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Temperature Dependent Thermal Properties of ^{40}Ca Nucleus

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***Abstract* – In this work, the thermal properties of double magic ^{40}Ca nucleus have been investigated. Mean field calculations are performed. An effective Hamiltonian is based on Nijmegen (Nigm.II) potential. The framework of the constrained finite temperature Hartree-Fock (FTHF) method is used. The calculations are performed in no-core model space consisting of six major oscillator shells (i.e. 21 single particle orbits). The sensitivity of the thermal properties such as: binding energy, nuclear radius, entropy and free energy, is investigated to the degree of heating. This study was carried in a temperature range zero to 8 MeV. As the temperature of nucleus is increased by 8 MeV, it shows about 310.917 MeV of excitation energy to achieve a 29.8% volume increasing during heating. It means that volume coefficient of expansion of the nucleus is increased with increased temperature. The specific heat of the nucleus is decreased as the temperature is increased. The free energy of the nucleus is inversely proportional with temperature. The volume of the nucleus approximately undergoes quadratic radial expansion with temperature. Finally the entropy behavior exhibits almost a linear dependence on temperature for T > 1MeV, the absence of response at low temperature is due to shell-closure effects.**

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I. Introduction

Investigating the properties of finite nucleus in its excitation state is very useful for understanding the products in heavy ion collisions, barrier heights or saddle point configuration in nuclear fission.

The study of nuclear thermodynamics is very important to understand heavy-ion experiments and nuclear reactions [1, 2]. This study of thermal excitations in finite nuclei is very interest because there is great important in nuclear properties above the ground state[3].Hot and highly excitation nuclei are very important to understand structure nuclear physics and ion beams collision. The experimental works depend on fission type or heavy ion collisions. The theoretical works are based on thermodynamical equilibrium and introduced the partition function with relevant quantities such as density, entropy, excitation energy, etc.

Realistic effective Hamiltonians have been adapted to the finite temperature Hartree-Fock (FTHF) method[4].The Hartree-Fock (HF) method is an approximate method for the determination of the ground-state wavefunction and ground-state energy of a quantum many-body system. The Hartree-Fock method assumes that the exact, N-body wavefunction of the system can be approximated by a single Slater determinant (in the case where the particles are fermions). Invoking the variation principle one can derive a set of N coupled equations for the spin-orbital. Solution of these equations yields the Hartree-Fock wavefunction and energy of the system, which are approximations of the exact ones. The Hartree-Fock method is also called, the self-consistent field method (SCF) because the resulting equations are almost universally solved by means of an iterative, fixed-point type algorithm. So by using computational methods we will start from an initial guess a trail wave function and a starting energy - then evaluate numerically the thermal properties, using a generated FORTRAN code developed for this purpose. The iteration will continue until convergence of the solution occurs.

The main aim of this paper is done same work of Bozzoloet.al.[5], but we adopt the different interaction, i.e. we use effective Nijmegen (Nigm.II) potential and the calculations are performed in no-core space. This is done to study of different interaction on nuclear thermal properties. Also, we increase scale of temperature to 8 MeV and also we calculate for other nuclear properties such as free energy, entropy and volume expansion. We use ^{40}Ca nucleus because it is double magic nucleus with magic number 20.

This paper is organized as follows: Sec.2 contains formalism. Sec. 3 specifies the results and discussions, while conclusion is given in Sec. 4.

II. Formalism

A nuclear system of A-nucleon (N neutrons and Z protons) is considered with its spin s and isospin τ are 1/2 for each. The Hamiltonian of this system consists of the single particle kinetic energy and the two-body interaction as:

$$\widehat{H} = \sum_{i=1}^{A} \hat{T} + \sum_{i<j}^{A} V_{ij} \quad (2.1)$$

where $\hat{T}_i$ denotes the single particle kinetic energy operator, which in terms of single particle momentum $\vec{p}$ is:

$$\hat{T}_i = \frac{\vec{p}^2}{2m} \quad (2.2)$$

here m is the nucleon mass. V_{ij} is the two-body interaction term. It is two body V_{NN} and Coulomb V_C interactions between protons that are included.

The exact solution of the Schrödinger equation in the full infinite Hilbert space of all possible nucleons many-body configurations was solved for light nuclei with mass number smaller than 20 only [6-9]. For mass number greater than 20, the infinite Hilbert space is replaced with a finite model space and an effective Hamiltonian, H_{eff}, is used in the truncated model space. So, Eq. (2.1) can be written as:

$$\widehat{H}'_{eff} = \sum_{i=1}^{A} \widehat{T}_i + \sum_{i<j}^{A} (V_{eff})_{ij} \quad (2.3)$$

A two-body effective Hamiltonian $\widehat{H}'_{eff}$ is introduced by using the relative kinetic energy operator $(T_{rel})_{ij}$ instead of the single particle energy operator.

$$\widehat{H}'_{eff} = T_{rel} + V_{eff} = T_{rel} + V_{eff}^{NN} + C_C \quad (2.4)$$

where $(T_{rel})_{ij}$ represents the pure two body natures. This is evident form the relative kinetic energy operator between pairs of nucleons

$$(T_{rel})_{ij} = (\vec{p}_i - \vec{p}_j)^2 / 2mA \quad (2.5)$$

The V_{eff}, however, is the sum of Brueckner G-matrix based on the Nijm. II interaction and the lower order folded diagram (2nd order in G) acting between pair of nucleons in the no-core model space [10, 11].

The matrix element of the two-body part of the effective Hamiltonian is constructed by using two-particle harmonic oscillator basis. They have good total angular momentum J and isospin τ.

There are two infinities: dimensional Hilbert space and short range repulsion of the core potential. The solution to the first is by truncating the full Hilbert space using Block-Horowitz theory. The second is removed by solving the Brueckner-Bethe Goldstone equation; the potential V matrix elements are replaced by the Brueckner G-matrix elements in the series expansion of V_{NN}.

$$G(\omega) = V + VQ/(\omega - H_0)G(\omega) \quad (2.6)$$

where the variable ω is the starting energy and Q is the Pauli operator. It prohibits particles from scattering into occupied states. H_0 is the unperturbed single particle Hamiltonian [12].

To evaluate matrix element of H'_{eff}, the harmonic oscillator basis are chosen with $\hbar\omega$ = 14.0 MeV. The relative and center of mass coordinates can be separated by using harmonic oscillator wave function. Therefore, a great simplification results in the calculation of the two-body matrix elements.

By applying the variation principle, the Hartree-Fock equation for nucleon orbits can be derived by using the effective Hamiltonian within the chosen model space. Compression is achieved by applying a static load. The radial constraint acts like an external force to compress or expand the nucleus. For details see Refs. [13-20].

In the present calculations, no-core oscillator model space that includes 6 major oscillator shells was used. In the 6 shells, 21 nucleon orbits were used: $0s_{1/2}$, $0p_{3/2}$, $0p_{1/2}$, $0d_{5/2}$, $1s_{1/2}$, $0d_{3/2}$, $0f_{7/2}$, $1p_{3/2}$, $0f_{5/2}$, $1p_{1/2}$, $0g_{9/2}$, $1g_{7/2}$, $1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$, $0h_{11/2}$, $0h_{9/2}$, $1f_{7/2}$, $1f_{5/2}$, $2p_{3/2}$ and $2p_{1/2}$. The picture of the model space which is used in this study was completed.

In particular, a no-core model space of six major shells was chosen in order to avoid calculating core polarization effects with realistic effective interaction. In addition, all nucleons were active, and hence there were no terms in the expansion that involves particle-hole excitations.In any microscopic calculation, the equilibrium state of a nuclear system at a nonzero temperature is found by minimizing the grand potential functional Ω. For T = 0, this is equivalent to minimizing the energy functional. The grand potential is a quantity used in statistical mechanics, especially for irreversible processes in open systems.

$$\Omega = E - TS - \mu N \quad (2.7)$$

Where E is the energy, T is the temperature of the system, S is the entropy, μ is the chemical potential and N is the number of particles in the system.

In the mean field approximation, the grand potential depends on the density ρand the minimization is done with respect to this density. The entropy and the particle number N are constrained by the temperature and the chemical potential.Thus, given an effective Hamiltonian H_{eff} for the nuclear system in a truncated model space, the variation of the functional is considered.

$$\Omega(T, \mu, D) = \langle H_{eff} \rangle - TS - \mu N$$
$$= tr(H_{eff} D) + Ttr(DlnD) - \mu tr(DN) \quad (2.8)$$

where (tr) denotes the trace of the matrix.With respect to the trial many body density matrix D, the usual requirement on D is that: $tr(D)$ = 1. Taking D as:

$$D = e^{-G}/tr(e^{-G}) \quad (2.9)$$

where

$$G = \sum_{\alpha,\beta} g_{\alpha\beta} a_\alpha^+ a_\beta \quad (2.10)$$

Here G is an arbitrary one-body operator, $a_\alpha^+ a_\beta$ are raising and lowering operators, respectively, and $\rho_{\alpha\beta}$ is defined as:

$$\rho_{\alpha\beta} = tr(D a_\alpha^+ a_\beta) \quad (2.11)$$

So that the radial density distribution is given by:

$$\rho = (1 + e^g)^{-1} \quad (2.12)$$

It can be written that:

$$\langle H_{eff} \rangle = tr(t\rho + 1/2\, \rho\, V_{eff}\, \rho\ ) \quad (2.13)$$

In Eq. (2.13), t is the kinetic energy operator, V_{eff} is the two body effective interaction of H_{eff}, and tr denotes the trace over the single particle indices.

The entropy is:

$$\begin{aligned} S = -tr(D\ln D) &= tr(DG) + \ln[tr(e^{-G})] \\ &= tr(\rho g) + tr\ln(1+e^{-g}) \\ &= -tr(\rho\ln\rho) \\ &\quad -tr\{(1-\rho)\ln(1-\rho)\ln(1-\rho)\} \end{aligned} \quad (2.14)$$

The number of particles in the system is:

$$N = tr(\rho) \quad (2.15)$$

Entropy is an extensive state function that accounts for the effects of irreversibility in thermodynamic systems, particularly in heat engines during an engine cycle. While the concept of energy is central to the first law of thermodynamics, which deals with the conservation of energy, the concept of entropy is central to the second law of thermodynamics, which deals with physical processes and whether they occur spontaneously. Spontaneous changes occur with an increase in entropy. Entropy change has often been defined as a change to a more disordered state at a microscopic level.

By using Eqs. (2.13 – 2.15) in Eq. (2.8), it can be obtained

$$\begin{aligned} \Omega(T,\mu,\rho) &= tr(t\rho + 1/2\rho V_{eff}\rho) \\ &\quad + Ttr(\rho\ln\rho) + Ttr\{(1-\rho)\ln(1-\rho)\} - \mu\, tr(\rho) \end{aligned} \quad (2.16)$$

Minimizing Eq. (2.16) with respect to ρ gives the temperature dependent Hartree-Fock equations.

$$\rho = \{1 - \exp[(h-\mu)/T]\}^{-1} \quad (2.17)$$

Where

$$h = t + \rho V_{eff} \quad (2.18)$$

At equilibrium, solution of the above equations at each T provides the entropy, radial density distributions and the free energy which define by the first and the second terms of the Hartree-Fock energy [21] as the Helmholtz free energy:

$$F = E - TS \quad (2.19)$$

The Helmholtz free energy is a measure of the amount of energy you have to put in to create a system once the spontaneous energy transfer to the system from the environment is accounted for.

Now, from the first and second laws of thermodynamics, it is possible to obtain the inequality

$$TdS \geq dE + dW \quad (2.20)$$

where dW is the work done by the nucleus under heating and the equality sign holds for a thermodynamically reversible process.

Finally, it is possible to express the specific heat (C_V) of the nucleus in terms of the free energy as:

$$C_V = -T\left\{\frac{\partial^2 F}{\partial T^2}\right\}_V \quad (2.21)$$

This formalism is commonly referred to as the finite temperature Hartree-Fock method.

III. Results and Discussion

The results of the properties of ^{40}Ca nucleus namely the binding energy, the root mean square radius (r_{rms}), free energy (F) and entropy (S) are presented. These results are obtained using the model space of six major oscillator shells within the constrained spherical Hartree-Fock (*CSHF*) approximation based on Nijm.II potential.

The adjusting parameters are listed in table (I). With these parameters, an equilibrium root mean square radius r_{rms} and E_{HF} are found using the Nigm.II potential. The value of λ_1 is less than unity. This is because the kinetic energy operator (T_{rel}) is a positive definite operator and if it is normalized by itself into a finite model space this will reduce its magnitude. The value of λ_2 is greater than unity in order to compensate for the lack of sufficient binding when the full Hilbert space is truncated to a finite model space.

Work	Potential	λ_1	λ_2	$\hbar\omega'$(MeV)
Our work	Nijmegen	0.915	1.000	6.800
Ref.[5]	Reid Soft Core	0.985	1.290	7.870

Table I: Values of adjusting parameters of the effective Hamiltonian for ^{40}Ca in six oscillator shells with *N-N* interaction to get an agreement between *HF* results and experimental data [22]. The binding energy (point mass r_{rms}) that was fitted was -342 MeV (3.484 fm) for ^{40}Ca.

The E_{HF} energies versus temperature using Nijm.II potential are displayed in figure (1). It can be seen from the figure that energy curve does not show any response to temperature at T<1*MeV*. After this range, the curve increases sharply with increasing temperature. This result is due to expansion that is happened to the nucleus. So that the binding energy of the nucleus is decreased with increases temperature.

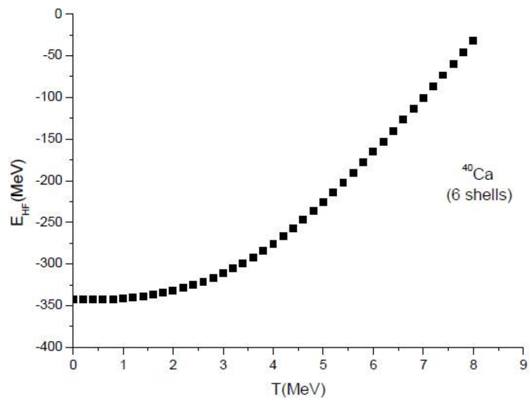

Fig. 1. Constrained spherical Hartree-Fock energy for ^{40}Ca in six-oscillator shells versus temperature by using Nijm.II potential.

It can be noted from the Fig.(1) that E_{HF} increases steeply towards zero binding energy under heating. As the temperature increased by 8 MeV, the binding energy will be about 310.917 MeV. That means, it shows 310.917 MeV of excitation energy to achieve a 8 MeV temperature increasing.

In this work, our results are the same behavior of figure 6 in Ref. [5]. There is different in values of excitation energiesfrom those reported in Ref. [5], because the calculations are done with different potentials.

In Fig. (2), the Helmholtz free energy as a function of temperature is displayed. The dependence of the free energy on temperature is initially constant and the turning approximately quadratic for $T > 1MeV$.

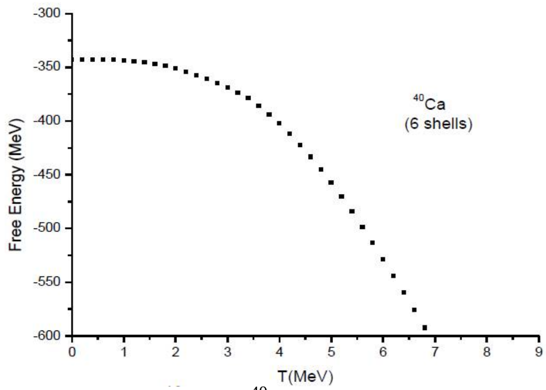

Fig. 2. The free energy for ^{40}Ca in six-oscillator shells as a function of temperature

Fig. (2) shows that the change of the free energy will decrease by an amount greater than work done by the nucleus. The usefulness of knowledge of the free energy arises also from its relation to other thermodynamic functions of the nucleus. For example, consider a reversible change in the nucleus such that the temperature change by 8 MeV and the only work done is that due to the expansion of the nucleus as its volume increases by 29.8%. It can be seen from Fig. (2), the specific heat, C_V, of the nucleus is decreased as the temperature is increased.

To compare our results with figure 7 of Ref. [23], the behavior of Helmholtz free energy is the same. The difference estimates of the calculations; our results are for block, but the results of Ref. [23] ware for surface with different space.

Figure (3) displays the root mean square radius (r_{rms}) as a function of temperature using Nigm.II as the N-N interaction. The curve shows that there is no response of r_{rms} to temperature for $T \leq 1$ MeV. This behavior can be understood as a result of shell-closure effects. It can be noted that the cure appears to show that the nucleus approximately undergoes a quadratic radial expansion with temperature(i.e., $r_{rms} \alpha T^2$).

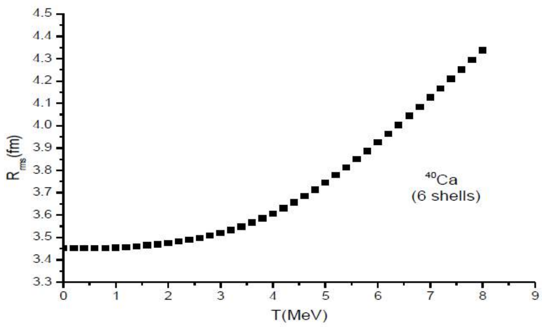

Fig. 3. The root mean square radius (r_{rms}) versus temperature for ^{40}Ca in a model space of six major oscillator shells.

Fig. (3) shows the change of volume of the nucleus with temperature. As the temperature of nucleus is increased by 8 MeV, it shows about 310.917 MeV of excitation energy to achieve a 29.8% volume increasing during heating. It means that volume coefficient of expansion of the nucleus is increased with increased temperature.Our results are consistent with figure 2 in Ref. [24] with different nuclei and methods.

Fig. (4) presents results for the entropy as a function of temperature. At low temperature ($T < 1$ MeV), the entropy does not give any response. Then the entropy behavior exhibits almost a linear dependence on temperature for (T > 1 MeV), the absence of response at low temperature is again due to shell-closure effects.

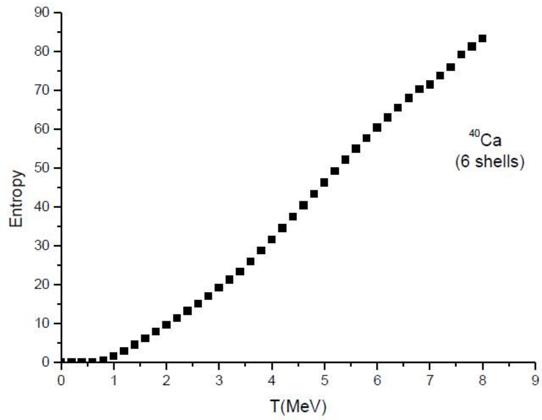

Fig. 4. The entropy versus temperature for the ^{40}Ca nucleus in a model space of six major oscillator shells by using the Nijm.II potential as *N-N* interaction.

It is interesting to note in Fig. (4) that the entropy is increased by 83.30 due to 8 MeV increased temperature. It is sometimes useful, however, to consider the entropy as being determined by the state of disorder of the nucleus. The increase in the entropy associated with the movement of the nucleons as the take up a more probable configuration will be accompanied by an increase in the disorder of the nucleus and by an increase in the observer's ignorance of the positions of nucleons.These result are approximately the same of figure 3 of Ref. [25]

Finally, for further efforts, the more current N-N interaction is used to obtain extended results. Therefore, our study will set a reference standard for judging the importance of the change in thermal properties to be obtained when future studies include the delta's degrees of freedom [26-34] to the heated nuclear system.

IV. Conclusion

The thermal properties of the double magic ^{40}Ca nucleus were evaluated. Mean field calculations is performed within the framework of finite temperature Hartree-Fock (*FTHF*) method. The response of several nuclear properties is investigated to temperature using realistic effective Hamiltonian in a mean field approach. The root mean square radius, Hartree-Fock energy, free energy and entropy are investigated as a function of temperature. These properties are evaluated in a model space of six major shells with an effective Hamiltonian based on Nijmegen potential.

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REFERENCES

[1] M Curtin, H Toki and D Scott, Phys. Lett. B123289, (1983)
[2] S Son, M Rivet, R Bimbot, B Borderie, I Forest, J Galin et.al. Phys. Lett.B13014 (1983)
[3] M LefortNucl. Phys. A3873C (1982)
[4] G Bozzolo and J Vary Phys. Rev. C311909(1985)
[5] G Bozzolo, O Civitarese and J Vary Phys. Rev. C371240(1988)
[6] G Miller Nucl. Phy. B112223 (2002)
[7] S Gandol, A Illarionov, S Fantoni, F Pederiva, and K Schmidt Phys. Rev. Lett,101132501 (2008)
[8] H Stoecker and C Sturm Nucl. Phys. A855506(2011)
[9] P Marshall, W Stocker, and T Chossy Phys. Rev. C60064302 (1999)
[10] Z Ma, N Giai, and H TokiPhys. Rev. C55 2385(1997)
[11] S Lenzi Journal of Physics: Conference Series168012009(2009)
[12] T Chossy and W Stocker Phys. Lett. B507109(2001)
[13] R Reid Ann. Phys. (N.Y.)50411 (1968)
[14] T Frick and H Mther Phys. Rev. C71 014313(2005)
[15] X Yong-Zhong, Z Yu-Ming, S Pornrad, Y Yu-Peng, and K Chinorat. Chin. Phys. Lett. 26 022501(2009)
[16] P Navr'til and W Ormand Phys. Rev C68 034305 (2003)
[17] I Stetcu, B Barrett, P Navr'til, and C Johnson Int. J. Mod. Phys. E1495(2004)
[18] J Vary, OAltramentov, and B Barrett, M. Hasan, A Hayes, R Lloyet. al.Eur. Phys. J. A25 475 (2005)
[19] M Hasan, J Vary, and P Navr'tilPhys. Rev. C69034332(2004)
[20] G Bozzolo and J Vary Phys. Rev. Lett,53 903 (1984)
[21] R Pathria. Statistical Mechanics. Academic Press, 3ed edition(2007)
[22] M Hasan, S Köhler, and J Vary. Phys. Rev. C36 2649(1987)
[23] B Agrawal, D Bandyopadhyay, J. De, and SSamaddarPhys. Rev. C89044320(2014)
[24] M Brack, and Ph Quentin PhysicaScripta, 10A163(1974)
[25] G Sauer, and H Chandra Nucl. Phys. A264221 (1976)
[26] M Abu-Sei'leek and M Hasan Comm. Theort. Phys.54339 (2010)
[27] M Abu-Sei'leek Comm. Theort. Phys. 55115(2011)
[28] M Abu-Sei'leek. International J. of Pure and Applied Phys. 773 (2011)
[29] MAbu-Sei'leek Pramana- J. of Phys.76573(2011)
[30] M Abu-Sei'leekTurk. J. Phys. 35 1 (2011)
[31] M Abu-Sei'leek Nucl. Phys. Rev. 27399(2010)
[32] M Abu-Sei'leek Nucl. Phys. Rev.28416 (2011)
[33] M Abu-Sei'leekJ. Phys. Soc. Jpn. 80104201 (2011)
[34] M Abu-Sei'leekTurk. J. Phys. 38 253 (2014)