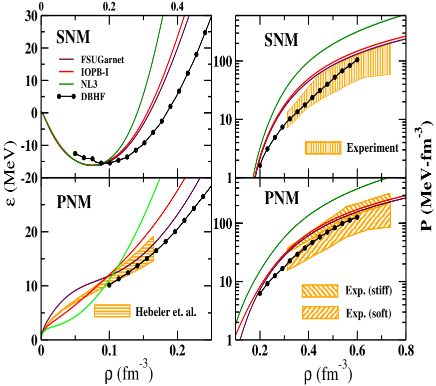
	NL3	FSUGarnet	IOPB-I
m_s/M	0.541	0.529	0.533
m_ω/M	0.833	0.833	0.833
m_ρ/M	0.812	0.812	0.812
$g_s/4\pi$	0.813	0.837	0.827
$g_\omega/4\pi$	1.024	1.091	1.062
$g_\rho/4\pi$	0.712	1.105	0.885
k_3	1.465	1.368	1.496
k_4	-5.688	-1.397	-2.932
ζ_0	0.0	4.410	3.103
Λ_ω	0.0	0.043	0.024
ρ_0 (fm^{-3})	0.148	0.153	0.149
$\mathcal{E}_0$(MeV)	-16.29	-16.23	-16.10
M^*/M	0.595	0.578	0.593
J^{NM}(MeV)	37.43	30.95	33.30
L^{NM}(MeV)	118.65	51.04	63.58
K_{sym}^{NM}(MeV)	101.34	59.36	-37.09

1

[1] NL3: PRC **55**, 540 (1997); FSUGarnet: PLB **748**, 284 (2015); IOPB1: Phys. Rev. C **97**, 045806 (2018).

Nuclear Matter

Results and discussion: Equation of state of nuclear matter



- FSUGarnet is the softer among the chosen parameter sets.

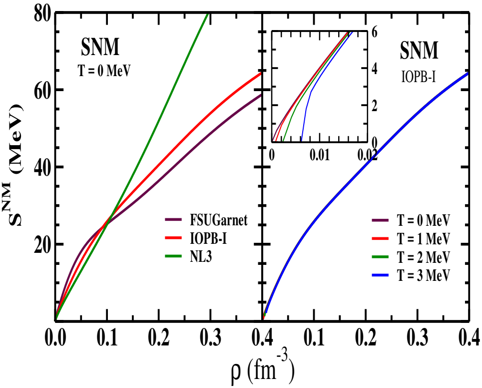
Ref:-

Hebeler: Astrophys. J. **773**, 11 (2013).

DBHF: Phys. Rev. C **45**, 2782 (1992); Phys. Rev. C **77**, 015801 (2008).

Exp.: Science **298**, 1592 (2002).

Results and discussion: Temperature dependent symmetry energy of nuclear matter



- The effect of temperature can be observed at higher temperature (T). Here, at low values of T, the symmetry energy is almost same with a little difference at low density.

Finite Nuclei

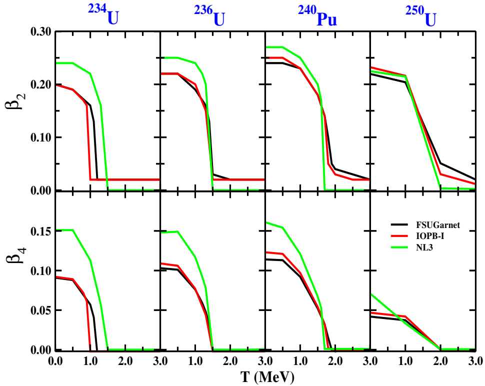
Results and discussion: Ground and excited state properties

Table: The calculated binding energy per particle (B/A) (MeV), charge radius (R_c) (fm) and deformation parameter β_2 of the nuclei ^{234,236,250}U and ^{240}Pu at finite temperature T (MeV) are tabulated and compared with the available experimental data [8].

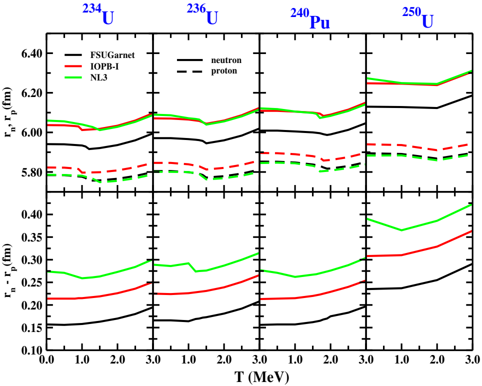
Temp.	^{234}U			^{236}U			^{240}Pu			^{250}U			Para.
	B/A	R_c	β_2	B/A	R_c	β_2	B/A	R_c	β_2	B/A	R_c	β_2	
T = 0	7.60	5.84	0.20	7.57	5.86	0.22	7.56	5.91	0.24	7.41	5.95	0.22	FSUG.
	7.61	5.88	0.20	7.59	5.90	0.22	7.57	5.95	0.25	7.43	5.99	0.23	IOPB
	7.60	5.84	0.24	7.58	5.86	0.25	7.55	5.90	0.27	7.42	5.94	0.22	NL3
	7.60	5.83	0.27	7.59	5.84	0.27	7.56	5.87	0.29	-	-	-	Exp.
T = 1	7.55	5.83	0.16	7.54	5.85	0.19	7.51	5.90	0.23	7.37	5.94	0.20	FSUG.
	7.56	5.85	0.02	7.55	5.89	0.20	7.52	5.94	0.23	7.39	5.99	0.22	IOPB
	7.51	5.84	0.22	7.50	5.85	0.24	7.47	5.90	0.25	7.33	5.94	0.21	NL3
T = 2	7.35	5.82	0.02	7.32	5.83	0.02	7.29	5.87	0.04	7.15	5.92	0.05	FSUG.
	7.35	5.86	0.01	7.33	5.88	0.02	7.29	5.91	0.03	7.16	5.96	0.03	IOPB
	7.28	5.81	0.00	7.26	5.82	0.00	7.22	5.86	0.00	7.09	5.91	0.00	NL3
T = 3	6.95	5.86	0.02	6.94	5.87	0.02	6.90	5.90	0.02	6.75	5.95	0.02	FSUG.
	6.94	5.90	0.01	6.93	5.91	0.02	6.89	5.95	0.02	6.75	6.00	0.01	IOPB
	6.87	5.84	0.00	6.85	5.86	0.00	6.82	5.91	0.00	6.68	5.94	0.00	NL3

[8] http://nndcbnl.gov

Results and discussions: β_2 and β_4

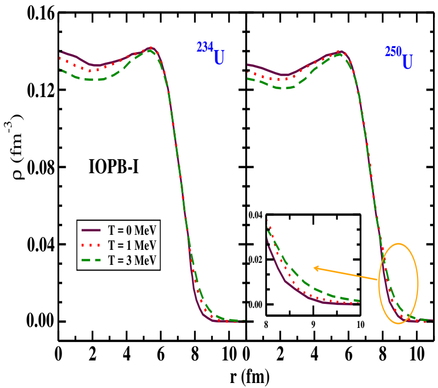


- Both β_2 and β_4 becomes zero at some finite T. This temp. is known as critical temp. (T_c) or transition temperature.
- At T_c, the shape of a nucleus changes from deformed to spherical and remain as it is even on further increasing the T.



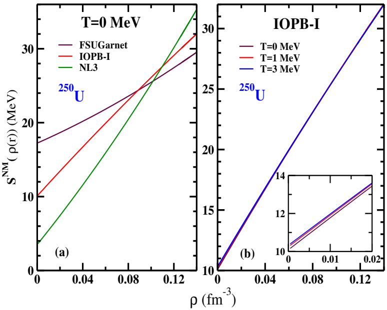
- Both r_n and r_p, first decrease and become minimum at $T = T_c$ and then gradually increase (nucleus expands with T).
- The skin thickness predicted by IOPB-I set is moderate to that predicted by FSUGarnet and NL3 parameters.

Results and discussion: Spherical equivalent density



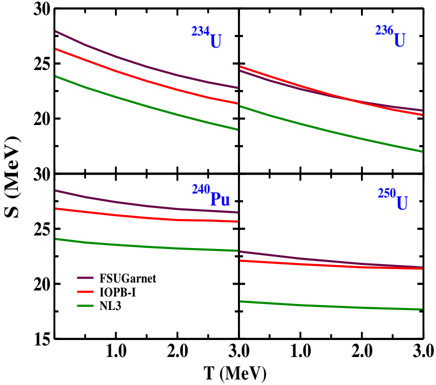
- With the application of T, random motion of nucleon is increased. Nucleons move toward the surface. As a results, the central density of a nucleus decreases and the surface density is enhanced slightly.

Results and discussion: Symmetry energy of nuclear matter at the local density of the nuclei



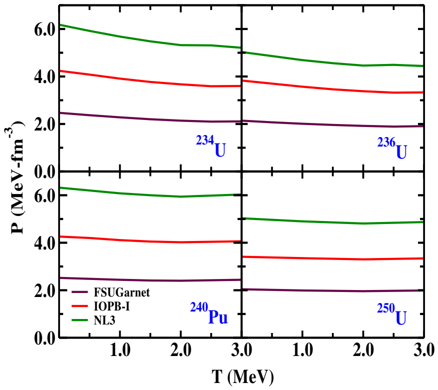
- The symmetry energy at the local density of the nuclei is large for softer EOS (FSUGarnet) and small for NL3 which is comparatively stiffer . But, this nature is get reversed at higher density $\sim 0.10 fm^{-3}$.
- The effect of T on the symmetry energy at the local density of the nuclei is again minuscule with the little difference which can be seen in the zoomed part of the figure.

Results and discussion: Symmetry energy coefficient



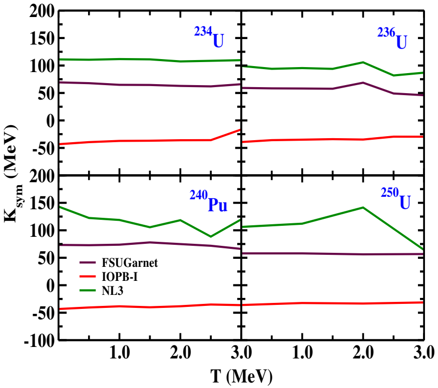
- The symmetry energy coefficient for ^{250}U is smaller as compared to the rest of the nuclei. This can be attributed to the large iso-spin asymmetry in ^{250}U.
- A small number of symmetry energy enhance the rate of conversion of protons to neutrons through electron capture. (Phys. Rep. **411**, 325 (2005).)

Results and discussion: Neutron pressure



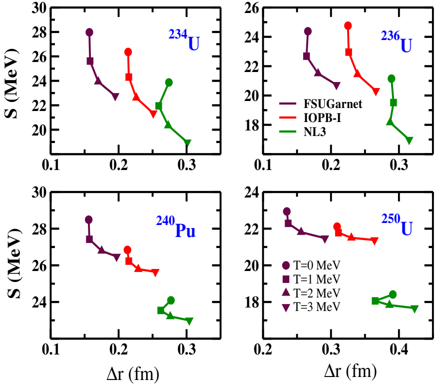
- The pressure of the nuclei is also decreased with increasing the T.
- Here, the nature corresponding to parameter sets is reversed to that observed in the case of symmetry energy curve. Stiffer the EOS, higher be the pressure of the nuclei. The same nature is observed for nuclear matter.

Results and discussion: Curvature coefficient



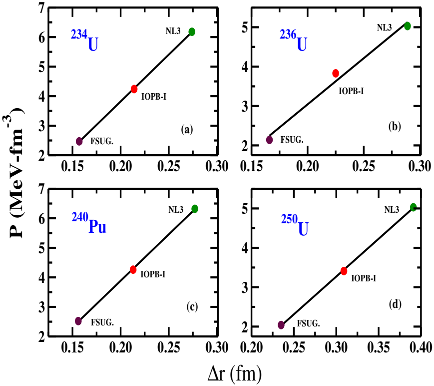
- The nature of the curvature coefficient is almost same as that of the pressure.
- It plays the role in the scattering phenomenon of nuclei. (Phys. Rev. C **82**, 064602)

Results and discussion: Symmetry energy and neutron skin thickness of the nuclei



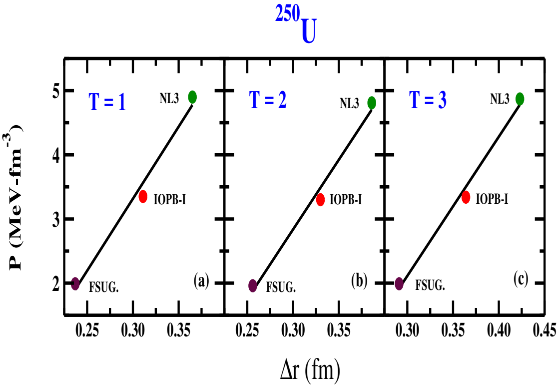
- As we have seen that skin thickness increases while symmetry energy decreases with increasing the T.
- It can be concluded that symmetry energy is decreased with growing of the skin thickness of a nucleus.

Results and discussion: Neutron pressure and skin thickness (at T=0)



- The figure exhibit that how the neutron pressure and the skin thickness are correlated corresponding to the parameter sets.
- It shows that the skin thickness of the nuclei is large corresponding to the stiffer EOS and vice versa.

Results and discussion: Neutron pressure and skin thickness (at finite T)



- The same quantities are plotted at the finite T for ^{250}U as the representative case. The correlation between these quantities exist even at finite T.

Conclusion:

- We have calculated the temperature dependent surface properties like neutron skin thickness, deformation parameters, symmetry energy coefficient, neutron pressure and curvature coefficient for thermally fissile nuclei.
- We have used IOPB-I and FSUGarnet parameter sets and compared the calculated results with the predictions of NL3 set.
- The calculated properties can be used for the production/synthesis of neutron rich/drip line nuclei.
- The properties can be used to constrain the EOS of neutron star.

Acknowledgment

- We are very grateful to Dr. Bharat Kumar, Prof B. K. Agrawal and Prof. J. N. De for their fruitful discussion.
- I am grateful to Institute of Physics, Bhubaneswar for providing necessary computer facility and great hospitality during the period of this work. Partial support from DST to carry out the work is greatly acknowledged.
- I am thankful to Science and Engineering Research Board (SERB), India for providing travel support to attend this Erice school and to Ettore Majorana Foundation for providing the fellowship, covering the full lodging and fooding during the school.
- Thankful to all the organizers of the school.

Thank You....