Correlations between nuclear landscape boundaries and neutron-rich $r$-process abundances

Q.Z. Chai, Y. Qiang, and J.C. Pe

State Key Laboratory of Nuclear Physics and Technology,
School of Physics, Peking University, Beijing 100871, China

Motivated by the newly observed $^{39}$Na in experiments, systematic calculations of global nuclear binding energies with seven Skyrme forces are performed. We demonstrate the strong correlation between the two-neutron separation energies ($S_{2n}$) of $^{39}$Na and the total number of bound nuclei of the whole nuclear landscape. Furthermore, with calculated nuclear masses, we perform astrophysical rapid-neutron capture process ($r$-process) simulations by using nuclear reaction code TALYS and nuclear reaction network code SkyNet. $r$-process abundances from ejecta of neutron star mergers and core-collapse supernova are compared. Prominent covariance correlations between nuclear landscape boundaries and neutron-rich $r$-process abundances before the third peak are shown. This study highlights the needs for further experimental studies of drip-line nuclei around $^{39}$Na for better constraints on nuclear landscape boundaries and $r$-process.

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I. INTRODUCTION

It is well known that studies of exotic nuclei close to drip lines are precious for understandings of the origin of elements in nature [1,2]. The rapid neutron capture process ($r$-process) involving high neutron densities is responsible for producing half of the elements heavier than iron and all elements beyond bismuth. The actual astrophysical sites for the occurrence of $r$-process is not definitely determined yet [1-4]. The developments of new-generation rare isotope beam facilities around the world provide unprecedented opportunities to access the nuclear drip lines. For example, the Facility for Rare Isotope Beams (FRIB) is expected to be fully operational in 2022 and will be able to reach the neutron drip line up to nuclei with charge number $Z = 40$ [5]. However, it is almost impossible to reach the neutron drip line in heavy nuclear mass region by terrestrial experiments. Therefore, the examination on correlations between existing experimental evidences and theoretical predictions is crucial for better exportations.

In a very recent experiment performed in RIKEN, $^{31}$F and $^{34}$Ne were reconfirmed to be the drip-line nuclei [6]. Surprisingly, this experiment also observed one event of $^{39}$Na [6], indicating it is weakly bound and mostly likely it is the drip line of sodium. This is an exciting progress to reach the neutron drip line since the last observation of $^{40}$Mg in 2007 [7]. It is known that different theoretical models can have remarkably divergent predictions about the neutron drip lines [8,11]. In contrast, the proton drip line has much reduced uncertainties. Therefore, the newly observed $^{39}$Na provides a great opportunity to constrain theoretical models. It is interesting to know how small discrepancies in drip lines of light nuclei propagate to large uncertainties in drip lines of heavy nuclei.

Consequently, the total number of bound nuclei in the nuclear landscape can be more accurately estimated.

So far it was known that binary neutron star mergers (NSM) [12,13] and ejecta from core collapse supernova (CCSN) [14,15] are possible scenarios for $r$-process. Following the gravitational wave event GW170817 of NSM, the $r$-process kilonova electromagnetic transient was observed, resulting from the ejection of $\sim 0.05$ solar masses of neutron-rich material [17]. These observations are becoming increasingly precise. NSM provides a much higher neutron density scenario to support a strong version of $r$-process to reach heavy elements such as uranium and thorium, while CCSN is associated with a larger electron faction $Y_e$. Therefore it is expected that $r$-process via NSM is more sensitive to properties of neutron drip lines compared to that via ejecta of CCSN. There have been extensive studies of the impacts of uncertainties of nuclear inputs for $r$-process abundances in the literature [2,15-21]. The $r$-process involves the neutron capture reactions, $\beta$-decays and fission properties. The fission is essential for appearance of the second peak ($A \sim 160$) in elemental abundance [22,23]. The uncertainties in ($n, \gamma$) reactions play a sensitive role. It was found that mass variations of $\pm 0.5$ MeV can result in up to an order of magnitude change in the final abundance [18]. The ($n, \gamma$) reaction is mainly determined by the nuclear masses and thus reliable predictions of nuclear mass by self-consistent microscopic framework are crucial.

In principle, the $ab$ initio calculations of nuclear drip lines are more reliable but it is problematic for heavy nuclei due to tremendous computing costs [24]. Semi-microscopic and phenomenological models can be precise for known nuclei but could be less reliable for explorations. As a suitable tool, the density functional theory with high-precision effective interactions are versatile for reasonable descriptions of global finite nuclei and neutron stars, including exotic structures and dynamics of halo nuclei, and nuclear fission [8,25,32]. Previously the properties of $^{39}$Na and neighboring drip line nuclei
have been studied [32]. The subsequent combined con-
strains on the whole nuclear landscape and r-process are
expected.

Compared to earlier studies of r-process by focusing on
the impact of uncertainties of nuclear inputs [18],
the aim of this work is to examine the correlations be-
tween theoretical discrepancies in $^{39}$Na, nuclear land-
scape boundaries, and r-process abundances based on
several effective nuclear forces. Firstly, the global nu-
clear masses are calculated with the Skyrme Hartree-
Fock-Bogoliubov (HFB) framework [33]. In particular,
the results are evaluated with the existing evidence of
the drip line nucleus $^{39}$Na. This results in very different
total number of bound nuclei and r-process paths. With
the calculated nuclear masses, the $(n, \gamma)$ reaction rates
are obtained with TALYS [34]. The updated reaction
rates are merged into REACLIB database [35], and then
the r-process simulations are performed with SkyNet [36]
which interfaces with REACLIB. Finally, the covariance
correlations between r-process abundances and nuclear
landscape boundaries are analyzed.

II. THE THEORETICAL FRAMEWORK

Firstly, the global nuclear masses at ground states are
calculated by the Skyrme HFB approach with the parallel
scheme. The HFB calculations are performed with the
HFBTHOv3.00 solver [33], in which wavefunctions are
calculated by the Skyrme HFB approach with the parallel
method after even-even nuclei are calculated with the
Skyrme Hartree-Fock-Bogoliubov (HFB) framework [33]. In particular,
the basis expansion of 22 harmonic oscilla-
tors is presented by the basis expansion of 22 harmonic oscilla-
tors. The default oscillator length $b_0 = \sqrt{\hbar/m\omega_0}$,
where $\hbar\omega_0 = 1.2 \times 41/A^{1/3}$. For each nucleus, the ground
state is determined by computing several quadrupole de-
formations from $\beta_2=-0.5$ to $0.5$, in case shape coexis-
tence present.

In HFB calculations, seven Skyrme type effective forces
have been adopted. SkM* force has good surface prop-
erties and has been widely applied in descriptions of fission [37]. SLy4 force has been widely used in descriptions
of neutron-rich nuclei and neutron stars [38]. SLy4 force
is a refitted force that improves global descriptions of
binding energies compared to the original SLy4 [39]. UN-
EDF0 has been well optimized for descriptions of global
binding energies with a high precision [39]. In addition,
we speculate that a single density dependent term in
standard Skyrme forces is not sufficient for the Skyrme
force to simulate many-body correlations. The extended
SLy4Eglobal [39], SkM*ext1 and UNEDF0ext1 forces [29]
with an additional high-order density-dependent term are
also adopted. In the particle-particle channel, a density-
dependent pairing interaction has been adopted [29, [30],

$$V_{pair}(r) = V_0 \left\{ 1 - \eta \left( \frac{\rho(r)}{\rho_0} \right)^\gamma \right\}, \quad (1)$$

where $\rho_0$ is the nuclear saturation density and we adopt
the constants as $\eta = 0.8$ and $\gamma = 0.7$. The pairing
strengths $V_0$ are fitted to the neutron gap of $^{120}$Sn of
1.245 MeV for different Skyrme forces. The pairing gaps
could be very different towards drip lines by using differ-
ent pairing interaction forms. The resulted pairing gaps
at the neutron drip lines are between the surface pairing
and the mixed pairing [29]. This is a reasonable choice
because the pairing gaps obtained with the surface pairing
interaction are too large toward the neutron drip lines
if the pairing strength is invariant for stable and weakly
bound nuclei. The global binding energies of odd-A and
odd-odd nuclei are obtained by the average pairing gap
method after even-even nuclei are calculated with the
HFB approach [8, [10, [11].

Secondly, we compute neutron capture rates with the
TALYS code [34] and the calculated nuclear masses. The
neutron capture rate is sensitive to the neutron separation
energy [18]. Calculated masses are used in TALYS
when no experimental masses are available. The reaction
rates are calculated at 24 temperatures ranging from $T_9$
= 0.1 to 10 GK. The reaction rates $\lambda$ are converted to
coefficients $a_0 \sim a_6$ in REACLIB format [35],

$$\lambda = \exp(a_0+a_1 T^{-1}_9+a_2 T^{-3/2}_9+a_3 T^{-1}_9+a_4 T_9+a_5 T^{3/2}_9+a_6 \ln T_9), \quad (2)$$

where $a_0 \sim a_6$ are obtained by the least square fitting
method and next we updates the REACLIB data. The
inverse $(\gamma, n)$ reaction rates are calculated with the
detailed balance [36]. In this work, we replaced 3825 $(n, \gamma)$
reaction rates for targets with $10 \leq Z \leq 83$ and 2453 $(n, \gamma)$
reaction rates for targets with $84 \leq Z \leq 112$ in REACLIB.
It was reported that r-process abundances are less
sensitive to uncertainties of $\beta$-decay rates compared to
neutron capture rates [29]. The present r-process nucle-
osynthesis calculation includes 7836 nuclear species and
95051 reactions rates. In SkyNet, the nuclear statistical
equilibrium (NSE) is adopted for all strong reactions
when $T_9 \geq 7.0$ GK [30]. The NSE is calculated with a
given temperature, density and $Y_e$ in SkyNet. This is
different from WinNet and XNet in which inverse rates
taken from REACLIB are not completely consistent with
NSE [30].

Finally, the abundance evolution is calculated with
SkyNet, which actually solves the reaction network equa-
tions, i.e., the coupled first-order non-linear ordinary dif-
fential equations, with a given set of rates [36]. The
initial NSE abundances are obtained with given temper-
ature $T$, entropy $S$ and $Y_e$. The initial density $\rho$ is
related to entropy that is proportional to $T^3/\rho$. After the
numerical convergence is obtained at the evolution time
of $10^5$ s ($T \approx 3 \times 10^5$ K, $Y_e \approx 0.4$), the final abundance
are obtained by the sum over all reaction species. In this
work, for the ejecta of NSM, the initial temperature is
taken as 7.1 GK; $Y_e$ is taken as 0.03 (within ranges sug-
gested in [13]); and initial density is taken as $2.2 \times 10^{11}$
g cm$^{-3}$ ($S=2.8$ $k_B$/baryon). For the ejecta of CCSN,
the initial temperature is taken as 10 GK; $Y_e$ is taken as
0.2 according to [16, 42]; and initial density is taken as
$2.0 \times 10^{8}$ g cm$^{-3}$ ($S=10$ $k_B$/baryon). The density expa-
sion timescales of the ejecta are taken as 1 ms and 20
ms for NSM and CCSN respectively. The combination of very low $\gamma_c$ and rapid expansion timescale guarantees the occurrence of a strong $r$-process \cite{11}. It is difficult to reproduce the solar $r$-process abundances by only one $r$-process scenario. SkyNet is a flexible modular library and has been successfully used for nucleosynthesis calculations in all astrophysical scenarios \cite{36}. For example, very recently, Jin et al. have investigated that the enhanced triple-$\alpha$ reaction reduces proton-rich nucleosynthesis in supernovae using SkyNet \cite{43}.

### III. RESULTS AND DISCUSSIONS

![FIG. 1. Calculated $S_{2n}$ of $^{39}$Na with seven Skyrme forces and the corresponding total number of bound nuclei from $Z=8$ to 120. The shadows show the confidential interval at 95%.](image)

The recent experiment on $^{39}$Na has attracted great interests for theorists \cite{32,45}. $^{39}$Na has a magic neutron number of $N=28$ but has a wide proton deformation and a deformed halo structure \cite{32}. The observation of $^{39}$Na provides a good opportunity for examination of various nuclear mass models. In Fig.1, the two-neutron separation energies $S_{2n}$ of $^{39}$Na are calculated with seven Skyrme-type forces. One can see SkM$, SkM^{*\text{ext1}}$, UNEDF0 and UNEDF0$^{\text{ext1}}$ forces could reproduce the existence of $^{39}$Na, while three SLy4-class forces obtain negative $S_{2n}$. SkM$^*$ gives the largest $S_{2n}$ of $^{39}$Na and predicts that $^{41}$Na is the drip line nucleus. Correspondingly, we performed global calculations of nuclear binding energies from $Z=8$ to $Z=120$ with seven Skyrme forces. The total number of bound nuclei of the nuclear landscape from $Z=8$ to $Z=120$ ranges from 7105 to 8761 with different Skyrme forces. Generally, we see that the Skyrme force obtains a large $S_{2n}$ of $^{39}$Na also predicts a large number of bound nuclei. The $S_{2n}$ of $^{39}$Na is strongly correlated with the total number of bound nuclei $N_b$ with a correlation $r=0.947$. The linear regression gives $N_b \sim N(b + aS_{2n}, \sigma^2)$, in which $a=638.5$, $b=7789.7$, and $\sigma=199.9$.

Once we know the experimental $S_{2n}$ of $^{39}$Na, we can immediately get a stringent prediction of the total number of bound nuclei of the nuclear landscape according to this linear regression.

Fig.2 displays the calculated nuclear landscape boundaries with seven Skyrme forces. Large uncertainties in nuclear landscape boundaries are shown in neutron drip lines. Furthermore, it can be clearly seen that uncertainties of boundaries in light and medium mass region are small but propagate to remarkable uncertainties in boundaries of heavy and superheavy mass region. The consistency between the $S_{2n}$ of $^{39}$Na and landscape boundaries is shown. SkM$^*$ results in the furthest extension of neutron drip line, while SLy4 results in the nearest boundaries. UNEDF0 results are close to that of SkM$^*$. SkM$^{*\text{ext1}}$ boundaries are between SLy4 and SkM$^*$, UNEDF0 results. The recent Bayesian mixing of eleven mass models infers that the total number of bound nuclei is $7708\pm534$ \cite{11}. This Bayesian-mixing inference is very close to the SkM$^{*\text{ext1}}$ prediction of 7671 as constrained by newly observed $^{39}$Na. Present calculations employ the HO basis while coordinate space calculations should be more accurate but are too costly. For example, with SkM$^{*\text{ext1}}$, $S_{2n}$ of $^{39}$Na by calculations in HO basis \cite{33} and in coordinate space \cite{10} are 0.23 MeV and 0.27 MeV, respectively.

It should be noted that SkM$^*$ systematically overestimates binding energies of neutron-rich nuclei \cite{8,28}. Thus SkM$^*$ is expected to overestimate the extension of neutron drip line and its prediction can be seen as an upper limit of nuclear landscape boundaries. In the literature, similar conclusions can be obtained that SkM$^*$ gives the largest number of bound nuclei while SLy4 gives the smallest number of bound nuclei $^{39}$Na. The symmetry energy $a_{\text{sym}}$ at the saturation density $\rho_0$ may play a role. However, the extended SkM$^{*\text{ext1}}$ has a close $a_{\text{sym}}$ to that of SkM$^*$. It has been pointed out that the symmetry energy at $\frac{3}{2}\rho_0$ (0.11 fm$^{-3}$) is strongly correlated with the neutron drip line location \cite{10}. Indeed, the symmetry energies at subsaturation (0.11 fm$^{-3}$) are 26.90, 26.54, 26.49, 25.69, 24.70, 24.37, 24.31 MeV for SLy4, SLy4global, SLy4, SkM$^{*\text{ext1}}$, UNEDF0, UNEDF0$^{\text{ext1}}$, SkM$^*$, respectively. These are strongly correlated with the total number of bound nuclei $N_b$, with a correlation $r=-0.989$. This exactly verified that the total number of bound nuclei is correlated with symmetry energy at subsaturation. We pointed out that SkM$^{*\text{ext1}}$ is a very reasonable force to describe the drip line nuclei around $^{39}$Na and the nuclear landscape boundaries.

The associated $r$-process paths vary with different models, which is defined as $S_{2n} \approx 2.0$ MeV \cite{8,10}. The kink patterns of $r$-process paths and boundary lines appear around neutron magic shells. Generally, the boundary lines have strong odd-even effects. For each isotope, the number of bound nuclei $N_{\text{drip}}$ can be determined as a function of charge number $Z$. In Fig.2 for different Skyrme forces, the uncertainties in $N_{\text{drip}}(Z)$ are particularly large just after the neutron magic number while
become much reduced towards the next neutron magic number. This feature is expected to impact the $r$-process uncertainties.

For detailed analysis of $r$-process evolutions, the abundances during freeze-out are also displayed in Fig. 4. The abundances at 1.2 s of NSM and abundances at 0.72 s of CCSN are shown. In NSM abundance, the significant uncertainties around $A\sim182$ present in the early phase, indicating that the dominate cause is from neutron capture rates close to neutron drip lines. It can be seen that the position of third peak in NSM is reproduced at 1.2 s but shifted slightly to heavier masses in Fig. 3. Indeed, it has been pointed out that the late neutron captures have a direct effect on the final position of the third peak, with neutrons released from fission of heavier nuclei. In NSM, the first peak is not yet produced at freeze-out and late fission fragments are essential to reproduce the first peak around $A\sim130$. Note that both $N=82$ neutron shell and $Z=50$ proton shell play a role in the first peak. The
Abundance

\( r \) neutron drip lines. This demonstrated that SLy4 with positive correlations between the denoted the variance. In the NSM case, we found strong where \( k \) obtains at 1.2 s and 0.72 s, respectively. freeze-out. For NSM (a) and CCSN (b), the abundances are much irregular and have strong odd-even effects in contrast to final abundances. The \( \beta \) decays and \( \beta \)-delayed decays in late phases would smooth out the abundances.

Finally, the statistical analysis is performed to look into the correlations between neutron drip lines and \( r \)-process abundances. The covariance correlation matrix is shown in Fig. 5. In the correlation analysis, the logarithm of abundances \( \log(Y(A)) \) in terms of nuclear mass \( A \) is adopted. For the other side, the relative value \( N^R(Z) = N_b(Z)/Z \) is used, where \( N_b(Z) \) is the number of bound isotopes for each charge number \( Z \). The relative uncertainties emphasize the correlations between drip-line light nuclei and \( r \)-process since drip-line heavy nuclei are not likely accessible. The correlation matrix is calculated as,

\[
\text{Corr}[\log(Y(i), N^R(j)) = \frac{1}{8} \sum_{k=1}^{7} [\log(Y(i,k) - \log(Y(i))) \cdot [N^R(j,k) - N^R(j)]}{\sqrt{\sigma[\log(Y(i))]^2 \sigma[N^R(j)]^2}}
\]

where \( k \) denotes the results of seven Skyrme forces and \( \sigma^2 \) denotes the variance. In the NSM case, we found strong positive correlations between the \( A \sim 180 \) abundance and neutron drip lines. This demonstrated that SLy4 with least extended nuclear boundaries would result in the underestimated \( r \)-process abundance around \( A \sim 180 \). This correlation is not an accident. The correlation matrix points out that boundaries of some isotopes are especially important. For example, the drip lines at \( Z = 11 \) are important, and the next is \( Z = 18 \). The analysis of evolution movies (see Supplemental Material) shows distinct features between SkM* and SLy4 in the early phase. The \( r \)-process with SkM* runs very quickly to heavy masses and considerable abundances are already accumulated just at the left side of the neutron magic number. It is understandable that SkM* with most extended boundaries has large early neutron capture rates. In contrast, SLy4 obtains much less abundances before the third peak due to much less early abundances just before \( N = 126 \). The in-between SkM* \( \text{ext1} \) obtains reasonable abundance in the NSM scenario. In all cases, it is surprising to see that there is no correlation between \( r \)-process abundance and neutron drip lines around proton shells at \( Z = 50 \) and 82. The early abundances of NSM has similar but smaller correlations in Fig. 5(b) due to larger variances, compared to that of final NSM abundance in Fig. 5(a). Fig. 5(c, d) shows that CCSN cases have no significant correlations between neutron drip lines and abundances around \( A \sim 180 \) in the less neutron-rich environment. There are some negative correlations in the transitional region around \( A = 150 \)–160. For some regions, such as the peaks around 130 and 195, there is no strong statistical correlations, since shell effects are dominated. It is encouraging that the statistical analysis can provide reasonable clues. In fact, \( r \)-process evolution

FIG. 4. Similar to Fig. 3 but for \( r \)-process abundance before freeze-out. For NSM (a) and CCSN (b), the abundances are obtained at 1.2 s and 0.72 s, respectively.

FIG. 5. The calculated correlation matrix between the \( r \)-process abundance and the number of bound isotopes. The results for NSM final abundance (a), NSM freeze-out abundance (b), CCSN final abundance (c), CCSN freeze-out abundance (d) are shown. In the correlation matrix, the logarithm of abundances \( \log(Y(A)) \) and the relative value of \( N_b(Z)/Z \) are used, where \( N_b(Z) \) is the number of bound isotopes for each \( Z \).
is so complex that a big data net analysis is inspiring from a different perspective [48].

IV. SUMMARY

In summary, we studied $S_{2n}$ of $^{39}$Na with seven Skyrme forces to constrain the neutron drip lines. We found strong linear correlation between $S_{2n}$ of $^{39}$Na and the total number of bound nuclei. The in-between SkM$^*$,ext1 predicts 7671 bound nuclei of the nuclear landscape, which is very close to the recent Bayesian mixing result. Our key motivation is to study the uncertainty propagation from neutron drip lines of light nuclei to heavy nuclei, which is crucial for $r$-process simulations but not accessible by terrestrial experiments. Based on obtained nuclear masses with different Skyrme forces, $r$-process abundances from ejecta of NSM and CCSN are calculated using the reaction rate code TALYS and reaction network code SkyNet. We see large uncertainties in NSM abundances before the third peak. Further covariance analysis indicate that the abundance uncertainties are strongly correlated with the extension of neutron drip lines. SLy4 predicts the least extended nuclear boundaries and results in the valley in abundances before the third peak. The statistical analysis shows that neutron drip lines of some isotopes are especially important to constrain $r$-process in neutron-rich environments. Our study highlights the further experimental study of $S_{2n}$ of $^{39}$Na would be very needed. In contrast, the $r$-process in CCSN is not sensitive to the neutron drip lines. Currently, the understandings of $r$-process still need comprehensive and accurate nuclear inputs, in particular, reliable fission predictions. The statistical analysis can provide reasonable clues and big data analysis is a promising perspective. It is reciprocal to develop highly accurate effective nuclear forces for consistent modelings of Equation of State, drip line nuclei, and nuclear reactions, for better exportations of nuclear astrophysics at extreme conditions.

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