# Thermodynamics properties of a system with finite heavy mass nuclei

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**Abstract:** The thermodynamics property of finite heavy mass nuclei, with the number of protons greater than the number of neutron is investigated. The core of the nucleus contains the neutron-proton pair that interacts harmonically; the excess neutron(s) reside(s) on the surface of the nucleus and introduce the anharmonic effect. The total energy is evaluated using ladder operator method and the quantum mechanical statistical expression of energy. The total energy, heat capacity and entropy are found to depend on the occupation number of states and the number of excess neutrons. At temperature near absolute zero the specific heat and entropy are lowest because a decreases in temperature leads to a decrease in particle interaction and energy.

**Keywords:** Anharmonic Oscillator, Transition Temperature, Heat Capacity and Entropy

## 1. Introduction

There are two kinds of nucleons (neutron (n) and proton (p)), which in principle can form four distinct type of correlated (cooper) pairs, *nn*, *pp* and *np,* each with the net orbital momentum of zero and thus strongly correlated in space. The *np* pair can either be isoscalar (T=O, S-1) or isovector (T=1, S=0). Generally, it is believed that the neutron-proton (*np*) pairing is important in finite nuclei with roughly equal number of neutrons and protons. Important insight on the *np* pairing correlation has been achieved in recent years in the content of exactly solvable models that include the various pairing correlation. The standard technique of treating this correlation is through the Barden Cooper Schrieffer (BCS) approximation that includes the *pn* pairing field in addition to the *nn* and *pp* fields [1-3]. The possibilities of transition from the BCS pairing to a Bose-Einstein condensation (BEC) in asymmetric nuclear matter at low density have elicited interest in the role of *np* pairing. For example, an analysis of triplet ${}^3S_1$ pairing in low density symmetric and asymmetric nuclear matter, show that as the system is diluted the BCS state with large cooper pair overlaps into BEC of tightly bound np pair [4]. BEC is purely a quantum statistical phase transition characterized by a macroscopic occupation in the ground state below some critical temperature $T_C$ [5]. The observation of BEC in ultracold trapped alkali gases has created a wave of renewed interest in theoretical and experimental investigation of this phenomenon. For example BEC of the ideal and the weakly interacting cold alkali gases confined by anisotropic harmonic oscillator potentials has been investigated by Xue-Xi Yi et al [6], to obtain the explicit expression for the condensation temperature, the internal energy and the specific heat. The transition point was shifted toward lower temperature because the trapped potentials and the specific heat below the transition point is no longer proportional to $T^{3/2}$. Sudip, K. H. et al [7] using a correlated many body method and realistic van der Waals potential studied measures of BEC like the specific heat, transition temperature and the condensate fraction of the interacting Bose gas trapped in an anharmonic potential. The anharmonic trap offers a more favorable condition to achieve BEC experimentally.

The pairing correlation in finite molecules can be analyzed via the interacting boson model (IBM), where neutrons and protons *np* pair up and act as a single particle with boson properties with integral spin of 0, 2 or 4. The interaction of the *np* pair can be approximated as an oscillator in a harmonic potential. In cases where the number of neutrons exceeds the number of proton, the interaction between *np* pair and unpaired neutrons introduces a small anharmonic effect. The thermodynamic functions of a system of

interacting bosons in the weak interaction approximation and in the neighborhood of the condensation line have been studied by the method of quantum field theory [8]. The many body perturbation theory has been used to calculate the total energy, binding energy per nucleon, specific heat and transition temperature of finite heavy nuclei in which the number of neutron is greater than the number of protons [9, 10]. Khanna, K. M., et al, 2010 [11] considered a heavy nuclei composed of Z protons and N neutrons, such that N>Z, the core of the nucleus is composed of Z $np$ pair and the N-Z unpaired neutron resides in the surface of the nuclei. The $np$ in the core of the nucleus interacts harmonically, while the interaction between the unpaired neutrons and the np pair leads to the anharmonicities in the $np$ pair interaction. The anharmonic interaction is approximated by the potential

$$\hat{f} = \alpha \hat{x}^3 + \lambda \hat{x}^4 \tag{1}$$

where $\alpha$ and $\lambda$ are perturbation parameters. The total energy of the heavy nuclei is the sum the energy of Z $np$ pair harmonic oscillators and N-Z anharmonic oscillators obtained using perturbation theory to second order. A thermal excitation factor $\exp\left(-\Delta E/\kappa T\right)$, where $\Delta E = \hbar\omega$ and $\kappa$ the Boltzmann constant, was added to the perturbed energy to introduce temperature dependence. The resulting expression was used to determine the transition temperature, specific eat and entropy of the heavy nuclei. A similar work by Sakwa, T.W, et al, 2013 [12], obtained the ground state properties of trapped atomic boson-fermion mixture at near absolute zero temperature Kelvin using second quantization technique. The energy, specific heat and the entropy of the boson-boson, boson-fermion, and fermion-fermion interactions system were established and analyzed. The total energy of the system was found to increase with increase in occupation number of the system and the entropy decreases with temperatures.

This work aims at evaluating the thermodynamic properties of a system with heavy finite nuclei, such that N>Z. The anharmonic potential for the N-Z excess electrons is give by (1). The energy of the anharmonic term is obtained using the quantum mechanical statistical average of an observable $\hat{f}$ in n-dimensional vector space as

$$\left\langle \hat{f} \right\rangle = \sum_{n} \rho_n \left\langle n \left| \hat{f} \right| n \right\rangle \tag{2a}$$

where the density operator

$$\rho_n = \exp\left(-\beta \Delta\right) \tag{2b}$$

$\Delta = n\hbar\omega$ is equally spaced single particle energy of the harmonic potential, $\beta = 1/\kappa T$ and the normalization constant is defined as [13]

$$\sum_{n} \rho_n = 1 \tag{2c}$$

where n=0, 1, 2, 3...is the occupation number. Then in (2a) the temperature dependence of perturbation energy is explicitly defined. The total energy which is the sum of the energy of the Z $np$ pair harmonic oscillator and the quantum statistical mechanic energy of the N-Z neutrons obtained using (2a), is used to obtain the transition temperature, specific heat and entropy of the heavy nuclei. We investigate the role of the excess (N-Z) neutrons residing on the surface of the nuclei play in determining the thermodynamic property of the nuclear system and study the dependence of the temperature and the occupation number of states on specific heat and entropy for selected heavy nuclei.

# 2. Theoretical Formulation

## 2.1. Operator Method for the Harmonic Oscillator

The quantum mechanical behavior of vibrating heavy nuclei in an atom that acts as a harmonic oscillator with frequency $\omega$, is described by the Schrödinger one dimension stationary state equation [13-15]

$$-\frac{\hbar^2}{2\mu}\frac{d^2\phi_n(x)}{dx^2} + \frac{\mu\omega^2}{2}x^2\phi_n(x) = E_{n_x}\phi_n(x) \tag{3a}$$

where

$$\mu = \frac{m_n m_p}{m_n + m_p} \tag{3b}$$

is the neutron proton reduced mass. The eigenfunctions that are solutions to the Schrodinger equation (3b) are

$$\phi_{n_x}(x) = \left(\frac{1}{\pi\gamma^2}\right)^{1/4}\frac{1}{\sqrt{2^n n!}}H_n\left(\frac{x}{\gamma}\right)\exp\left(\frac{-x^2}{2\gamma^2}\right) \tag{3c}$$

where $\gamma = \sqrt{\hbar/\mu\omega}$ and $H_n\left(x/\gamma\right)$ are Hermite polynomials. The eigenvalues of the Harmonic oscillator are

$$E_{n_x} = \left(n_x + \frac{1}{2}\right)\hbar\omega \tag{3d}$$

If the normalized eigenfunctions for the oscillator $\phi_{n_x}(x)$ in an n-dimensional vector space is denoted by eigenstates $\left|n_x\right\rangle$, the representation of the eigenvalue spectrum, $E_{n_x}$ for the oscillator, can be obtained by defining the lowering and raising operator,

$$a_x = \sqrt{\frac{\mu\omega}{2\hbar}}\left(\hat{x} + i\frac{\hat{p}_x}{\mu}\right);$$
$$a_x^+ = \sqrt{\frac{\mu\omega}{2\hbar}}\left(\hat{x} - i\frac{\hat{p}_x}{\mu}\right) \tag{4a}$$

which satisfy the relation [14]

$$a_x\left|n_x\right\rangle = \sqrt{n_x}\left|n_x-1\right\rangle; \quad a_x^+\left|n_x\right\rangle = \sqrt{n_x+1}\left|n_x+1\right\rangle \tag{4b}$$

From equation (4a), the position and momentum operator are defined as

$$\hat{x} = \sqrt{\frac{\hbar}{2\mu\omega}}\left(a_x + a_x^+\right);$$
$$\hat{p}_x = i\sqrt{\frac{\mu\omega\hbar}{2}}\left(a_x^+ - a_x\right) \tag{4c}$$

Using equation (4c) the quantum mechanical anharmonic operator (1) becomes

$$\hat{f} = \alpha\left(\frac{\hbar}{2\mu\omega}\right)^{3/2}\left(a_x + a_x^+\right)^3 + \lambda\left(\frac{\hbar}{2\mu\omega}\right)^2\left(a_x + a_x^+\right)^4 \qquad (4d)$$

Substitute equation (4d) in (2a), the potential of the form $\alpha\hat{x}^3$ vanishes, due to the symmetry of the problem and the perturbation, the quadratic term of the form $\lambda\hat{x}^4$ as a nontrivial first-order effect [14, 16], resulting in

$$\langle n_x|\hat{f}|n_x\rangle = \frac{3\lambda\hbar^2}{2\mu^2\omega^2}\left(n_x^2 + n_x + \frac{1}{2}\right) \qquad (4e)$$

The energy of the anharmonic term becomes

$$E_{n_x}' = \frac{3\lambda\hbar^2}{2\mu^2\omega^2}\sum_{n_x}\left(n_x^2 + n_x + \frac{1}{2}\right)\exp\left(-n_x\hbar\omega/\kappa T\right) \qquad (4f)$$

Using equations (3d) and (4f), the total energy for the finite nuclei composed of Z np pair that interacts harmonically and the (N-Z) unpaired neutron is expressed as

$$E_{n_x} = ZE_{n_x}^{(0)} + (N-Z)E_{n_x}' = \sum_{n_x}\mathcal{E}_{n_x} \qquad (5a)$$

where

$$\mathcal{E}_{n_x} = Z\left(n_x + \frac{1}{2}\right)\hbar\omega + \frac{3\lambda\hbar^2(N-Z)}{2\mu^2\omega^2}\left(n_x^2 + n_x + \frac{1}{2}\right)\exp\left(-n_x\hbar\omega/\kappa T\right) \qquad (5b)$$

and $n_x = 0, 1, 2, 3\ldots\ldots$ is the occupation number.

The important properties of the heavy nuclei in a harmonic trap is normally considered using a three dimensional oscillator potential approximated with the quadratic form

$$V(\mathbf{r}) = \frac{1}{2}Kr^2 = \frac{\mu}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right) \qquad (6a)$$

where $\omega_x$, $\omega_y$ and $\omega_z$ are oscillator frequencies in the x, y and z directions. The investigation of the three dimensional oscillator starts as application of non-relativistic quantum mechanics for identical one-dimension particles in a harmonic potential as outlined in equations (3a-5b). Individual equations for the one dimensional particles in the y and z direction are obtained by replacing x with y and z in equations (3a-5b). The resulting many-body Hamiltonian is the sum of single particle Hamiltonian whose eigenfunctions and eigenvalues have the form

$$\Phi_{n_x n_y n_z}(x,y,z) = \phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z) \qquad (6\,b)$$

and

$$E_{n_x n_y n_z} = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z \qquad (6\,c)$$

respectively. The three dimensional oscillator are labeled by three quantum numbers $\{n_x, n_y, n_z\}$ each of which can take any values between zero and infinity. When all the three quantum numbers are equal to 0, we have the ground state with energy $E_{000} = \frac{3}{2}\hbar\omega$, changing the quantum numbers from 0 to 1 result in six excited states with energy $E_{100} = E_{010} = E_{001} = \frac{5}{2}\hbar\omega$. In a similar way we can find six states with energy $\frac{7}{2}\hbar\omega$, ten states with energy $\frac{9}{2}\hbar\omega$, and so on. The degeneracy arises because the Hamiltonian for the three-dimensional oscillator has rotational and other symmetries.

### 2.2. Heat capacity, Transition Temperature and Entropy

The relation between the internal energy and the heat capacity is

$$C_x = \frac{d\mathcal{E}_{n_x}}{dT} = \frac{3\lambda\hbar^2(N-Z)}{2\mu^2\omega^2}\left(\frac{n_x\hbar\omega}{\kappa T^2}\right)\left(n_x^2 + n_x + \frac{1}{2}\right)\exp\left(-n_x\hbar\omega/\kappa T\right) \qquad (7a)$$

after substituting (5b). The transition temperature $T_C$ is obtained under the condition

$$\left(\frac{dC_x}{dT}\right)_{T=T_C} = 0 \;\Rightarrow\; T_C = \frac{n_x\hbar\omega}{2\kappa} \qquad (7b)$$

Using (7a), the entropy $S(T)$ of the system becomes

$$S(T) = \int\frac{dQ}{T} = \int\mu C_x\frac{dT}{T} = \frac{3\lambda\hbar^2(N-Z)}{2\mu\omega^2}\left(n_x^2 + n_x + \frac{1}{2}\right)\left(\frac{\kappa}{n_x\hbar\omega} + \frac{1}{T}\right)\exp\left(-n_x\hbar\omega/\kappa T\right) \qquad (7c)$$

The perturbation potentials in (1) has the dimensions of energy, then the parameter $\gamma$ in (5b), (7a) and (7c) can be approximated as $\gamma = \hbar\omega/a_0^4$, where $a_0 = 1.3\times10^{-13}A^{1/3}\,cm$ (A mass number) is the scattering length and angular frequency $\omega = 6\times10^{22}\,s^{-1}$ [11]. In equations (5b), (7a) and (7c), the Boltzmann constant $\kappa = 1.38\times10^{-23}\,JK^{-1}$, reduced Planck constant $\hbar = 1.055\times10^{-34}\,Js$, and neutron-proton reduced mass $\mu = 8.369\times10^{-25}\,g$. The mass number A, atomic number Z and neutron number N for arbitrary selected elements is presented in table 3.1

**Table 3.1.** *Values for A, Z, N and N-Z for selected elements with heavy mass nuclei*

| Element | A | Z | N | N-Z |
|---|---|---|---|---|
| Zinc | 64 | 30 | 34 | 4 |
| Ruthenium | 101 | 44 | 57 | 13 |
| Samarium | 150 | 62 | 88 | 26 |

The mass number and neutron proton difference for isotopes of $^{64,66,68}Zn$, is presented in table 3.2

**Table 3.2.** *Values for A, Z, N and N-Z for $^{64,66,68}Zn$*

| Element | A | Z | N | N-Z |
|---|---|---|---|---|
| Zinc | 64 | 30 | 34 | 4 |
| Zinc | 66 | 30 | 36 | 6 |
| Zinc | 68 | 30 | 38 | 6 |

## 3. Results and Discussion

The plot of the internal energy (5b) of the nuclei in table 3.1 against occupation number of states at absolute zero temperature is given in figure 3.1.
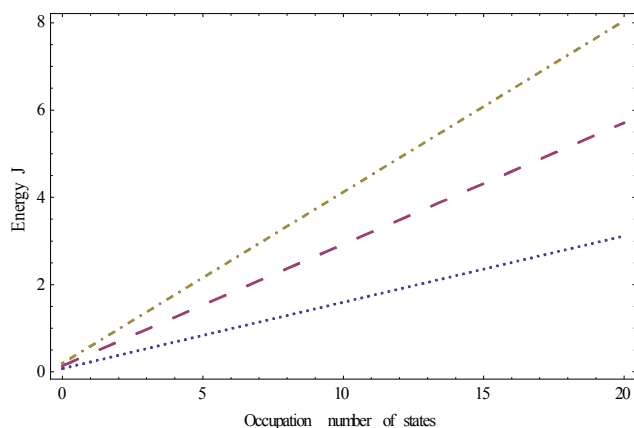
*Figure 3.1. The total energy of the nuclei against the occupation number of states at absolute zero temperature, dash dotted ($^{64}$Zn), dashing large ($^{101}$Ru) and dashing tiny ($^{150}$Sm).*

The variation between the total energy the occupation number state was found to increase linearly with the increase in the mass number nuclei. The gradient corresponding to each nucleus is approximately 0.4, 0.3 and 0.2 for $^{150}$Sm, $^{101}$Ru and $^{64}$Zn respectively. Then the total energy of the nuclei largely depends on the mass number and the occupation number of particles. Around the ground state, n=0 the energies of the nuclei were approximately equal.

Figure 3.2 shows the plot of for the specific heat (7a) of the nuclei in table 3.1 against temperature at occupation number $n_x$=1.
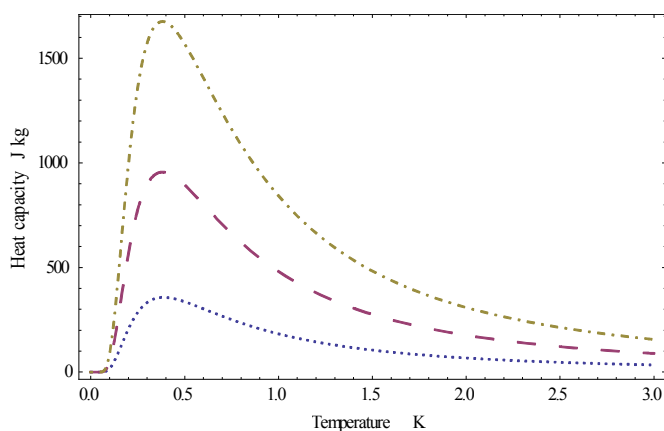


*Figure 3.2. The heat capacity against temperature for occupation number $n_x=1$ , dash dotted ($^{64}$Zn), dashing large ($^{101}$Ru) and dashing tiny ($^{150}$Sm).*

The three elements $^{64}$Zn, $^{101}$Ru and $^{150}$Sm have transition temperature of about 0.4 K corresponding to the occupation of particle state $n_x$=1. However the maximum values of the heat capacity increases with the increase in the neutron-proton difference. As the temperature of the nuclei cools to near the absolute zero temperature the heat capacity of the three nuclei decreases rapidly as energy is being released to the surrounding by the nuclei as it cools.

The plot for the entropy (7c) of the nuclei in table 3.1 against temperature at occupation number of state $n_x$=1 is given in figure 3.3.
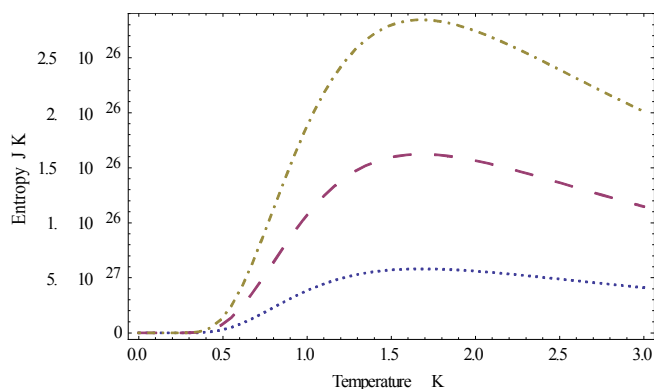


*Figure 3.3. The entropy of the nuclei versus temperature for occupation number of state $n_x$=1, dash dotted ($^{64}$Zn), dashing large ($^{101}$Ru) and dashing tiny ($^{150}$Sm).*

The entropy of the nuclei increases is lowest up to the temperature 0.4K, where it rises to a maximum at about 1.5 K, followed by decrease with increase in temperature. Below 0.4 K. the energy of the nuclei decreases, resulting in reduced interaction for the particles in the nuclei.

The plot of the heat capacity (7a) of $^{64}$Zn against temperature for $n_x$=1, 2, 3 is given in figure 3.4
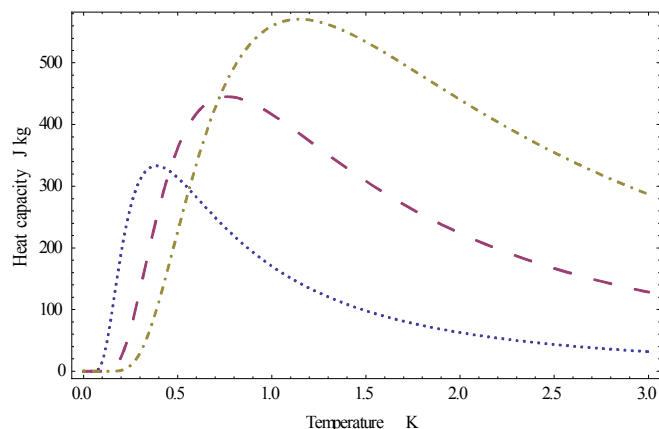


*Figure 3.4. The heat capacity against temperature for $^{64}$Zn,  , dash dotted ($n_x$=3), dashing large ($n_x$=2) and dashing tiny ($n_x$=1)*

The low value of heat capacity around the absolute zero temperature is an indication that as the nuclei is cooled to and releases energy to the surrounding. It is noted that the heat capacity increase with increase in the occupation number. The transition temperature for occupation number $n_x$=1, $n_x$=2 and $n_x$=3 is approximately equal to 0.4 K, 0.7 K and 11 K respectively. Then the transition temperature of the nuclei depends on the occupation number as in (7b).

Figure 3.5 shows the plot for the heat capacity (7a) for the isotopes of $^{64,66,68}Zn$ in table 3.2 against temperature for occupation number $n_x = 1$.
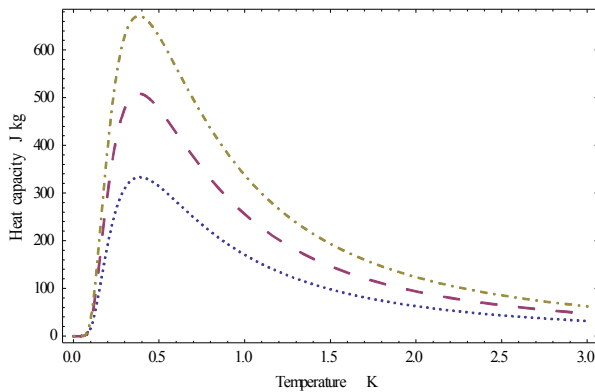
***Figure 3.5.*** *The heat capacity against temperature for occupation number* $n_x=1$*, dash dotted (*$^{64}Zn$*), dashing large (*$^{66}Zn$*) and dashing tiny (*$^{68}Zn$*).*

Figure 3.5 shows the peak value of the heat capacity for the isotopes of $^{64,68,68}$Zn increases with the increase in neutron-proton difference as already outlined in figure 3.2.

## 4. Conclusion

In the article the weak interaction of heavy finite nuclei composed of Z np pair interacts harmonically and the N-Z excess neutrons that introduce the anharmonicities is considered. The energy total energy of the nuclei is the sum of the harmonic component and that of the anharmonic part evaluated the using the expression for the quantum mechanical statistical average of an operator $\hat{f}$. The latter introduces the dependence on temperature and occupation number of states. The total energy, heat capacity and entropy for arbitrary selected elements of $^{64}_{30}Zn$, $^{101}_{44}Ru$ and $^{150}_{62}Sm$ with different number of excess neutrons were evaluated. It was noted that $^{150}_{62}Sm$ with the highest number of excess neutrons had the highest values of total energy, heat capacity and entropy. The main reason being the excess neutrons stay on the surface of the nuclear resulting in perturbation of the core which leads to increases the perturbation energy and entropy. Similar result was obtained for the heat capacity of the isotopes of $^{64,66,68}$Zn. The heat capacity and entropy of the nuclei were lowest near absolute zero, because a decrease in temperature leads to a reduced particle interaction with a decrease in energy. The heat capacity curve had a Gaussian shape with the transition temperature dependent on the occupation number. Similar results have been obtained by Khanna K .M, 2010 [11] where the temperature dependence is introduced to the perturbation energy by multiplying it by a thermal excitation factor that does not contain occupation number of states.

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