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The role of the surface energy in nuclear octupole excitations

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Octupole excitations of atomic nuclei can be viewed as fluctuations around an equilibrium shape. These fluctuations in turn can be seen as probes of nuclear matter properties to the extent that the shape changes explore changes in compression, surface to volume ratio, or isospin overlap. In the present work we use a series of Skyrme interactions, which were fitted to provide a systematic range of surface energies, to explore the surface energy dependence of octupole excitations in ^{208}Pb. We find a strong positive linear corelation between the surface energy of a Skyrme interaction and its prediction of the first 3^- octupole excitation energy.

Keywords: Octupole Excitation; Nuclear Matter; Nuclear Surface Energy

1. Introduction

The representation of bulk properties of nuclear matter in terms of coefficients in mass formulae remains a useful way of classifying nuclei and the forces that act in them. A basic form of the semi-empirical mass formula, as given in Bohr and Mottelson's textbook,[1] following Weizsäcker,[2] and Bethe and Bacher[3] can be expressed as

$$\mathcal{B} = b_{\mathrm{vol}}A - b_{\mathrm{surf}}A^{2/3} - \frac{1}{2}b_{\mathrm{sym}}\frac{(N-Z)^2}{A} - \frac{3}{5}\frac{Z^2e^2}{R_c} \tag{1}$$

where $\mathcal{B}$ is the total binding energy of a nucleus of N neutrons and Z protons, with total mass number $A = N + Z$. The coefficient b_{vol} characterises the volume term, accounting for the nearest-neighbour interaction of each nucleon with its surrounding nucleons. The b_{surf} surface coefficient corrects the volume term for those nucleons which lack a full set of nearest-neighbour due to being at the surface of the nucleus. The b_{sym} term accounts for the preference for a like number of protons and neutrons in the nucleus while the final term, in which e is the elementary charge and R_c the charge radius of the nucleus, gives a contribution from the Coulomb force.

From a fit to observed binding energies, numerical values of each coefficient can be obtained. For example, the value for b_{surf} quoted by Bohr and Mottelson is $\simeq 17$ MeV. One may then go on to link this macroscpic view with any microscopic theory that is able to calculate these coefficients and other derived properties alongside more detailed structure , thereby linking structure details to the bulk properties.[4,5]

The surface energy of nuclear matter has been studied relatively less than other terms, as it does not apply in the calculationally simple case of infinite nuclear matter. However, it has recently become of increasing interest as the ability to make useful calculations of e.g. heavy-ion reactions[6] and fission[7] have become possible with effective interactions in the density funcional framework. This has combined with the availability of paramters sets for Skyrme effective interactions in which the surface energy is systematically varied.[8,9]

The purpose of the present work is to study the effect of the systematic variation of the surface energy on shape vibrations in the form of the lowest octupole state in doubly-magic ^{208}Pb. The vibration can be thought of as dynamical shape-changing processes in which the surface area of the nucleus stretches and contracts.

2. Methodology

We employ the time-dependent density functional theory, through the published Sky3d code[10,11] using the set of Skyrme interactions developed by Jodon *et al.*[8] The time-dependent density function theory (TDDFT)[12] is the general microscopic theory of quantum dynamics truncated at the one-body level. Formally, theories such as the random phase approximation (RPA) can be derived from it,[12] and the practical correspondence between TDDFT and RPA for the case of resonance states has been demonstrated.[13] While RPA is a more widespread theory used in practice for microscopic calculation of vibrational excitations, we use TDDFT to get a real-time picture of the shape changes when a nucleus is undergoing a vibrational excitation.

The set of Skyrme forces used in our study were fitted so that each had identically-constrained values of many nuclear matter and finite nuclear properties, while being adjusted to particular values of the surface energy – essentially the b_{surf} coefficient of equation 1. Since extracting the b_{surf} parameter from a Skyrme interaction depends on the particular method used, Jodon *et al.* presented different values. For our analysis we use their $a_{\mathrm{surf(HF)}}$ value as the surface energy.

In order to calculate the octupole vibrational state in ^{208}Pb, we first run the Sky3d code in static Hartree-Fock mode to generate a ground state, then apply an instantaneous octupole boost to each single particle wave function $\psi(r,t)$ of the form

$$\psi(r,0^+) = \exp^{ikr^3 Y_{30}} \psi(r,0), \tag{2}$$

where $\psi(r,0)$ are the static ground state wave functions. $r^3 Y_{30}$, where Y_{30} is a spherical harmonic, is the octupole excitation operator and initialises the octupole shape excitation. Once the boost is applied, the single-partice states are evolved forward in time by the TDDFT equations, and the nucleus allowed to respond to the octupole excitation. The octupole operator $O(t)$ is followed in time to analyse the response

$$O(t) = \langle r^3 Y_{30} \rangle (t) \tag{3}$$

The nuclear strength is given by

$$S(E) = \frac{1}{\hbar k} \tilde{O}(\omega) \tag{4}$$

where $\tilde{O}(\omega)$ is the Fourier Transform of the time-dependent response and k is the boost strength parameter featured in equation (2). In this work, we stick to the linear RPA limit with a boost strength of $k = 0.0001$ fm^{-3}.

In order to extract peak energies from a finite time signal, the data is enveloped as described in ref.,[11] with a linear interpolation made between the discretised energy grid points to estimate the peak location and height.

3. Results

For each of the eight SLy5sX forces with $X = 1..8$, we calculated the response of the ^{208}Pb nucleus to an octupole boost, and performed the Fourier analysis. The tabluated peak positions for each force, along with the given surface energy, is shown in Table 1

Table 1. Lowest octupole state in ^{208}Pb for each SLy5sX force

Force Name	Surface Energy $a_{\mathrm{surf}}^{(\mathrm{HF})}$ [MeV]	E_{3^-} [MeV]
SLy5s1	17.55	3.122
SLy5s2	17.74	3.153
SLy5s3	17.93	3.182
SLy5s4	18.12	3.211
SLy5s5	18.31	3.241
SLy5s6	18.50	3.268
SLy5s7	18.70	3.298
SLy5s8	18.89	3.323

The correlation between the surface energy and the 3^- energy is shown in Figure 1. Here, the straight line fit is shown. It is made with linear regression with the resulting equation

$$E_{3^-} = 0.1506 a_{\text{surf}}^{(HF)} + 0.4812. \tag{5}$$

The plot includes a 1σ envelope from the fit, but the conspicuous linearity of the fit and subsequent high confidence means that the uncertainty band is narrow and barely perceptible in the plot.

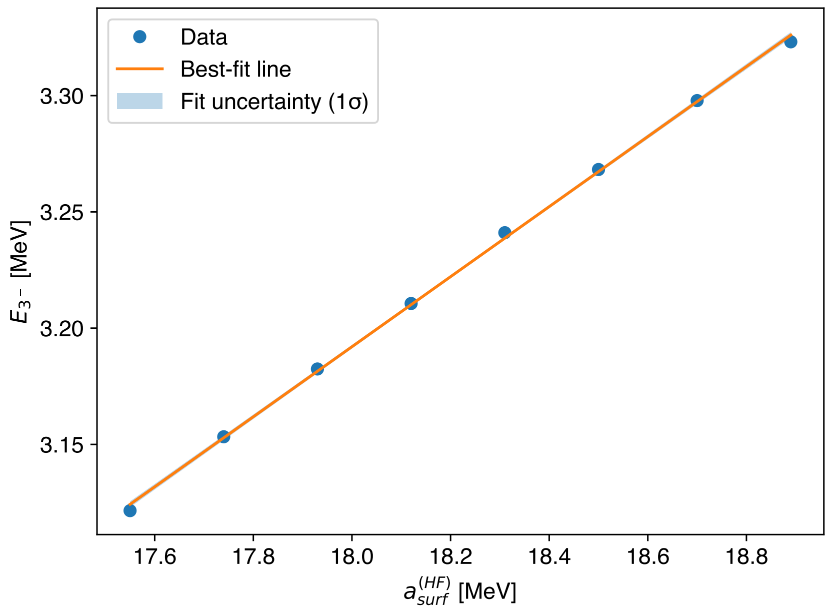

Fig. 1. Correlation between the surface energy and the predicted octupole peak position for each Skyrme interaction in the SLy5sX series.

To further visualise the results, Figure 2 shows the strength function as described by equation (4). Here, the peaks are shown at the points calculated through the interpolation method discussed in section 2. The peak height includes an error bar given by the height of the highest neighbouring point in the Fourier transform not included in the interpolation. For the forces SLy5s1 and SLy5s8 the raw Fourier transformed strength is shown which shows both the discretisation of the energy grid caused by the finite sampling time of the octupole signal, and the spreading of strength between neighbouring energy points caused by the envelope technique[11] used in the Fourier analysis.

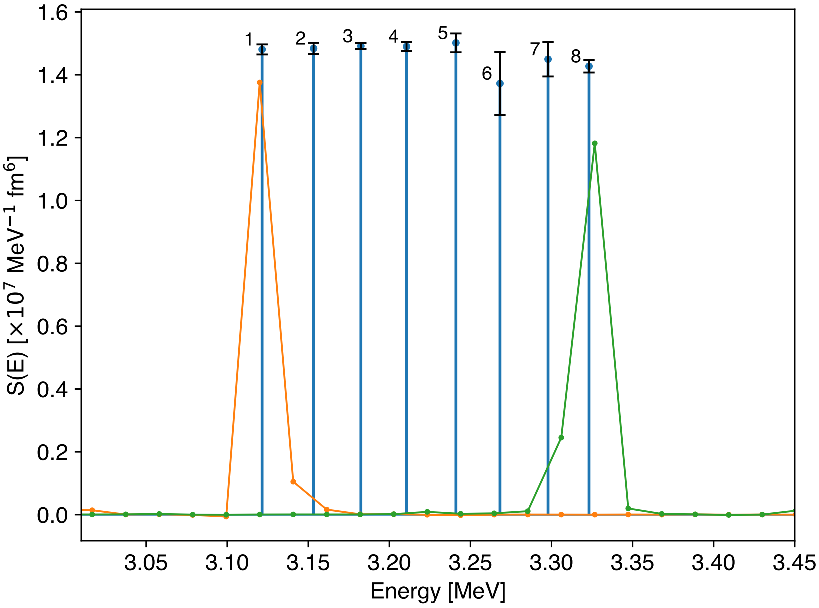

Fig. 2. Octupole strength in ^{208}Pb for the forces SLy5sX forces for $X = 1..8$ in the region of the low-lying excited 3^- state. Peak positions and strenghts are shown for all eight forces.

4. Discussion and Conclusion

The results from section 3 suggest that the there is a strong linear relationship between surface energy and the position of the octupole state in ^{208}Pb. We hypothesise that this is due to the fact that an octupole vibration involves a change in the surface area of a nucleus, and where the cost of generating the nuclear surface is low, the corresponding excitation energy of the nuclear state is lower.

The experimental value for the first 3^- energy in ^{208}Pb is 2614 keV.[15] This is substantially lower than the values coming from any of the SLy5sX forces. We do not suggest here that an extrapolation for this particular level makes sense, as other systematic effects in the Skyrme fits should be taken into account, with existing Skyrme forces showing a wide variation in reproduction of this energy level.[14] However, the linear fit shown in equation (5) appears robust, and could form a low-cost way of including pseudodata in future fits or studies.

In conclusion, we hypothesised a correlation between the surface energy which characterises an effective nuclear interaction, and the position of shape-vibrational excited octupole states. We shows there to be a strong linear correlation between the two quantities in the case of the well-known first excited state in ^{208}Pb, which is octupole in nature.

Data Availability

All data produced in this work was produced with published codes and using parameters as noted in the manuscript. No further data than that presented is required for reproduction.

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