SURFACE CONTOURS AND SHAPES OF SUPERHEAVY ELEMENTS

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Abstract

The enormity of data obtained in scientific experiments often necessitates a suitable graphical representation for analysis. Surface contour is one such graphical representation which renders a pictorial view that aids in easy data interpretation. It is essentially a two-dimensional visualization of a three-dimensional surface plot. Very recently, it has been shown that Super Heavy Elements can exist in a variety of shapes - spherical, spheroidal and ellipsoidal with or without shape co-existence. The shapes of such nuclei as predicted by us by diagonalizing the triaxial Nilsson Hamiltonian in cylindrical representation and using the Strutinsky-BCS corrections are graphically displayed by surface contours with Origin software. The obtained results are highly useful in the analysis of the stability of the Super Heavy Elements. Further, they yield a surprising result that the doubly magic spherical nucleus after lead (Z=82 and N=126) is SHE (Z=126 and N=184) in the macroscopic-microscopic method itself.

INTRODUCTION

Even though the predicted doubly magic superheavy nucleus having a lifetime comparable to the age of the earth should have a spherical shape, there could be other superheavy nuclei having ellipsoidal shapes (axial and non-axial) with predictable longer lifetimes. Such a possibility is considered theoretically in this work by the macroscopic-microscopic method namely the triaxial Nilsson-Strutinsky-BCS approach. Ellipsoidal shapes for alpha decaying and fissioning heavy nuclei are not new but well-known since the time of Hill and Wheeler. After reproducing some well established experimental quantities for heavy nuclei like alpha decay Q values, our calculations were extended to the fertile region of the transitional superheavy nuclei recently synthesized to determine their shapes by surface contours. The present macroscopic-microscopic calculations and the resulting contour diagrams further lead to the fact that the spherical doubly magic nucleus is $^{310}126_{184}$ instead of $^{298}114_{184}$

SUPER HEAVY ELEMENT

A superheavy nucleus is one which is doubly magic beyond $^{208}_{82}$Pb and has a spherical shape, according to theoretical predictions. While the predicted magic number for proton beyond 82 is 114, 120, 124 or 126 according to non-self-consistent [1], self-consistent [2] and relativistic theories [3], the neutron magic number after 126 is to be 172 or 184 according to those theories. Further, the size of the superheavy region, whether narrow or broad, is another interesting problem to tackle. After the advent of recent experiments by Oganessian *et al*. [4] at Dubna, a remarkable finding is emerging, according to which there could be a broad region of long-lived metastable superheavy nuclei having prolate, oblate or ellipsoidal shapes with very small deformations. Such a possibility of metastable superheavy elements directly accessible in heavy ion reactions has already been predicted by Bengtsson *et al*. [5] as early as 1975 with the triaxial Nilsson-Strutinsky method. However, at that time, the main focus was the on the stability of such superheavy elements against spontaneous fission decay. But presently, it has become clear that the predominant mode of decay of superheavy nuclei is mainly by a chain of alpha decays which terminate only at the end by spontaneous asymmetric fission. It seems now that Z=114 and N=172 are not the final destination but the starting points for a fertile land of transitional superheavy nuclei closing on sphericity around Z=126 and N=184 having all possible ellipsoidal shapes, axial as well as non-axial with small deformations. This is a dramatic turning point for the quest for superheavy nuclei.

THE METHOD

Our macroscopic-microscopic method [6, 7, 8] essentially has two components for the evaluation of the potential energy of nuclei, namely a smooth macroscopic liquid-drop model energy part(E_{LDM}) and a fluctuating microscopic part consisting of shell and pairing corrections ($\Delta E_{shell}\ and\ \Delta E_{pair}$). Thus the total energy E is given by,

$$E(Z,N,\varepsilon,\gamma) = E_{LDM}(Z,N,\varepsilon,\gamma) + \Delta E_{shell}(Z,N,\varepsilon,\gamma) + \Delta E_{pair}(Z,N,\varepsilon,\gamma) \quad (1)$$

ε and γ being the elongational and the non-axial parameters. The traditional liquid drop model energy is [9],

$$E_{LDM} = 17.9439\left(1 - 1.7826\left(\frac{N-Z}{A}\right)^2\right)A^{\frac{2}{3}}((B_S - 1) + 2x(B_C - 1)) \quad (2)$$

where B_S and B_C denote, respectively, the surface and coulomb potential energy in units of the spherical values

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assuming a homogeneous charge distribution bounded by a sharp ellipsoidal surface and the fissility parameter [10]

$$x = \frac{(Z^2/A)}{50.88\left(1 - 1.7826\left(\frac{N-Z}{A}\right)^2\right)}$$

The single particle energies are obtained by diagonalizing the triaxial Nilsson-Newton Hamiltonian

$$\begin{aligned} h^0 = -\frac{\hbar^2}{2m}\nabla^{'2} + \frac{m}{2}(\omega_x x^{'2} + \omega_y y^{'2} + \omega_z z^{'2}) \\ + C\ell.\mathbf{s} + D(\ell^{'2} - \frac{1}{2}N(N+3)) \end{aligned} \quad (3)$$

in cylindrical representation [11, 12] in the basis states

$$|N_\rho N_z \Lambda\Sigma >= |N_\rho\Lambda > |\Lambda > |N_z > |\Sigma >, \quad (4)$$

where $|\Sigma >$ is the spin eigen function and

$$\begin{aligned} |\Lambda >= (2\pi)^{-\frac{1}{2}} e^{i\Lambda\phi} \\ |N_z >= (\sqrt{\pi} N_z! 2^{N_z})^{-\frac{1}{2}} e^{-z^2/2} H_{N_z}(z) \\ and\ |N_\rho\Lambda >= \left(\frac{2\Gamma(n+1)}{\Gamma(|\Lambda|+n+1)^3}\right)^{\frac{1}{2}} e^{-\rho^2/2}\rho^{|\Lambda|} L_n^{|\Lambda|}(\rho^2). \end{aligned} \quad (5)$$

Here we have substituted $n = \frac{1}{2}(N_\rho - |\Lambda|)$. The functions $L_n^{|\Lambda|}$ and $H_{N_z}(z)$ are the Laguerre and Hermite polynomials. The κ and μ values used for the Nilsson Hamiltonian are those given by Bengtsson *et al*. [13]. The shell and pairing corrections are then evaluated using the Strutinsky and the BCS methods [14].

The shell correction is given by,

$$\begin{aligned} \Delta E_{shell}(N) = E_N - \tilde{E}(N) \\ \text{where } E_N = \sum_{n=1}^{N} \epsilon_n \\ \text{or } \Delta E_{shell}(N) = \sum_{n=1}^{N} \epsilon_N - \int_0^N \tilde{\epsilon}(n)dn \end{aligned} \quad (6)$$

Because neither the smoothing range nor the order p represent physical quantities, the shell correction should be approximately independent of them as long as they are chosen suitably. The value of γ should be large enough to average over the levels between major shells, but must not be too large, because then levels far from the fermi surface would strongly affect the shell correction. The value $\gamma = 1.2\hbar\omega_0^0$ where $\hbar\omega_0^0 = \frac{45.30}{(A^{1/3}+0.77)}$ MeV in a sixth-order correction ($p = 6$) is near the optimum choice.

The pairing correction for either neutrons or protons is given by

$$\Delta E_{pair} = E_{pc} - \tilde{E}_{pc}$$

The pairing strength G for neutrons and protons usually are adjusted to reproduce the average mass differences of neighboring nuclei that differ by one neutron or one proton. This average odd-even mass difference is given by the semi-empirical result

$$\tilde{\Delta} = \frac{12}{\sqrt{A}} \text{ MeV} \quad (7)$$

In the above formulation of the pairing correction, the value of G for either neutrons or protons is taken from Dudek et. al [15]. When parametrizing the pairing constants (average matrix elements) [16, 17] they took as a starting point the pairing force strength parameters from

$$\begin{aligned} G_n = \frac{1}{A}[18.95 - 0.078(N-Z)] \\ G_p = \frac{1}{A}[17.90 + 0.176(N-Z)] \end{aligned} \quad (8)$$

where they have been adjusted to experimental data on normal nuclei by applying the pairing-self-consistent Bogolyubov formalism without the proton-neutron pairing. When used within the particle projection formalism, these values have to be decreased, by about 15%. In the present application we use the reduction factor of 0.85 for both the neutrons and the protons, i.e., we apply $0.85G_n$ and $0.85G_p$ in the monopole pairing Hamiltonian.

Table I. Q-values for alpha decay of some very heavy and superheavy nuclei

A_p	Z_p	A_d	Z_d	Q_α (MeV) Calculated	Q_α (MeV) Experimental [4]
271	106	267	104	8.37	8.65
275	108	271	106	9.50	9.44
279	110	275	108	9.75	9.84
283	112	279	110	9.42	9.67
286	114	282	112	10.21	10.35
290	116	286	114	10.63	11.00
294	118	290	116	11.42	11.81

We then apply the present model to reproduce the recently measured alpha decay Q values for nuclei in the very heavy and superheavy region. Our results are shown above in table I and it is seen that the experimentally measured Q values for the very heavy and superheavy nuclei are reproduced within a deviation of 0.4 MeV. Considering the fact that the present model is a simple one, it is gratifying to note its success in closely reproducing the alpha decay Q values for the very heavy and superheavy nuclei considered.

SURFACE CONTOURS

- A contour plot is a two-dimensional version of a three-dimensional surface plot.
- Given a function v=f(x, y), a surface contour consists of all the curves that connect all the (x, y) points for a constant v.
- In this work, we use Origin software to generate the contour plots given the values x, y and f(x,y).

The advantages of contour plotting are:

- Easy detection of areas of rapid change and areas of constant value.
- Well suited to monochrome and gray scale reproduction and easy to annotate within the field.
- Widely used, generally understood by others and can easily be transformed and projected

Hence, results of our calculations are given in the form of Potential Energy Surface Contours (normalized to spherical-liquid-drop energy) in the (Q_{20}, Q_{22}) plane, where Q_{20} and Q_{22} are the quadrupole moments which can be related to the Hill - Wheeler polar deformation parameters Q_0 and γ through the usual relations: $Q_{20} = Q_0 cos\gamma$ and $Q_{22} = \frac{Q_0}{\sqrt{2}} sin\gamma$. Q_0 is proportional to the quadrupole deformation β for weakly deformed systems. The non-axial parameter γ gives the degree of triaxiality. While $\gamma = 0^\circ$ denotes prolate shapes, $\gamma = 60^\circ$ denotes oblate shapes. Intermediate values of γ correspond to triaxial shapes.

We first apply our triaxial Nilsson-Strutinsky calculations to the doubly magic spherical nucleus $^{208}_{82}$Pb, which produce a spherical shape with a shell energy of -12 MeV as is well-known. Then, we consider the long-lived superheavy nucleus $^{285}_{112}$X which was found to be the starting point of the transitional region with a deformation $\beta < 0.1$ and prone to shape coexistence and triaxiality [18] thereby inhibiting the alpha decay and enhancing its lifetime [19, 20]. The superheavy nucleus $^{286}_{114}$X which was expected to be closing on sphericity turns out to be transitional and is non-spherical. The nucleus $^{300}_{124}$X is oblate with $\gamma = 60^\circ$, $\beta = 0.2$ and a fission barrier of 2.5 MeV. This result is exactly the same as that obtained by Bengtsson *et al*. [5] which is used as a benchmark for testing the precision of our calculations. To track down the doubly magic nucleus after lead, we next consider $^{310}_{126}X_{184}$. It is seen from the figure 1 that the nucleus $^{310}_{126}X_{184}$ is spherical showing that it is doubly magic. This result is in accordance with the predictions of the density functional method. However, it is to be noted that while the doubly magic nucleus $^{208}_{82}$Pb is robust, the doubly magic superheavy nucleus $^{310}_{126}X_{184}$ is fragile having a shell energy of about -7 MeV and a fission barrier of about 3 MeV. Between this nucleus and the nucleus $^{285}_{112}$X we have the transitional region which is very rich in structure and is important since it may yield long-lived species of superheavy nuclei. The even Z nuclei with Z=114 - 126 and N=184 are spherical but all of them except Z=126 become non-spherical when N=172. This leads to the neutron magicity of N=184 and proton magicity of Z=126.

To summarize, the macroscopic-microscopic calculation namely the triaxial Nilsson-Strutinsky-BCS approach and surface contour plotting have been revisited. These closely reproduce the experimental alpha decay Q-values of very heavy and superheavy nuclei recently synthesized. Further, they lead to the fact that the doubly magic spherical nucleus after $^{208}_{82}Pb_{126}$ is $^{310}_{126}X_{184}$ instead of $^{298}_{114}X_{184}$. It is felt that this result is due to the role of triaxial degree of freedom in weakly deformed alpha decaying superheavy nuclei. Undoubtedly, we have reached an exciting phase in our quest for superheavy elements.

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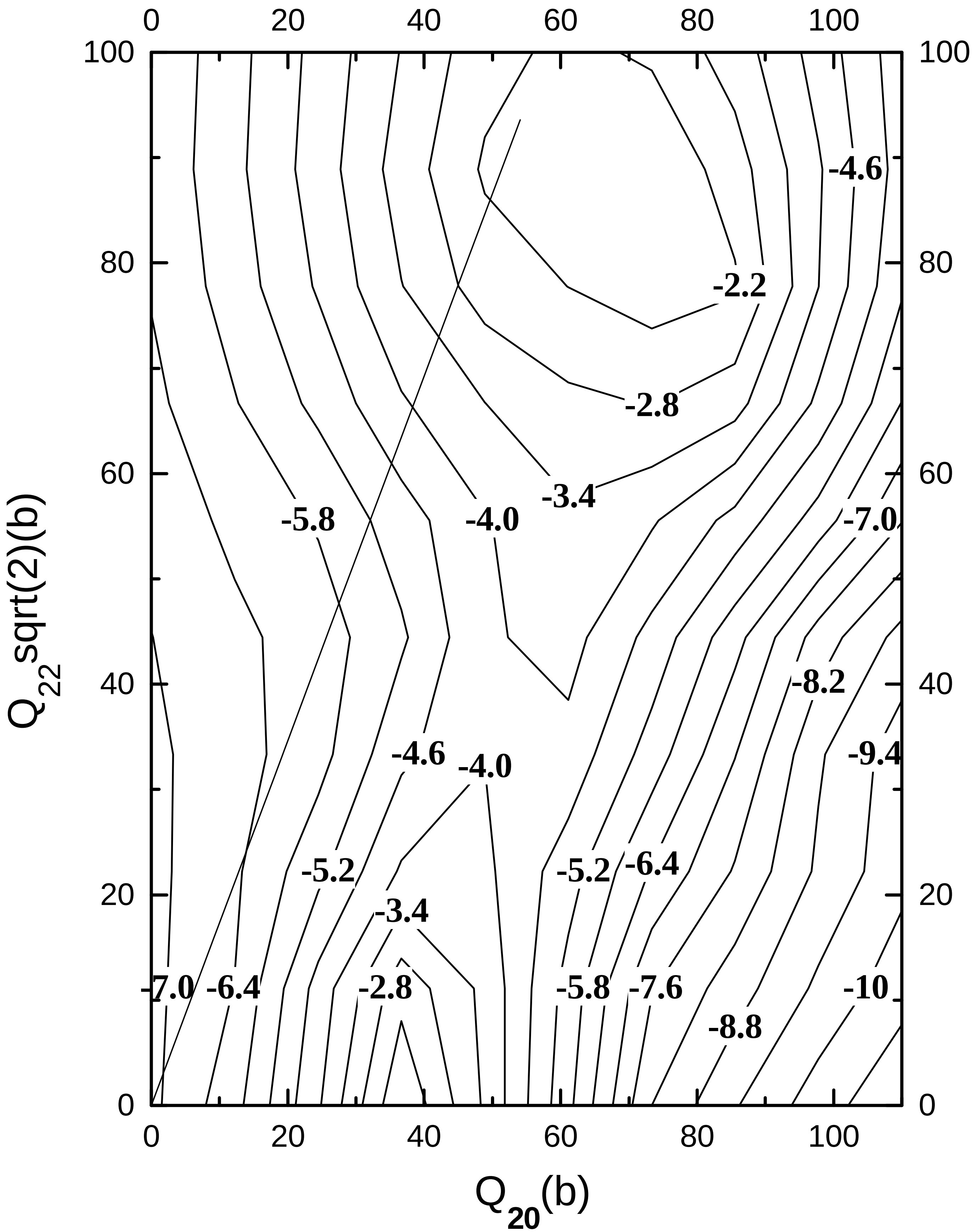

Figure 1: Potential Energy Surface Contour(normalized to spherical-liquid-drop energy) for $^{310}_{126}$X