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Shell-model study on properties of proton dripline nuclides with Z,N =30-50 including uncertainty analysis

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Part I

Overview

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Abstract

- use the non-parametric Bootstrap method to estimate the stablity of protons emission for each nuclide
- propose 2 formulas to calculate the binding energy and proton separation energy
- use the S_p and S_{2p} energy to predict the boundary of the region
- find a new dripline by extrapolation
- predict the unstable nuclides to bound about proton-emission

Key Words

Shell Model, Proton Separation, Binding Energy

Part II

Introduction

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P Nuclei

- neutron-deficient stable nuclei(from ^{74}Se to ^{196}Hg)
- related to p-process(γ process) with photodisintegration reactions of (γ, n), (γ, p),(γ, α)

Mass And Half-lives of Nuclei

Before

- semi-empirical droplet model of nuclei masses and deformations
- finite-range liquid-droplet model
- ...

Now

- full f_5pg_9 shell model calculation

Part III

Formulas And Statistic Method

f_5pg_9 Shell Model Space

$p_{3/2}$, $f_{5/2}$, $p_{1/2}$, $g_{9/2}$

Effective Interaction

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Binding Energy of Valence Nucleon

$E_{BE,SM}(Z,N)$:ignore the Coulomb interaction ,just refers to the binding energy between the valence nucleons in the shell model calculations

Binding Energy

$$E_{BE}(Z,N) = E_{BE,SM}(Z,N)+const+a(Z-28)+b(Z-28)^2+c(N-28)^2+d(N-28) \quad (1)$$

consider the core , $const = E_{BE}(^{56}Ni)$

$$E_{BE}(Z,N) = E_{BE,SM}(Z,N)+E_{BE}(^{56}Ni)+a(Z-28)+b(Z-28)^2+c(N-28)^2+d(N-28) \quad (2)$$

consider the isospin, the $(Z-N)^2$ is added

$$E_{BE}(Z,N) = E_{BE,SM}(Z,N)+const+a(Z-28)+b(Z-28)^2+c(N-28)^2+d(Z-N)^2 \quad (3)$$

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Binding Energy

the last 2 terms show a hyperholoid-like distribution

$$E_{BE}(Z,N) = E_{BE,SM}(Z,N) + const + a(Z-28) + b(Z-28)^2 + c(Z-30)(Z-2N+50) \quad (4)$$

Separation Energy

$$S_p = E_{BE}(Z,N) - E_{BE}(Z-1,N) \qquad S_p = E_{BE}(Z,N) - E_{BE}(Z-2,N) \quad (5)$$

$$S_p(Z,N) = E_{BE,SM}(Z,N) - E_{BE,SM}(Z-1,N) + aZ + bN + d \quad (6)$$

$$S_{2p}(Z,N) = E_{BE,SM}(Z,N) - E_{BE,SM}(Z-2,N) + aZ + bN + d \quad (7)$$

consider the isospin, the $(Z-N)^2$ is added

$$S_p(Z,N) = E_{BE,SM}(Z,N) - E_{BE,SM}(Z-1,N) + aZ + bN + c(Z-N)^2 + d \quad (8)$$

$$S_{2p}(Z,N) = E_{BE,SM}(Z,N) - E_{BE,SM}(Z-2,N) + aZ + bN + c(Z-N)^2 + d \quad (9)$$

Calculation of Binding Energy And Separation Energy

Separation Energy

	$\sigma_{total}{}^{*}$	$\sigma_{stat}{}^{*}$	$\sigma_{sys}{}^{*}$	$\sigma_{total}{}^{\#}$	$\sigma_{stat}{}^{\#}$	a	b	c	d	e	f
$E_{BE}(Eq.2)$	0.731	0.122	0.721	0.774	0.281	-9.15 (5)	-0.0954 (25)	0.0188 (12)	-0.276 (31)	—	—
$E_{BE}(Eq.3)$	0.316	0.0482	0.312	0.416	0.275	-9.61 (1)	-0.0944 (8)	0.0245 (5)	-0.0262 (9)	—	—
$E_{BE}(Eq.4)$	0.317	0.0399	0.315	0.374	0.202	-9.12 (1)	-0.0921 (7)	-0.0309 (5)	—	—	—
$E_{BE}(Eq.5)$	0.305	0.0563	0.300	0.779	0.719	-9.45 (8)	-0.118 (1)	0.425 (98)	0.0221 (158)	-0.0939 (244)	0.363 (96)
$S_p(Eq.6)$	0.286	0.0362	0.284	0.294	0.0781	-0.242 (6)	0.0548 (52)	—	-4.28 (19)	—	—
$S_p(Eq.8)$	0.276	0.0404	0.273	0.375	0.257	-0.186 (16)	0.00385 (1541)	0.00335 (88)	-4.36 (19)	—	—
$S_p(Eq.10)$	0.275	0.0331	0.273	0.278	0.0519	-0.182 (5)	—	0.00359 (27)	-4.36 (19)	—	—
$S_p(Eq.22)$	0.231	0.0328	0.228	0.233	0.0447	-0.183 (4)	—	0.00364 (25)	-4.14 (16)	-0.302 (33)	—
$S_{2p}(Eq.7)$	0.306	0.0449	0.303	0.320	0.102	-0.478 (8)	0.105 (7)	—	-8.36 (22)	—	—
$S_{2p}(Eq.9)$	0.265	0.0439	0.261	0.390	0.289	-0.360 (19)	-0.00125 (1794)	0.00736 (111)	-8.55 (21)	—	—
$S_{2p}(Eq.11)$	0.264	0.0355	0.261	0.267	0.0527	-0.361 (5)	—	0.00729 (34)	-8.55 (20)	—	—

* Calculated uncertainties for these nuclides with experimentally known data.
\# Calculated uncertainties for these nuclides without experimentally known data.

b is no more robust ,which is neglected.

$$S_p(Z,N) = E_{BE,SM}(Z,N) - E_{BE,SM}(Z-1,N) + aZ + c(Z-N)^2 + d \quad (10)$$

$$S_{2p}(Z,N) = E_{BE,SM}(Z,N) - E_{BE,SM}(Z-2,N) + aZ + c(Z-N)^2 + d \quad (11)$$

Total Uncertainty

The total uncertainty : the experimental uncertainty,the statistical uncertainty and the systematic uncertainty.But the experimental uncertainty is neglected.

Residual

$$r(Z,N,S_{BS,i}) = y_{cal}(Z,N,S_{BS,i}) - y_{exp}(Z,N) \quad (12)$$

$S_{BS,i}$ is the ith Bootstrap sample in the M Bootstrap samples

Statistical Uncertainty

$$\sigma^2_{stat}(Z,N) = \frac{1}{M-1}\sum_{i=1}^{M}(y_{cal}(Z,N,S_{BS,i}) - \bar{y}_{cal}(Z,N))^2 \quad (13)$$

The global statistical uncertainty of a formula: K is the number of the combinations of protons and neutrons in the datasets

$$\sigma^2_{stat} = \frac{1}{K}\sum_{k=1}^{K}\sigma^2_{stat}(Z,N) \quad (14)$$

Systematic Uncertainty

$$\begin{aligned} \sigma^2_{sys}(Z,N) &= \left(\sum_{i=1}^{M} \frac{y_{cal}(Z,N,S_{BS,i})}{M} - y_{exp}(Z,N)\right)^2 \\ &= \left(\frac{1}{M}\sum_{i=1}^{M} r(Z,N,S_{BS,i})\right)^2 \end{aligned} \quad (15)$$

the global systematic uncertainty:

$$\sigma^2_{sys} = \frac{1}{K}\sum_{k=1}^{K}\sigma^2_{sys}(Z,N) = \frac{1}{K}\sum_{k=1}^{K}\bar{r}^2(Z,N) \quad (16)$$

total uncertainty and prediction uncertainty

$$\sigma^2_{total}(Z,N) = \frac{1}{M}\sum_{i=1}^{M} r^2(Z,N,S_{BS,i}) = \frac{M-1}{M}\sigma^2_{stat}(Z,N) + \sigma^2_{sys} \quad (17)$$

$$\sigma^2_{total} = \sigma^2_{sys} + \sigma^2_{stat} \quad (18)$$

$$\sigma^2_{pred}(Z,N) = \sigma^2_{sys} + \sigma^2_{stat}(Z,N) \quad (19)$$

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Bootstrap Method

The original dataset is divided in 2 parts: training group(Bootstrap sample) and test group.

$$\sigma_{tr}(S_{BS,i}) = \sqrt{\frac{1}{n_{i,tr}} \sum_{k=1}^{n_{i,tr}} r^2(Z_k, N_k, S_{BS,i})} \quad (20)$$

$$\sigma_{ts}(S_{BS,i}) = \sqrt{\frac{1}{n_{i,ts}} \sum_{k=1}^{n_{i,ts}} r^2(Z_k, N_k, S_{BS,i})} \quad (21)$$

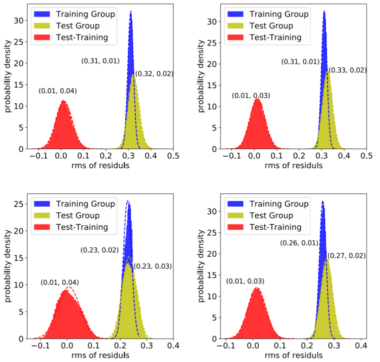

FIG. 1. Distribution of uncertainties of training group, test group and their difference. The top two are for Eq. (3) and Eq. (4). The bottom two are for Eq. (22) and Eq. (11). The dash lines are the fitted normal distribution, of which the parameters, mean and standard deviation, are listed in the nearby parentheses.

Part IV

Result and Discussion

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Parameter

	σ_{total}^*	σ_{stat}^*	σ_{sys}^*	$\sigma_{total}^\#$	$\sigma_{stat}^\#$	a	b	c	d	e	f
$E_{BE}(Eq.2)$	0.731	0.122	0.721	0.774	0.281	-9.15 (5)	-0.0954 (25)	0.0188 (12)	-0.276 (31)	—	—
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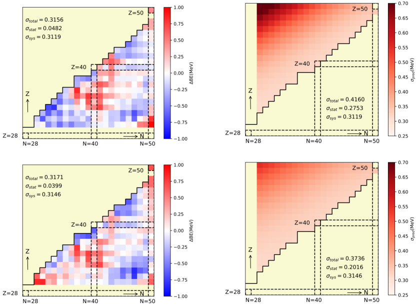
$E_{BE}(Eq.5)$	0.305	0.0563	0.300	0.779	0.719	-9.45 (8)	-0.118 (1)	0.425 (98)	0.0221 (158)	-0.0939 (244)	0.363 (96)

Repulsion,Neutron Shell Effect, Isospin Effect

- repulsion between protons decreases the single particle energy of orbit and the released energy
- residual:the competition between the neutron shell effect and the isospin effect
- less parameters to control the uncertainty



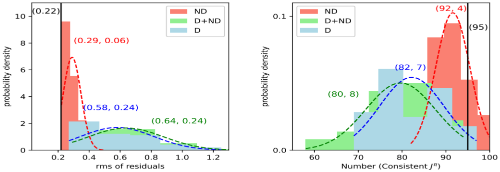
Binding Energy

Decomposed Uncertainty

The dataset is divided into 2 parts: $N < 45, \&Z > 33$(middle region), and the outer region.

	objective region	parameter region	σ_{total}	σ_{stat}	σ_{sys}
Eq. (3)	middle	middle	0.317	0.0849	0.305
		outer	0.557	0.0569	0.554
		whole	0.379	0.0437	0.377
	outer	outer	0.254	0.0473	0.250
		middle	0.867	0.305	0.812
		whole	0.286	0.0499	0.281
Eq. (4)	middle	middle	0.327	0.0768	0.317
		outer	0.382	0.0724	0.375
		whole	0.355	0.0431	0.352
	outer	outer	0.295	0.0426	0.292
		middle	0.461	0.153	0.434
		whole	0.300	0.0385	0.298

Random Perturbation



- The influence of the perturbation on ND TBME is weak
- The rms is sensitive to the diagonal TBMEs
- Calculated spin and parity of ground state are consistent with the experimental data

Separation Energy

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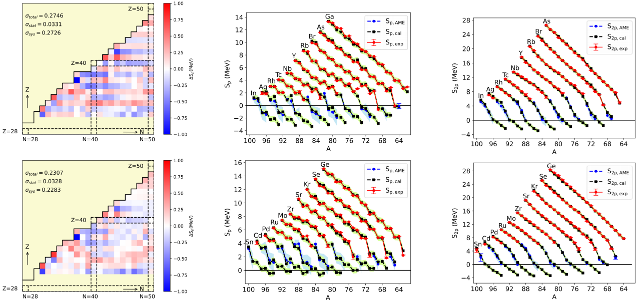
Correction

Equation (10) overestimate the odd-Z nuclides but underestimate the even-Z nuclides, which indicates the pairing strength may not be well described in shell model.

$$S_{2p}(Z,N) = E_{BE,SM}(Z,N) - E_{BE,SM}(Z-2,N) + aZ + c(Z-N)^2 + d + e\delta_Z \quad (22)$$

$\delta_Z = 0$,if Z is even,$\delta_Z = 1$,if Z is odd.



Thanks!

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