EAPAS

East African Journal of
Pure and Applied
Science

East African Journal of Pure and Applied Science Vol. 2 (1): 16-24 (2012)

DESIGNER NUCLEI AND SOME OF THEIR PROPERTIES

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Abstract

Recently 'designer' nuclei with large neutron excess, such as ${}^{11}_{3}Li$, have been produced to understand the role played by excess neutrons in studying the properties of new isotopes and to develop new nuclear theory, and to understand how such isotopes can be used to develop new fission and fusion processes for the development of nuclear energy. Using the idea of a nuclear core composed of neutron-proton pairs (np-pairs) surrounded by unpaired neutrons and the Bogoliubov technique, we have calculated the binding energy, binding fraction, specific heat, entropy, and transition temperature of such nuclei, and particularly the isotopes for which the ratio of neutron to proton number is approximately
1.554 or more since this is the ratio for fissile materials.

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 ISSN 2070 0903

Introduction

During the last decade, chemists and physicists have tried a fabrication process at the scale of atomic nuclei. It is a new method of producing in large quantities, the so called "designer" atomic nuclei, which are new rare isotopes with large excess numbers of neutrons or protons, and with unusual decay modes [Geesaman et al 2006]. There are various reasons why there is a demand for unusual type of new isotopes. New isotopes may hold key to the understanding of the significant properties of large finite nuclei with large neutron excess such as the pairing phenomena, constitution of the core region of the nucleus, the size of the nucleus, decay phenomena from the nucleus, the role of neutron excess in studying the creation of nuclear energy and nuclear fission. There could be a host of other properties and phenomena that may be studied in future depending upon what kind of isotopes we are able to produce.

The ability to produce and study single atoms depends on the scientific and technological capability to produce super heavy isotopes of light nuclei. For instance a superheavy lithium isotope $\left({}^{11}_{3}Li\right)$ may have large ratio of neutrons such that the binding energy of the neutrons in the nucleus may be decreased. The size of such a nucleus may be very large. For instance, ${}^{11}_{3}Li$ stretches to the extent that its volume is roughly 10 times the volume of a normal ${}^{6}Li$ nucleus [Tanihata 1996, Sherill 2008]. Unlike normal nuclei, ${}^{3}_{11}Li$ has diffused surface of neutron matter, and its size is of the order of a much heavier ${}^{220}_{88}Ra$ nucleus [Sherill 2008].

Quantum mechanically, the wave function of the neutrons can extend far beyond the normal range of the nucleus. The existence of nuclei with abnormal neutron excess can allow researchers to study the inter-actions of neutrons with protons in the nucleus, and also to study the charge radius of ${}^{11}_{3}Li$, and such a study can provide key information to develop a new nuclear theory [Sanchez 2006].

The discovery of new isotopes (nuclei) with very typical characteristics has shown that the quantum magic numbers in nuclei are not generally the same, and this is centrally to what is observed for electrons in atomic physics. For instance, a nucleus with 28 neutrons (28 is a magic number for nuclei) is sometimes but not always magic [Bastin 2007]. On the other hand, a change in the magic numbers in rare isotopes is not always found. A recent mass measurement of rare isotope ${}^{132}_{50}Sn$, with a proton number $Z = 50$ and the neutron number $N = 82$, found it to have the largest measured shell gap, which is energy difference between the field shell model orbit and the next unfilled one [Dworschak 2008].

It is well known that the atomic nuclei fuel the fission and fusion processes that are responsible for the creation of energy on the Earth and the Sun and Stars. Transuranic elements, like ${}_{92}$U and ${}_{94}$Pu are used in fission (reactors) reactions and ${}^{2}_{1}H$ and ${}^{3}_{1}H$ are used in fusion reactions. These nuclei have sufficient neutron excess; for ${}^{235}_{92}U$, it is of the order of $\frac{N}{Z} = \frac{143}{92} = 1.554$ and ${}^{3}_{1}H$, it is 2. Thus, if we can produce nuclei with this ratio=1.554 or more and smaller Z, it should be from the above, we can come to the conclusion that the key to the development of future nuclear theory and nuclear science will

be to create nuclei with large neutron excess,

and study their properties experimentally and theoretically.

In this manuscript we have studied some of the properties ,such as binding energy, binding fraction, specific heat, entropy and transition temperature using ideas developed by us in an earlier attempt [Khanna et al 2010] in which we assumed that a nucleus may be composed of a core of neutron-proton(np-pairs) pairs surrounded by an envelop of unpaired neutrons. We have specifically studied the

properties of ${}^{11}_{3}Li$ and ${}^{125}_{49}In$ and some isotopes

for which

$\frac{N}{Z} \approx 1.554$ or more. Isotopes whose ratios

of $\frac{N}{Z}$ are higher than this will be studied in

another communication.

Theory:

Assuming that a nucleus with large neutron excess is composed of a core made of n-p

pairs, and the excess neutrons constitute the diffused neutron surface, we have used the Bogoliubov technique [Bogoliubov 1959] to

obtain an expression for the energy E_n of a

nucleus with mass number A, atomic number Z (proton number) and neutron number N such that $A = Z + N$, and $(N - Z)$ is large.In this method we use a trial wave function that exhibits the interaction of an unpaired neutron in the surface region with the np-pairs in the core region of a large A nucleus. The trial wave can be written as,

$$\psi = a_l^+ (U_k + V_k a_k^+ a_k^+) |0\rangle \quad \text{......................(1)}$$

where $a_k^+ a_k^+$ will refer to the neutron-proton pair in the core of the nucleus, and a_l^+ refers to the perturbing neutron that exists in the surface region of the nucleus. The perturbation H is written as,

$$H' = \beta x^3 + \gamma x^4 \quad \text{..(2)}$$

where β and are constants of perturbation and are defined in the section on calculations. The expectation value of the perturbation is,

$$\langle \psi | H' | \psi \rangle = \langle 0 | a_l (U_k + V_k a_k a_k) H' (U_k + V_k a_k^+ a_k^+) a_l^+ | 0 \rangle \quad \text{................................ (3)}$$

$$\text{Where } U_k^2 + V_k^2 = 1 \quad \text{........................ (4)}$$

Depending upon the values of U_k and V_k ,

the trial wave function ψ can account for the following possibilities[9].

$$U_k = 0 \text{ and } V_k = 0 \text{.................................... (5)}$$

$$U_k = 1 \text{ and } V_k = 0 \quad \text{..........................(6)}$$

$$U_k = \frac{1}{\sqrt{2}} \text{ and } V_k = \frac{1}{\sqrt{2}} \quad \text{..................(7)}$$

Possibilities given in Eqs.(5) and (6) lead to unacceptable situations since the model is based on the existence of np-pairs in the core and unpaired neutrons in the surface region. Only the possibility given in Eq.(7) leads to the existence of the term

$\frac{1}{\sqrt{2}} a_l^+ a_k^+ a_k^+ |0\rangle$ which implies that the np-pair exists as a separate entity

Assuming that the neutron and proton in the np-pair interact with each other harmonically, the displacement x will be written as,

Following rigorous derivations the energy E_n of the nuclear system can now be written as,

$$x = \frac{1}{\alpha\sqrt{2}}\left(a^{+} + a\right) \quad \text{……….......... (8)}$$

$$\begin{aligned} E_n &= E_n^0 + E_n^{/} \\ &= Z\left(n + \frac{1}{2}\right)\hbar\omega + (N - Z)\frac{\gamma}{4\alpha^4}\frac{1}{2}\left(6n^5 + 86n^4 + 467n^3 + 1180n^2 + 1378n + 585\right) \end{aligned} \quad \text{…………(9)}$$

Binding fraction f

From Eq. (9) we get an expression for the binding fraction f for $n = 0$, when the nucleus is in the ground state, i.e.,

$$f = \frac{E_{n=0}}{A} = \frac{Z}{A}\cdot\frac{1}{2}\hbar\omega + \left(\frac{N-Z}{A}\right)\left(\frac{\gamma}{8\alpha^4}\right)\cdot(585) \quad \text{.. (10)}$$

In Eq. (10), the quantity $\frac{N-Z}{A}$ is called neutron excess parameter , i.e.

$$\eta = \frac{N-Z}{A} \quad \text{.. (11)}$$

Specific Heat C

To calculate the specific heat C, it is necessary to include the probability amplitude Green's function factor. The corresponding thermal activation factor is $e^{\frac{-\hbar\omega}{\kappa T}}$. Using this in Eq. (9) and writing,

$$C = \frac{\partial E_n}{\partial T}$$

$$= (N - Z)\frac{\gamma}{8\alpha^4}\cdot\frac{\hbar\omega}{\kappa T^2}\left(6n^5 + 86n^4 + 467n^3 + 1180n^2 + 1378n + 585\right)e^{\frac{-\hbar\omega}{\kappa T}} \quad \text{…………………................ (12)}$$

we get the value of the specific heat C as a function of temperature T.Entropy S.The expression for the entropy S is,

$$dS = \frac{dQ}{T} \quad or \quad \int dS = \int\frac{dQ}{T} = \int\frac{mCdT}{T} \quad \text{.. (13)}$$

T T T

where m = mass of the nucleus

Carrying out the integration and substituting for C from Eq.(12) we obtain explicit expression for S.

$$S = (N - Z)\frac{\gamma}{8\alpha^4}\cdot\frac{\hbar\omega}{\kappa}\left(6n^5 + 86n^4 + 467n^3 + 1076n^2 + 1378n + 585\right)\left(\frac{\kappa}{\hbar\omega T}e^{\frac{-\hbar\omega}{\kappa T}} + \frac{\kappa^2}{\hbar^2\omega^2}e^{\frac{-\hbar\omega}{\kappa T}}\right) \quad \text{................................ (14)}$$

Transition Temperature T_C

The transition temperature of the nucleus is given by

$$\left(\frac{\partial C}{\partial T}\right)_{T=T_C} = 0 \quad (15)$$

Substituting for C from Eq.(12), we get T_C from Eq.(15) as

$$T_C = \frac{\hbar\omega}{2\kappa} \quad \text{...(16)}$$

Methodology

Our model of the nucleus conceptualizes a large neutron excess finite nucleus as comprising a core region containing neutron- proton (n-p) pairs and a surface region in which the unpaired neutrons exist. The n-p pairs are considered to interact harmonically while the interaction of the unpaired neutrons with the n-p pairs is considered to be

anharmonic perturbation. This model has been solved using Bogoliubov method [Bogoliubov 1959] and Eqs.10, 11, 12, 14 and 16 obtained.

These relationships describe the properties of a large neutron excess nuclear system. Using these relationships explicit parameters are calculated and compared with those obtained with other models.

Since γx^4 must have the dimensions of energy ML^2T^{-2}, the dimensions of should be $ML^{-2}T^{-2}$, since x which is the displacement operator has the dimension of length L. Therefore, a parameter a_0 which is

assumed to be fundamental to the perturbation parameters has been introduced. This parameter a_0 is defined as the bond length

between the nucleons in the nucleus.

Results and Discussions

We can define the bond length parameter a_0 and perturbation parameter respectively as,

$$a_0 = 1.3\times10^{-15} A^{\frac{1}{3}}\ \mathrm{m} \quad \text{............................ (17)}$$

and

$$\gamma = \frac{\hbar\omega}{a_0^4} \quad \text{.......................................(18)}$$

The following values for different physical quantities have been used with the derived relationships to obtain numerical values of the various properties.

Plank’s constant/ $2\pi = \hbar$ is given as 1.054

The neutron-proton reduced mass is given as 8.369×10^{-28} kg.

Boltzmann's constant is given as 1.3807×10^{-23} J/K

The angular frequency/ 2π = $\omega = 6 \times 10^{22}\, S^{-1}$

Variation of f with A, Z, N and

Eq.(10) for f and Eq.(11) for , we get the values of binding fraction and neutron excess parameter. The variation of f with A is

shown in Fig.1.

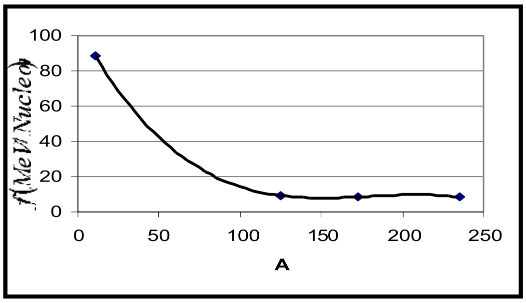

Figure 1: Binding fraction $f\left(MeV / Nucleon\right)$ against mass number A

Giving appropriate values to A, Z , and N for the nuclei, ${}^{11}_{3}Li,\ {}^{125}_{49}In,\ {}^{163}_{66}Dy$ and ${}^{235}_{92}U$ and using

Variation of C with E_n

Using Eq.(9) in Eq.(12), we get,

$$C = \frac{\hbar\omega}{\kappa T^2}\left[E_n - Z\left(n + \frac{1}{2}\right)\hbar\omega\right] \quad (19)$$

Eq.(19) can now be used to calculate the variation of C with E_n. Eq.(19) shows that C

varies directly as the difference of the total energy and the proton energy and it should be so since as Z increases, repulsive energy between the protons increases, and this changes the total energy of the nucleus [Khanna et al 2010]. The variation of C with E_n for the nuclei ${}^{11}_{3}Li,\ {}^{125}_{49}In,\ {}^{163}_{66}Dy$ and ${}^{235}_{92}U$ is shown in Fig.2.

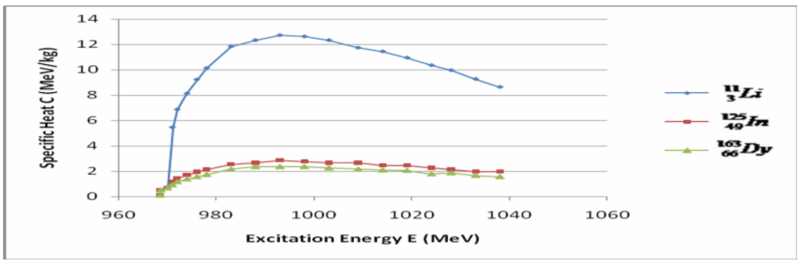

Fig.2: Variation of specific heat C (MeV/kg) against excitation energy E (MeV) for ${}^{11}Li,\ {}^{125}In$

The calculated values of specific heat C for $^{163}_{66}Dy$ at the various values of excitation

E_n are equivalent to those of $^{235}_{92}U$ the reason for this being that the two nuclei have equal neutron excess parameters to two places of decimal. Thus the curve representing the variation of C against E_n in Fig.2 for $^{163}_{66}Dy$ also represents variation of C against E_n for $^{235}_{92}U$.

Fig.2 also shows that the specific heat C is large for nuclei with large neutron excess parameter ($^{11}_{3}Li$) at any excitation energy E.

This effect is shown to be greater by the characteristics of the three nuclei as they go through the liquid-gas phase transition [Saauer 1976, Siemens 1964].

Using Eq.12 we have calculated the variation of C with mass number A and this is shown in Fig.3. In this figure, it is seen that the nucleus

$^{11}_{3}Li$ with an abnormally high number of

neutrons has a very large specific heat and is thus a strongly bound system. The specific heat decreases as the mass number increases because the protons increase with mass number thus reducing the total energy of the nucleus.

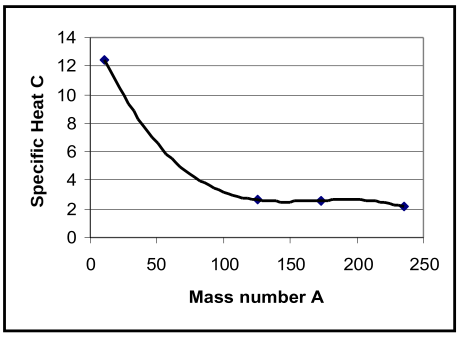

Fig 3: Specific heat C (MeV/kg) at $T=T_C$ against mass number A.

Variation of S with A and with T

Using Eq.14 we have calculated the variation of entropy S (MeV/T) with mass number A for nuclei with large neutron excess parameter . This variation is shown in Fig.4.

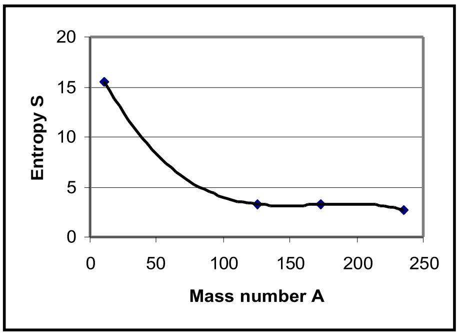

Fig 4: Entropy S (MeV/T) at $T=T_C$ against mass number A

Fig.4 shows that for large neutron excess

systems the entropy S is high for low mass and

decreases with increase in mass number A.

Using Eq.(14), we have calculated the variation of S with T for the nuclei $^{11}_{3}Li$, $^{125}_{49}In$, $^{163}_{66}Dy$ and $^{235}_{92}U$. The variation of S with T for these nuclei is shown in Fig.5 .

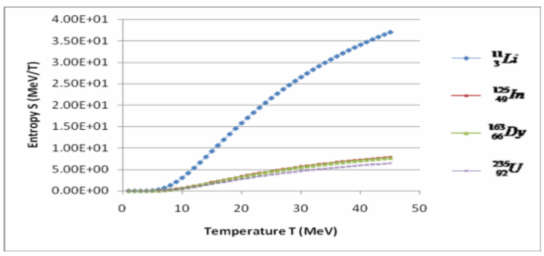

Fig.5: Variation of entropy S (MeV/kg) with temperature T (MeV) for

$^{11}_{3}Li$, $^{125}_{49}In$, ^{163}Dy and ^{235}U .

Fig.5 shows that the curves are approximately s-shaped and similar to those obtained using other methods [Khanna et al 2010]. It is also seen in the figure that the critical transition temperature T_c is at about 20 MeV where the curves have maximum gradient and that in large neutron excess nuclear systems light nuclei may be identified by their larger rate of change of entropy S with temperature T.

Transition Temperature T_C

The transition temperature is the temperature at which phase transition occurs. At the transition temperature T_C the free energies of the two phases must be equal and the specific heat must show a bump at this temperature.

Using Eq.16 the value of the transition temperature $T_C\kappa = \frac{h\omega}{2}$, and this turns out to be 19.602MeV.

Conclusions

The calculations of this study provide the result that the binding fraction of ${}^{11}_{6}Li$ with large number A. This proves that the nuclei with exceptionally large neutron numbers are more strongly bound and less susceptible to disorder which is a measure of entropy.

The variation of entropy S with temperature T for the four nuclei ${}^{11}_{3}Li$, ${}^{125}_{49}In$, ${}^{163}_{66}Dy$ and ${}^{235}_{92}U$ was also determined. The super heavy lithium isotope ${}^{11}_{3}Li$ was found to have the highest entropy S over the range of variation considered. This was consistent since it has the largest ratio $\frac{N}{Z}$ in the group. These excess neutrons stay in the surface region and contribute to the perturbation of the core resulting in an increase of perturbation energy and hence an increase in entropy [Khanna et al 2010, Saauer 1976, Siemens 1964].

A transition temperature $T_C = 19.602$ MeV was obtained, and this was within the expected range of 10-20MeV as pointed out earlier [Khanna et al 2010, Dean 2003, Elliot 2002].

Overall, this study emphasizes that a nucleus with exceptionally large neutron excess will be neutron excess is very large. This points to the fact that the neutrons when added to a nucleus contribute a lot of attractive energy and thus increases the binding fraction. This result confirms the fact that strongly bound neutron stars can exist as stable systems. Because of the very large binding fraction, such nuclei with large neutron excess cannot be used as fissile materials.

The variation of specific heat against excitation energy is faster for large neutron excess light nuclei than for heavy nuclei for the same variation of excitation. Such is the influence of the abnormal neutrons in ${}^{11}_{3}Li$ that its specific heat at the liquid gas phase transition [Saauer 1976, Siemens 1964] is found to be approximately six times that of ${}^{163}_{66}Dy$ or ${}^{235}_{92}U$.

The increase observed in the specific heat as A increases especially for nuclei with large neutron excess is in good agreement with earlier work [Khanna et al 2010, Dean 2003].

This study has also revealed that the entropy of abnormally large neutron excess systems is high and decreases with increase in massa strongly bound system; thus confirming the existence of neutron stars as stable systems.

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