YITP Workshop
"Fundamentals in density functional theory (DFT2022)"
December 7–20, 2022, Kyoto U., Japan

Quantum computing for nuclear structure properties?

Haozhao LIANG（梁豪兆）

Department of Physics, The University of Tokyo, Japan

December 19, 2022

東京大学
THE UNIVERSITY OF TOKYO

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Quantum computing (or machine learning) for nuclear structure properties?

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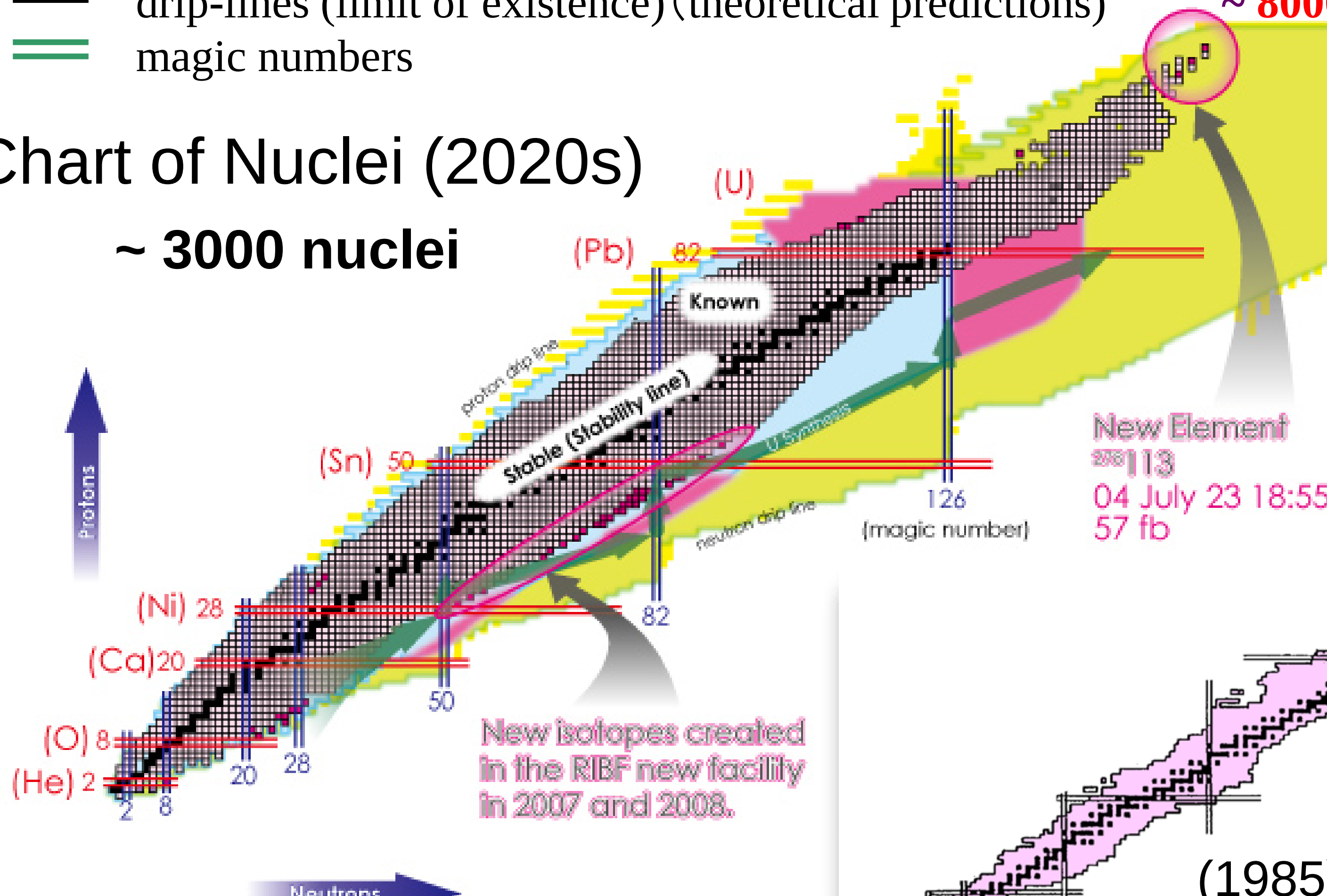
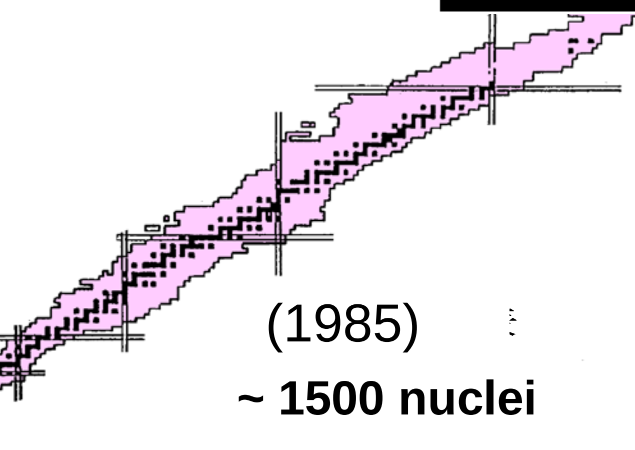
Nuclear chart

■	stable nuclei	~ **300 nuclei**
□	unstable nuclei observed so far	~ **3000 nuclei**
—	drip-lines (limit of existence) (theoretical predictions)	~ **8000 nuclei**
=	magic numbers	

Chart of Nuclei (2020s)

~ 3000 nuclei





(1985)

~ 1500 nuclei

https://www.nishina.riken.jp/

Nuclear chart

■	stable nuclei	~ 300 nuclei
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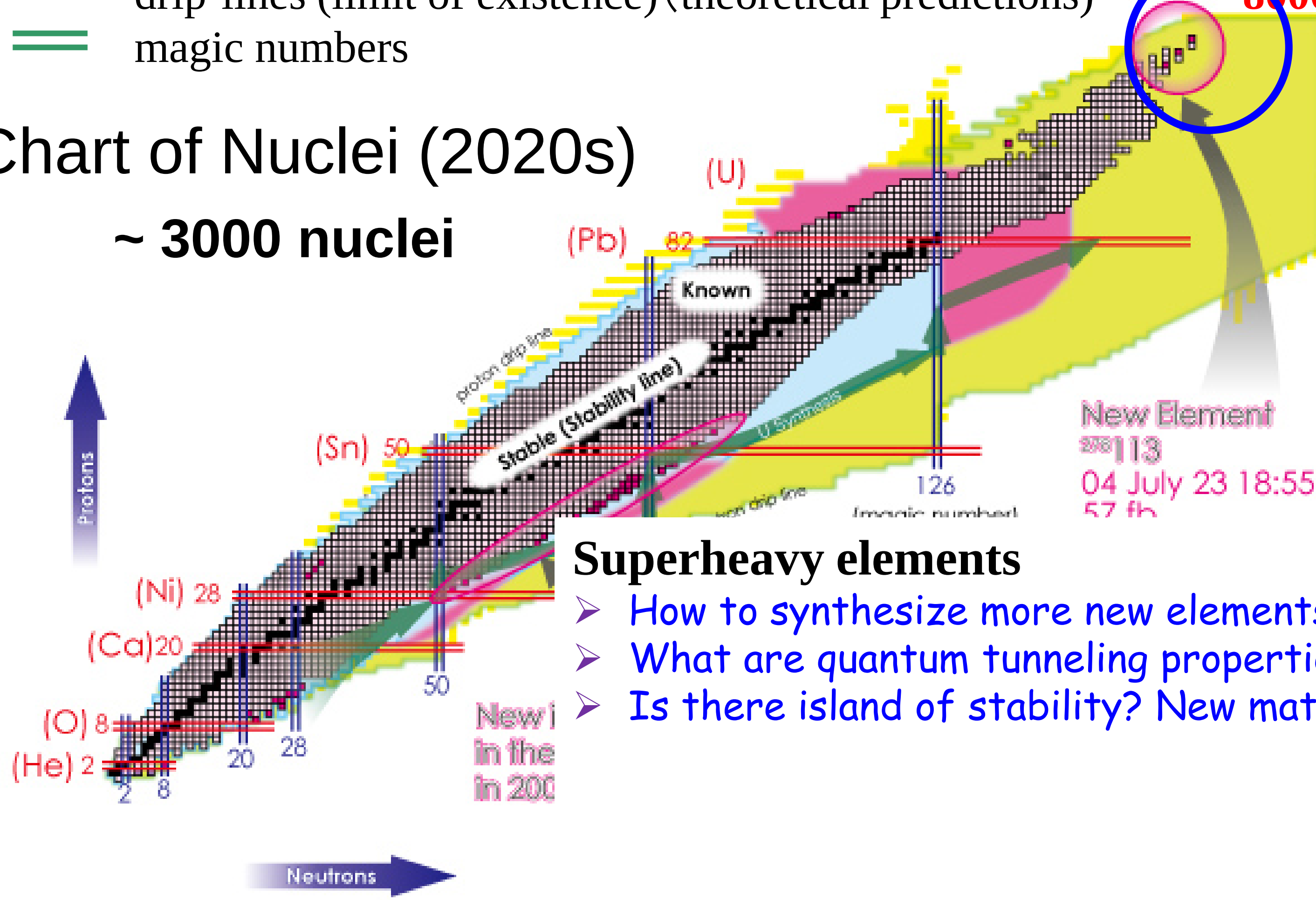
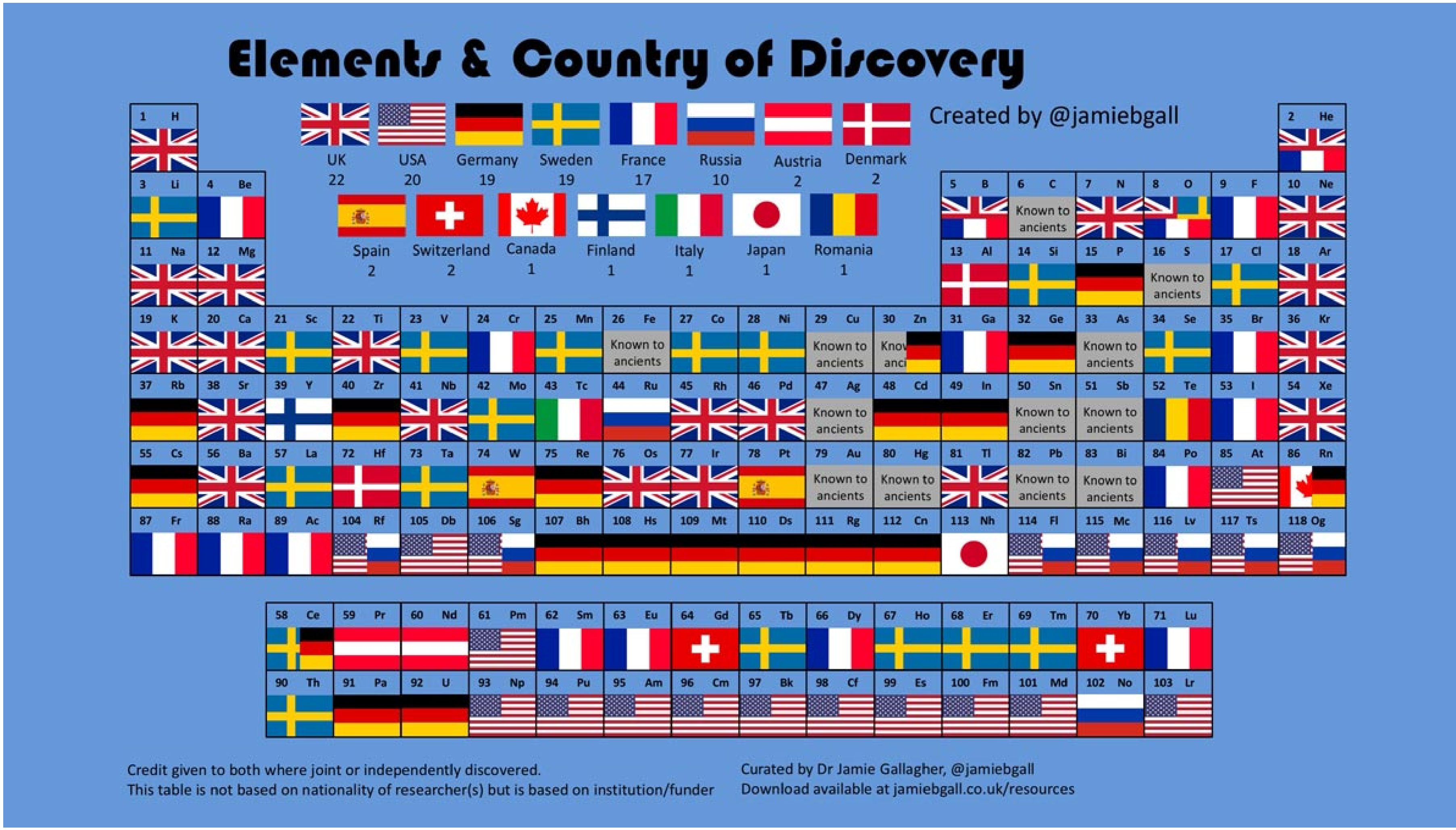


Superheavy elements

- *How to synthesize more new elements?*
- *What are quantum tunneling properties of SHE?*
- *Is there island of stability? New materials?*

https://www.nishina.riken.jp/

Periodic Table with National flags



Open question:

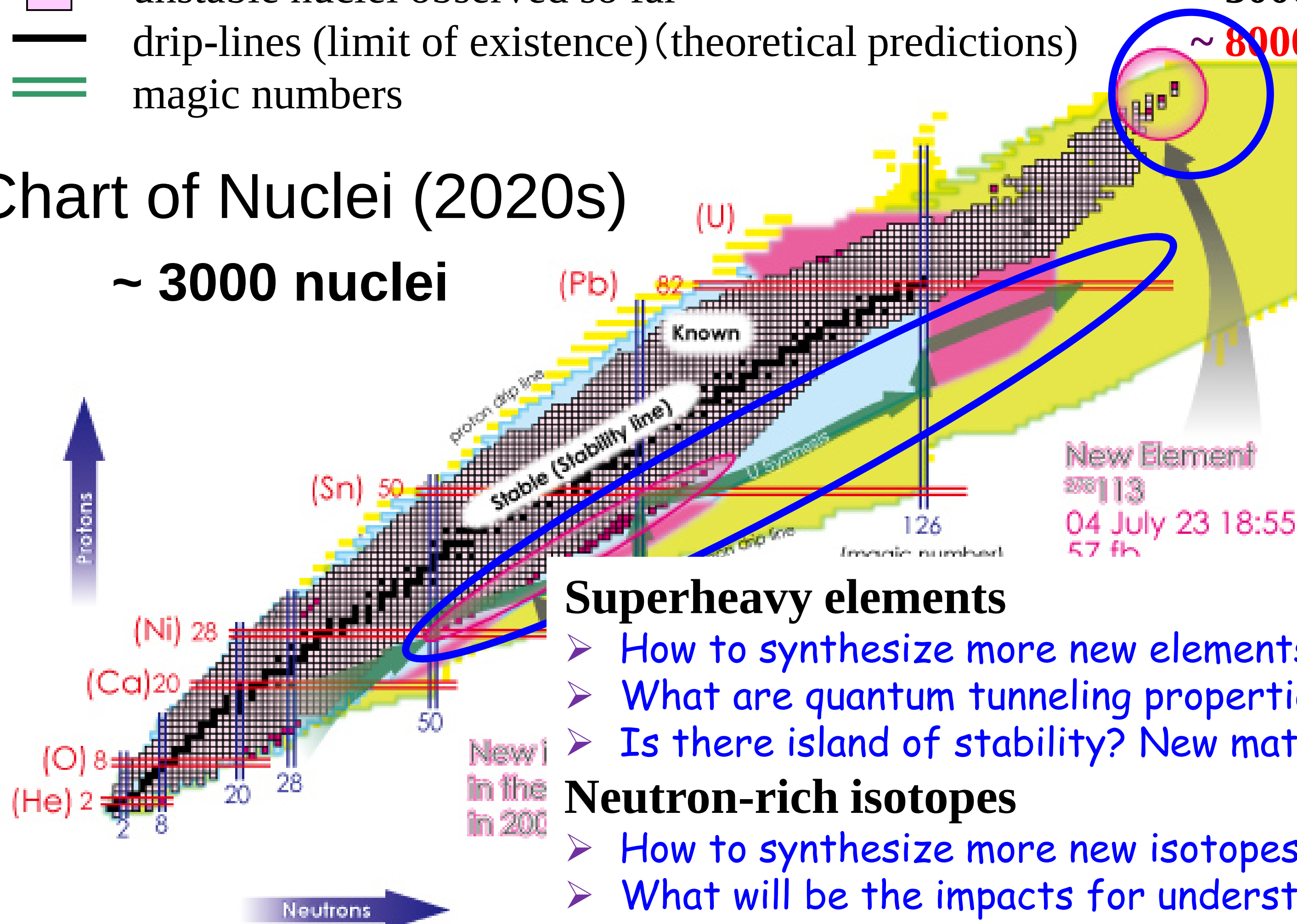
- Is there or where is **the end** of the periodic table?

Nuclear chart

■	stable nuclei	**~ 300 nuclei**
□	unstable nuclei observed so far	**~ 3000 nuclei**
—	drip-lines (limit of existence)（theoretical predictions)	**~ 8000 nuclei**
=	magic numbers	

Chart of Nuclei (2020s)

~ 3000 nuclei



https://www.nishina.riken.jp/

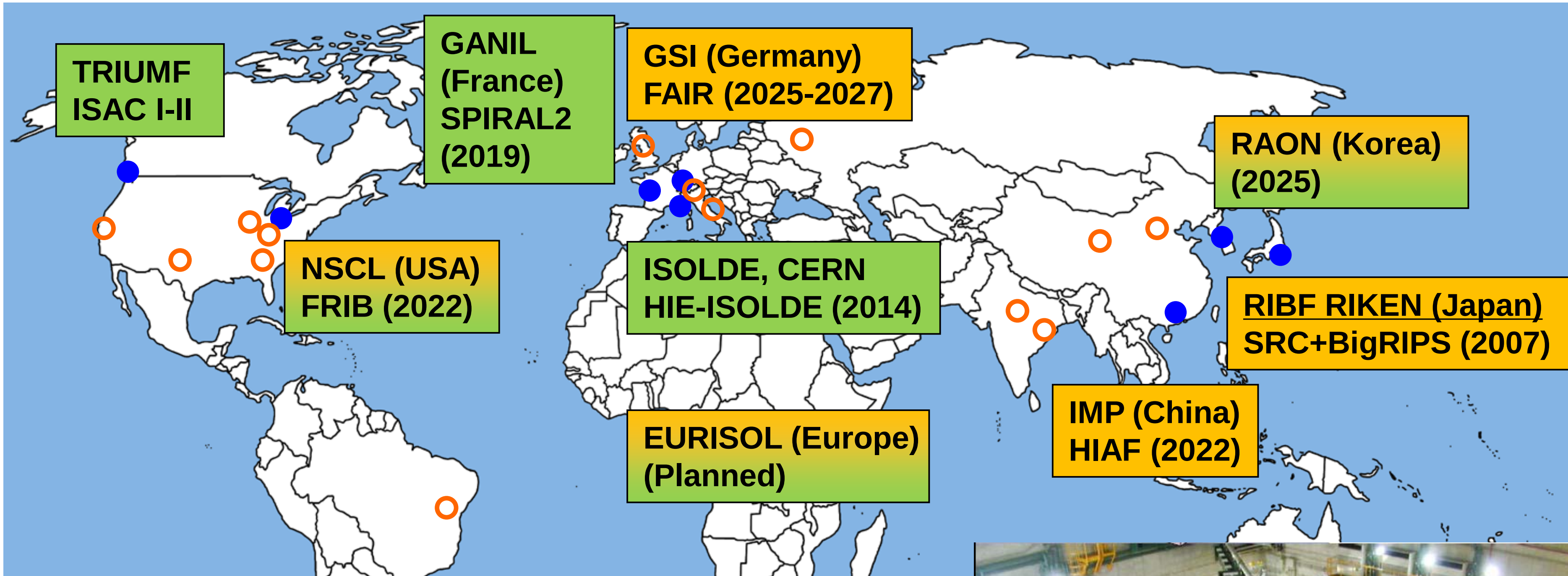
Superheavy elements

- How to synthesize more new elements?
- What are quantum tunneling properties of SHE?
- Is there island of stability? New materials?

Neutron-rich isotopes

- How to synthesize more new isotopes?
- What will be the impacts for understanding origins of heavy elements?
- What will be the impacts for handling nuclear wastes?

Radioactive isotope beam facilities



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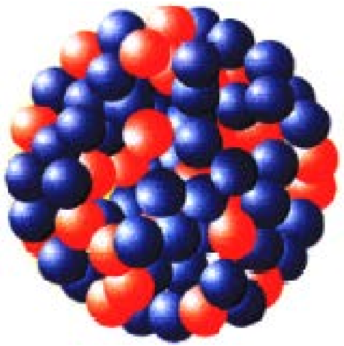
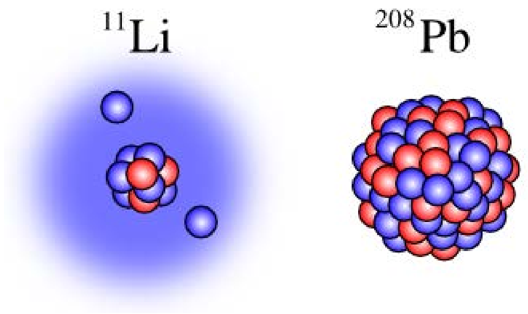
Atomic nuclei

Atomic nucleus is a rich system in physics

- quantum system
- many-body system (A ~ 100, spin & isospin d.o.f.)
- finite system (surface, skin, halo, …)
- open system (resonance, continuum, decay, …)



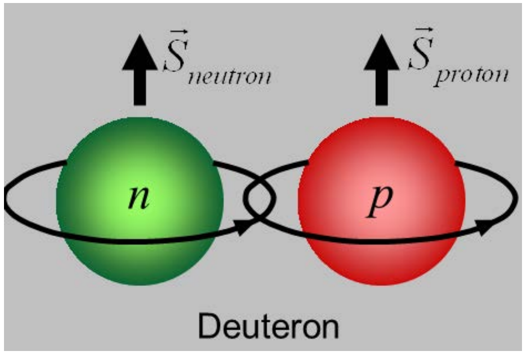
Neutron halos



***R* ~ *A*$^{1/3}$? Not always!**
^{11}Li: a size as ^{208}Pb

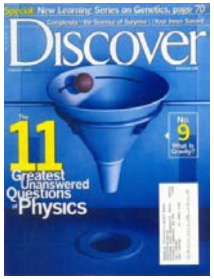
Tanihata:1985

Spin and **Isospin** are essential degrees of freedom in nuclear physics.

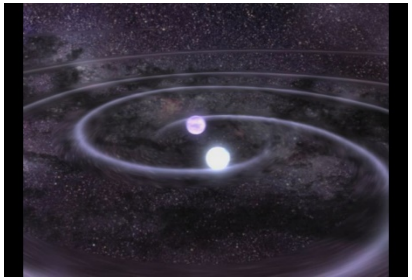


r-process nucleosynthesis and nuclear inputs

The 11 greatest unanswered questions of physics



Question 3
How were the heavy elements from iron to uranium made?



★ Nuclear data inputs for r-process

Quantity		Effects
S_n	neutron separation energy	path
$T_{1/2}$	β-decay half-lives	abundance pattern, time scale
P_n	β-delayed n-emission branchings	final abundance pattern
Y_i	fission (products and branchings)	endpoint, degree of fission cycling
		abundance pattern (?)
G	partition functions	path (very weakly)
$N_A \langle \sigma \nu \rangle$	neutron capture rates	conditions for waiting point approximation
		final abundance pattern during freezeout (?)

Nuclear inputs for r-process

Key exp. @ RIKEN

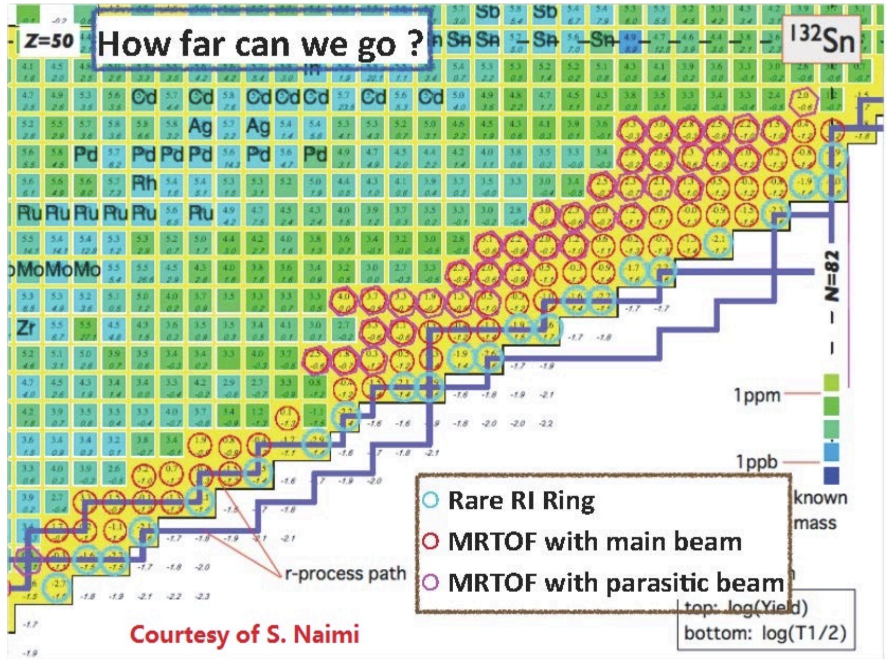
masses

***β*-decay half-lives**

***β*-delayed *n*-emissions**

(*n*, *γ*) cross-sections

……



- To provide and organize **all these inputs** in a systematic and consistent way
  - e.g., changes in mass ➔ changes in half-lives, capture rates …

    (not hybrid databases !)
  - more exp. data ➔ more reliable extrapolation / smaller uncertainties

    (higher accuracy ?)

Machine learning

Machine Learning for physics?

- We learn what we need ……
- We learn what we have less control ……
- We learn what we are guaranteed ……
  e.g., Imoto's talk & works by Nagai, Akashi, Sugino, et al.

NATURE REVIEWS | PHYSICS VOLUME 4 | JUNE 2022 | 357

Machine learning and density functional theory

Ryan Pederson[1], Bhupalee Kalita[2] and Kieron Burke[1,2]

Over the past decade machine learning has made significant advances in approximating density functionals, but whether this signals the end of human-designed functionals remains to be seen. Ryan Pederson, Bhupalee Kalita and Kieron Burke discuss the rise of machine learning for functional design.

Machine learning

Machine Learning for physics?

- We learn what we need ……
- We learn what we have less control ……
- We learn what we are guaranteed ……

  e.g., Imoto's talk & works by Nagai, Akashi, Sugino, et al.

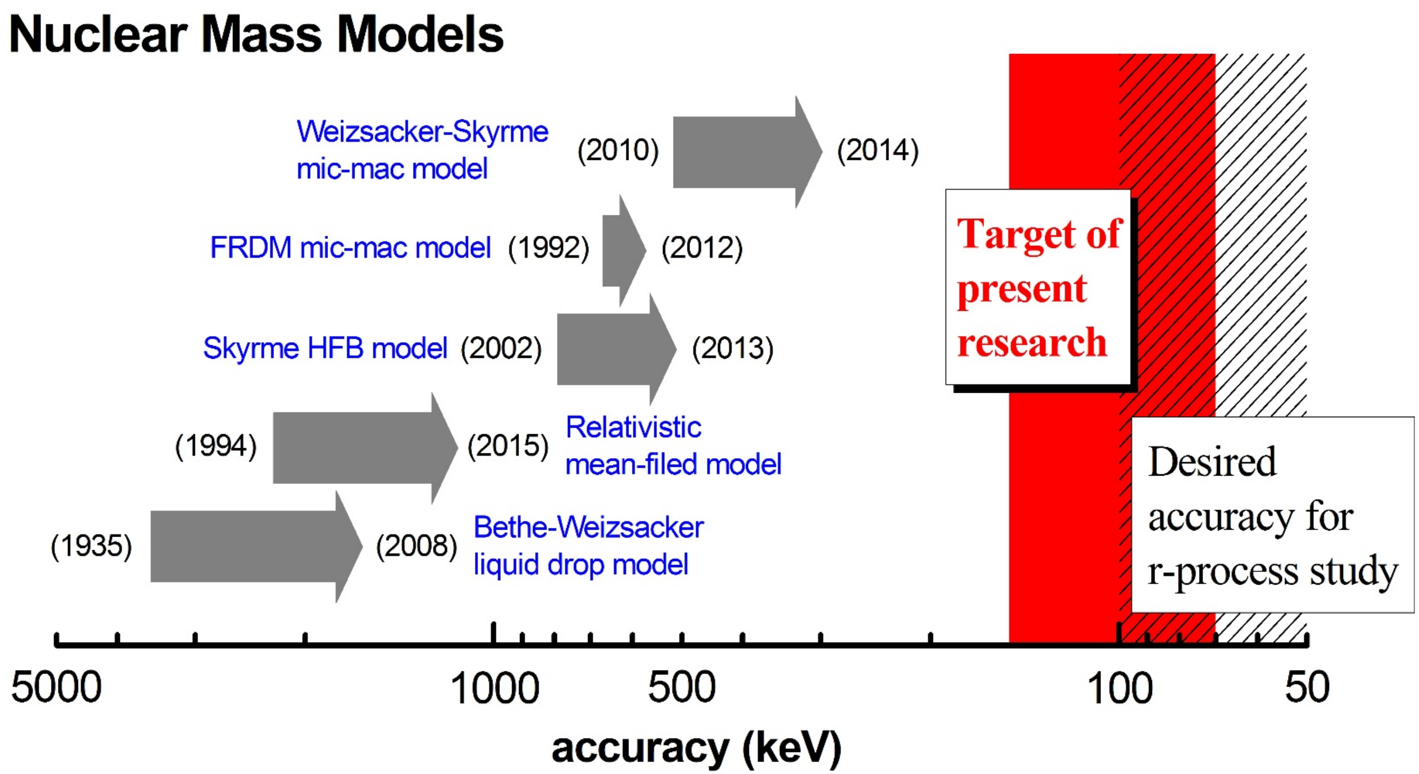
Or

We build physics (space and time) in neural networks …

e.g., Koji Hashimoto's talk

Nuclear mass models

- Theoretically, the development of nuclear mass model can be traced back to the early age of nuclear physics, known as Bethe-Weizsacker liquid drop model in 1935.
- To take into account the nuclear shell effects: the microscopic models and the microscopic-macroscopic (mic-mac) models.

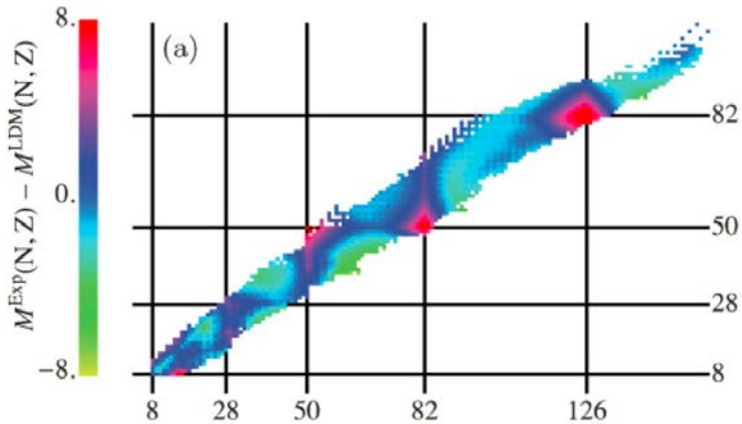


Theories + Bayesian approaches

Strutinsky's energy theorem:
The nuclear binding energy may be separated into two main components: one large and smooth and another one small and fluctuating.

$$M(Z,N) \equiv M_{\rm LDM}(Z,N) + \delta_{\rm LDM}(Z,N)$$

Strutinsky, *NPA* **95**, 420 (1967)



LDM: $\sigma_{\rm RMS}$ ~ 3.6 MeV

cf. Morales *et al.*, *PRC* **81**, 024304 (2010)

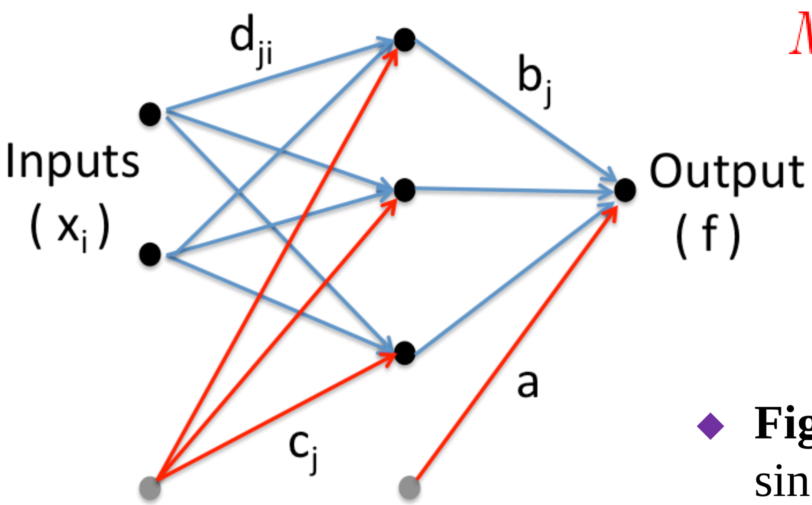
PHYSICAL REVIEW C **93**, 014311 (2016)

Nuclear mass predictions for the crustal composition of neutron stars: A Bayesian neural network approach

R. Utama,* J. Piekarewicz,† and H. B. Prosper‡

Key ideas

- "To account for the small and fluctuating contribution, we ***train* a suitable neural network** on the mass residuals between the LDM predictions and experiment, as given in the latest Atomic Mass Evaluation (AME2012)."
- "Once trained, we used the resulting **universal approximator $\boldsymbol{\delta_{\mathrm{LDM}}(Z, N)}$** to validate the approach and later to make predictions in regions where experimental data are unavailable."



$$M(Z,N) \equiv M_{\mathrm{LDM}}(Z,N) + \delta_{\mathrm{LDM}}(Z,N)$$

Bayesian Neural Network

- **Figure 1**: A feed-forward neural network with a single hidden layer, two inputs ***Z*** and ***A***, and a single output $\boldsymbol{f = \delta_{\mathrm{LDM}}(Z, A)}$

Utama, Piekarewicz, and Prosper, *PRC* **93**, 014311 (2016)

Contents

- **Nuclear inputs with Bayesian approaches**
  - Nuclear Masses
  - Nuclear β-decay half-lives

Theories + Bayesian approaches

Nuclear mass predictions based on Bayesian neural network approach
with pairing and shell effects

Z.M. Niu (牛中明)[a,b], H.Z. Liang (梁豪兆)[b,c,d,*]

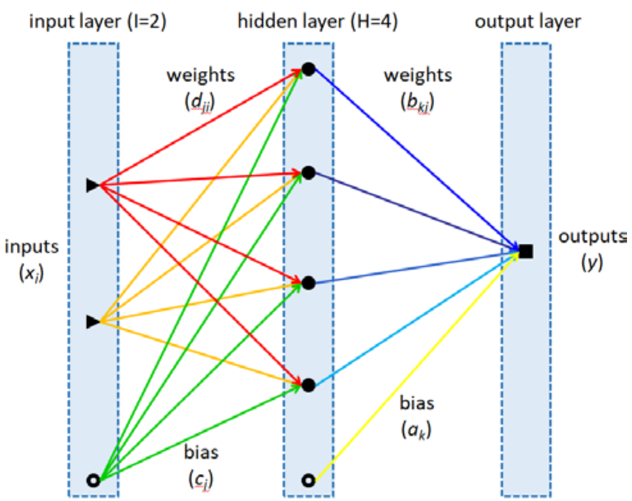
Physics Letters B 778 (2018) 48–53

- Posterior distributions of parameters are Neal1996Springer

$$p(\omega|D)=\frac{p(D|\omega)p(\omega)}{p(D)}\propto p(D|\omega)p(\omega),\quad D=\{(x_1,t_1),\ (x_2,t_2),\ \ldots,\ (x_N,t_N)\}$$

- likelihood function $p(D|\omega)$

$$p(x,t|\omega)=\exp(-\chi^2/2),\ \chi^2=\sum_{n=1}^{N}\left[\frac{t_n-y(x_n,\omega)}{\sigma_n}\right]^2$$



$$y(x,\omega)=a+\sum_{j=1}^{H}b_j\tanh\left(c_j+\sum_{i=1}^{I}d_{ji}x_i\right)$$

$$\tanh x=\frac{\sinh x}{\cosh x}=\frac{e^x-e^{-x}}{e^x-e^{-x}}$$

Numerical details

Likelihood function $p(D|\omega)$

$$p(D\,|\,\omega) = \exp(-\chi^2/2),\ \ \chi^2 = \sum_{n=1}^{N}\left[\frac{t_n - y_n(x,\omega)}{\sigma_n}\right]^2$$

$$t_n = M_n^{\rm exp} - M_n^{\rm th},\ y(x,\omega) = a + \sum_{j=1}^{H} b_j \tanh\left(c_j + \sum_{i=1}^{I} d_{ji} x_i\right) \Rightarrow M_n'^{\rm th} = M_n^{\rm th} + y(x,\omega)$$

- Inputs:
  - ✓ 2 inputs (I=2): Z, A
  - ✓ 4 inputs (I=4): Z, A, δ, P;

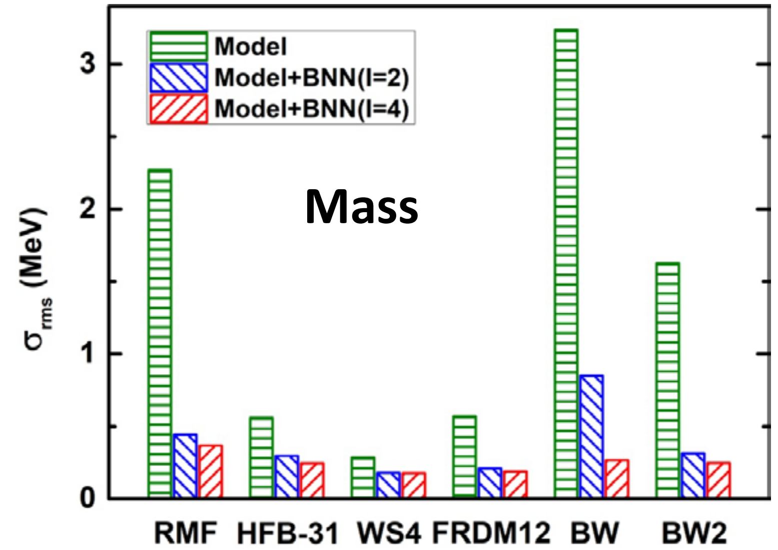
$\delta=[(-1)^Z+(-1)^N]/2$, $P=\nu_n\nu_p/(\nu_p+\nu_n)$

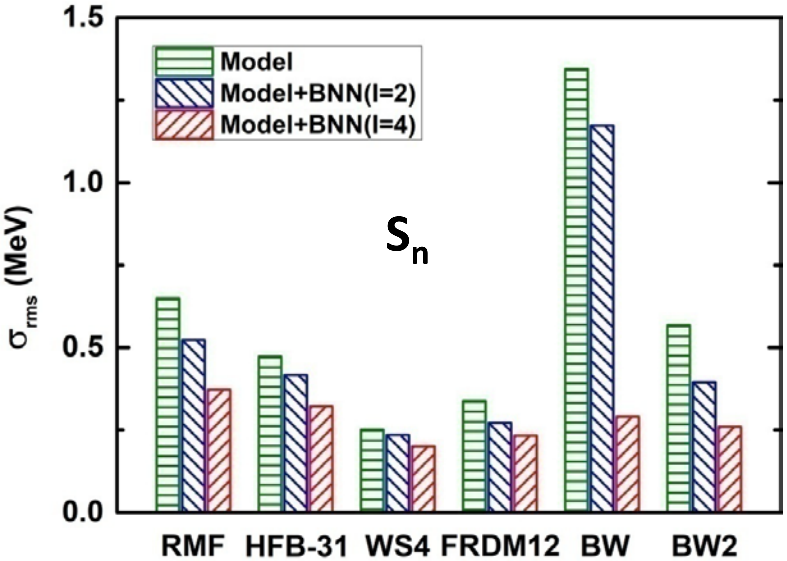
$\nu_p = \min(|Z - Z_0|),\ \ \nu_n = \min(|N - N_0|)$

cf. Utama, Piekarewicz, and Prosper, *PRC* **93**, 014311 (2016)

- Hidden units:
  - ✓ 2 inputs (I=2): H=42
  - ✓ 4 inputs (I=4): H=28
- Number of parameters: 169
- **Data:** Huang et al., CPC 41 030002; Wang et al., CPC 41 030003.
  - ✓ **Entire set**: 2272 nuclei in AME2016 (Z, N>=8 and $\sigma^{\rm exp}$<=100 keV)
  - ✓ **Learning set**: 1800 data randomly selected from entire set
  - ✓ **Validation set**: the remaining 472 data in entire set

Rms deviations of mass and S_n





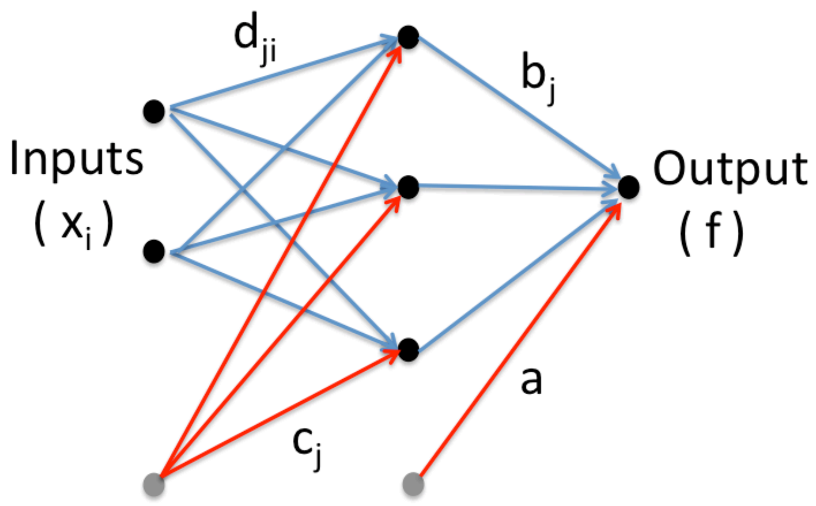
- The predictions of nuclear mass and neutron-separation energy are **significantly improved** with the BNN approach.
- After the improvement using the BNN approach with four inputs, the rms deviations are generally around **200 keV**.
- The BNN **with four inputs** is more powerful than the BNN with two inputs, especially for the neutron separation energy.

Niu and HZL, *PLB* **778**, 48-53 (2018)

Designs of BNN

In order to take into account as much physics as possible

- To design appropriate **output(s)**
- To design appropriate **inputs**
- To design appropriate **network structure**



In this work

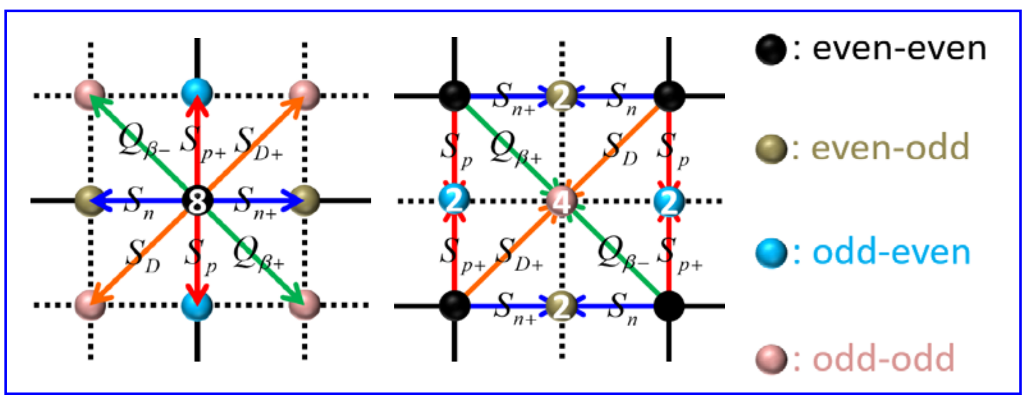
- **Outputs:** $\boldsymbol{E_{\text{mic}}, S_*, Q_*}$
- **Inputs:** $\boldsymbol{N, Z, E_{\text{mic}}}$**(model)**
- **Network: 9 different Bayesian networks**

Reference mass models

- Macroscopic mass model: BW2
- Macro-microscopic mass models: KTUY, FRDM12, and WS4
- Microscopic models: RMF and HFB-31
- High-precision global mass models: Bhagwat and DZ28

Even-odd effects and BNN designs

1. $S_n(Z,N) = M(Z,N-1) + m_n - M(Z,N) \quad \Rightarrow \quad M(Z,N-1) = M(Z,N) - m_n + S_n(Z,N)$
2. $S_{n+}(Z,N) = S_n(Z,N+1) = M(Z,N) + m_n - M(Z,N+1) \quad \Rightarrow \quad M(Z,N+1) = M(Z,N) + m_n - S_{n+}(Z,N)$
3. $S_p(Z,N) = M(Z-1,N) + m_p - M(Z,N) \quad \Rightarrow \quad M(Z-1,N) = M(Z,N) - m_p + S_p(Z,N)$
4. $S_{p+}(Z,N) = S_p(Z+1,N) = M(Z,N) + m_p - M(Z+1,N) \quad \Rightarrow \quad M(Z+1,N) = M(Z,N) + m_p - S_{p+}(Z,N)$
5. $S_D(Z,N) = M(Z-1,N-1) + m_D - M(Z,N) \quad \Rightarrow \quad M(Z-1,N-1) = M(Z,N) - m_D + S_D(Z,N)$
6. $S_{D+}(Z,N) = S_D(Z+1,N+1) = M(Z,N) + m_D - M(Z+1,N+1) \quad \Rightarrow \quad M(Z+1,N+1) = M(Z,N) + m_D - S_{D+}(Z,N)$
7. $Q_{\beta-}(Z,N) = M(Z,N) - M(Z+1,N-1) \quad \Rightarrow \quad M(Z+1,N-1) = M(Z,N) - Q_{\beta-}(Z,N)$
8. $Q_{\beta+}(Z,N) = M(Z,N) - M(Z-1,N+1) - 2m_e \quad \Rightarrow \quad M(Z-1,N+1) = M(Z,N) - Q_{\beta+}(Z,N) - 2m_e$



$$\bar{M}(Z,N) = M(Z,N)$$

$$\bar{M}(Z,N+1) = \sum_{i=1}^{2} M^i(Z,N+1)$$

$$\bar{M}(Z+1,N) = \sum_{i=1}^{2} M^i(Z+1,N)$$

$$\bar{M}(Z+1,N+1) = \sum_{i=1}^{4} M^i(Z+1,N+1)$$

Niu and HZL, *PRC* **106**, L021303 (2022)

A benchmark to FRDM12

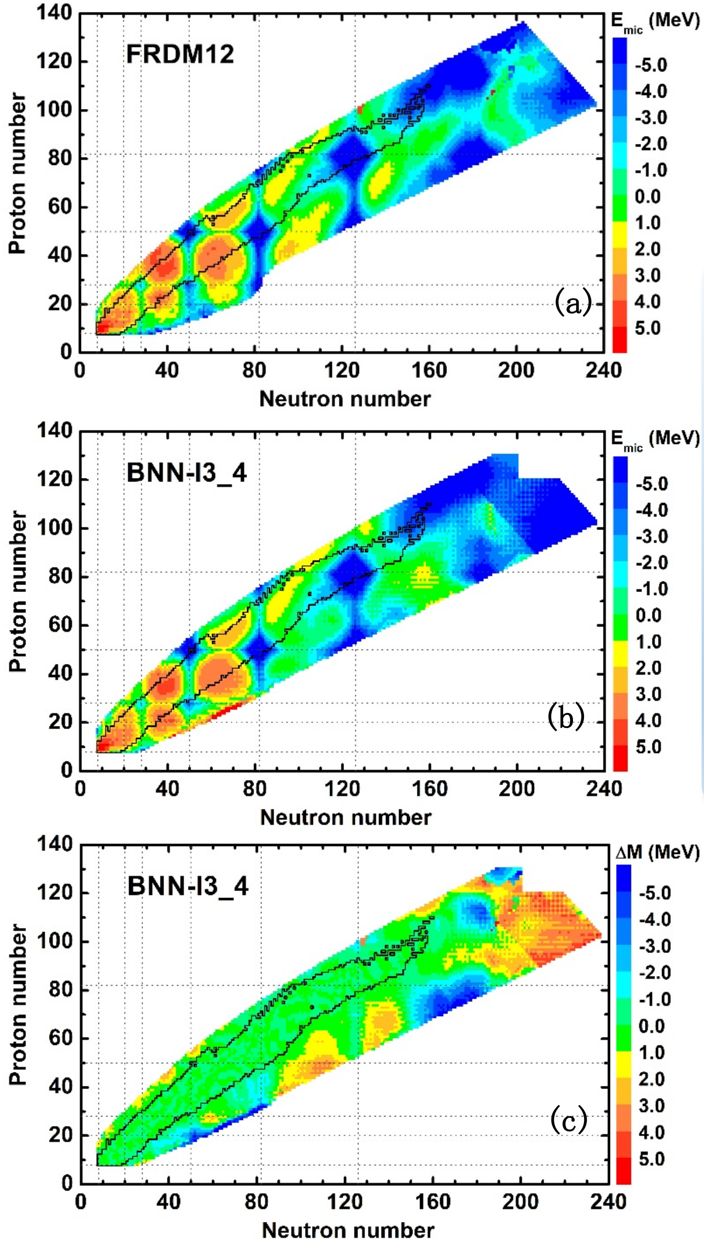


Fig: Panels (a) and (b) represent E_{mic} of FRDM12 and BNN predictions. Panel (c) represents ΔE_{mic} between E_{mic} of FRDM12 and those predicted by BNN approach.

- BNN_{FRDM12} predictions are **in excellent agreement** with the E_{mic} of FRDM12 for nuclei in and not very far from the training region, which also shows clear shell structure information.
- The deviations between BNN_{FRDM12} predictions and E_{mic} of FRDM12 are **relatively large** for very neutron-rich nuclei and super heavy nuclei.

Model	M	S_n	S_{2n}	S_p	S_{2p}	S_D	Q_β
BNNI3_4	0.093	0.092	0.125	0.097	0.130	0.113	0.109

Table: The rms of M, S_x, and Q_x between FRDM12 and BNN_{FRDM12} predictions for nuclei in T_{set} and other nuclei in FRDM12.

A benchmark to FRDM12

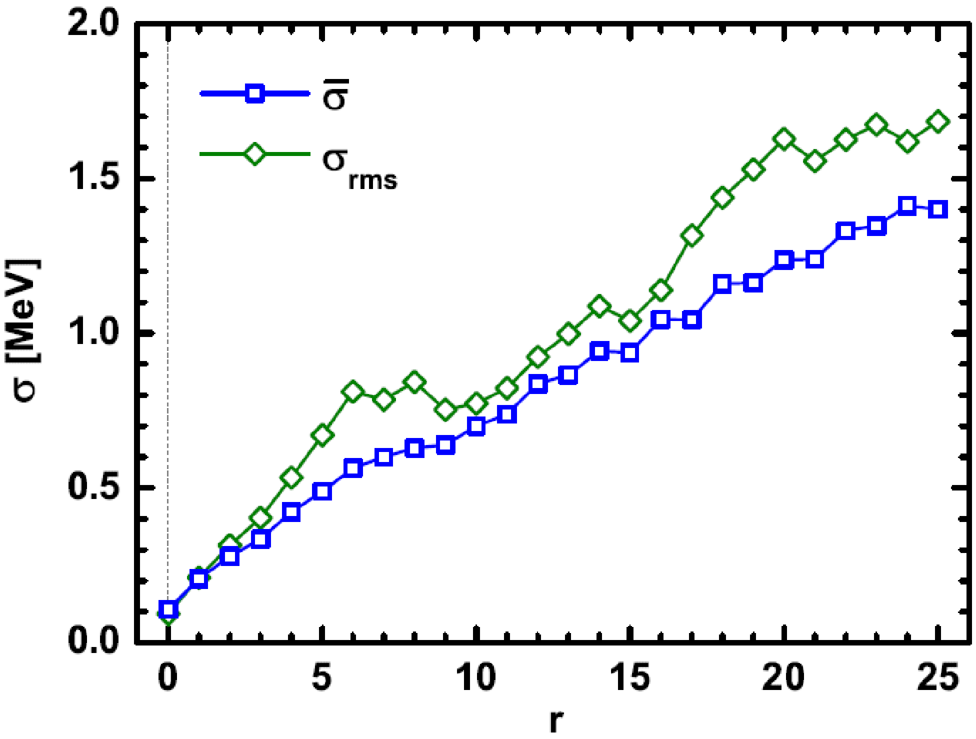
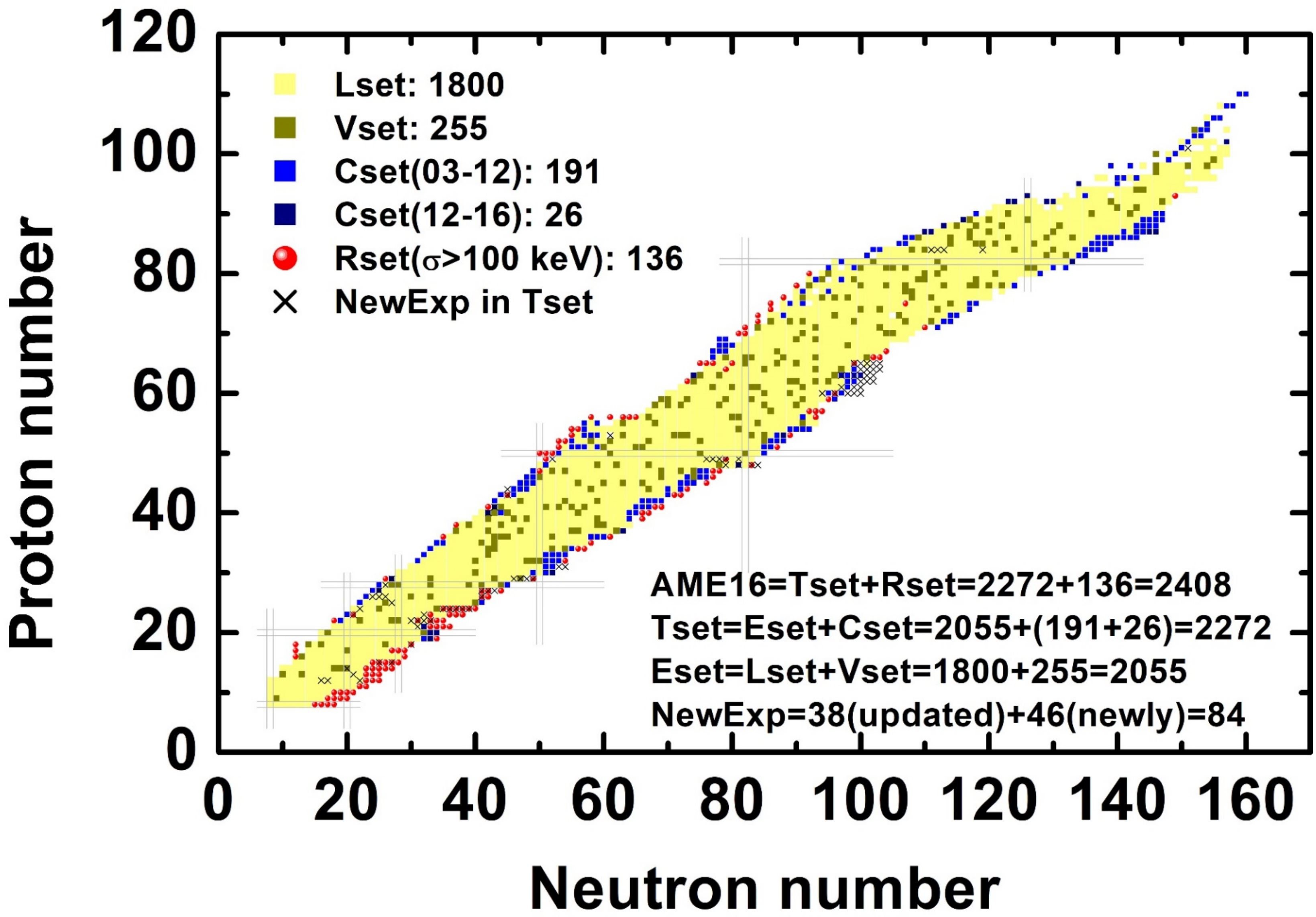


Fig: The rms deviations of BNN mass predictions with respect to the mass predictions of FRDM12 as a function of the minimum distance *r* to the isotopes in the training region. The squares and circles denote the average errors of BNN_{FRDM12} and BMM for the nuclei with the same *r*.

- The BNN_{FRDM12} can well reproduce the FRDM12 masses within **100 keV** for nuclei in Lset.
- The rms deviation between BNN_{FRDM12} predictions and FRDM12 masses increases as the increase of the distance *r*. It is very similar to the average error of BNN_{FRDM12}, which indicates **the BNN can give reasonable evaluations of the theoretical uncertainties**.

Experimental data



New Mass Model --- BMM

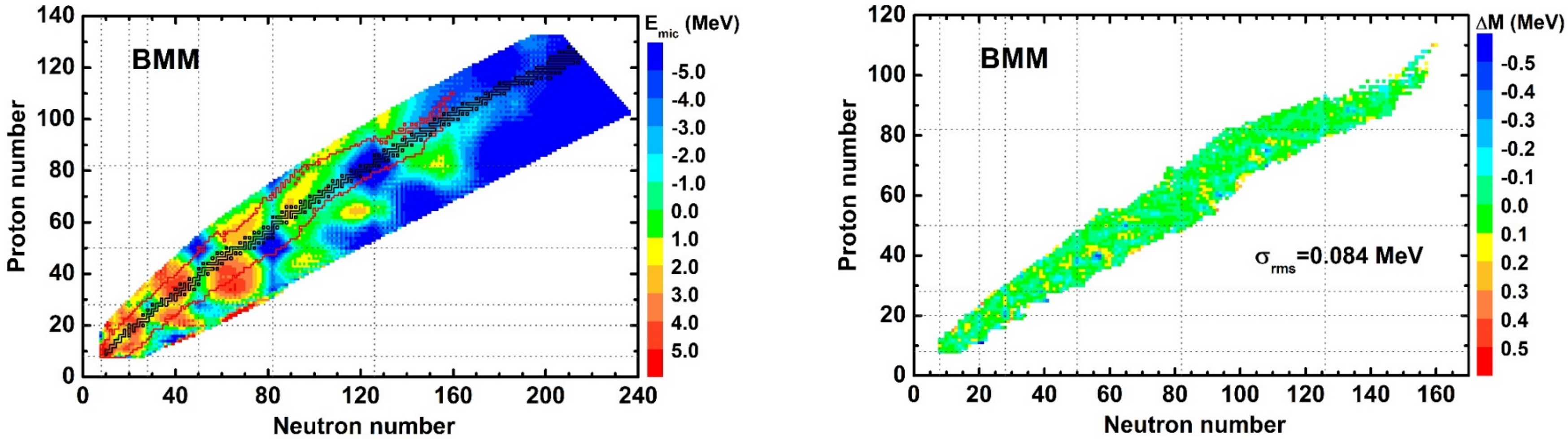
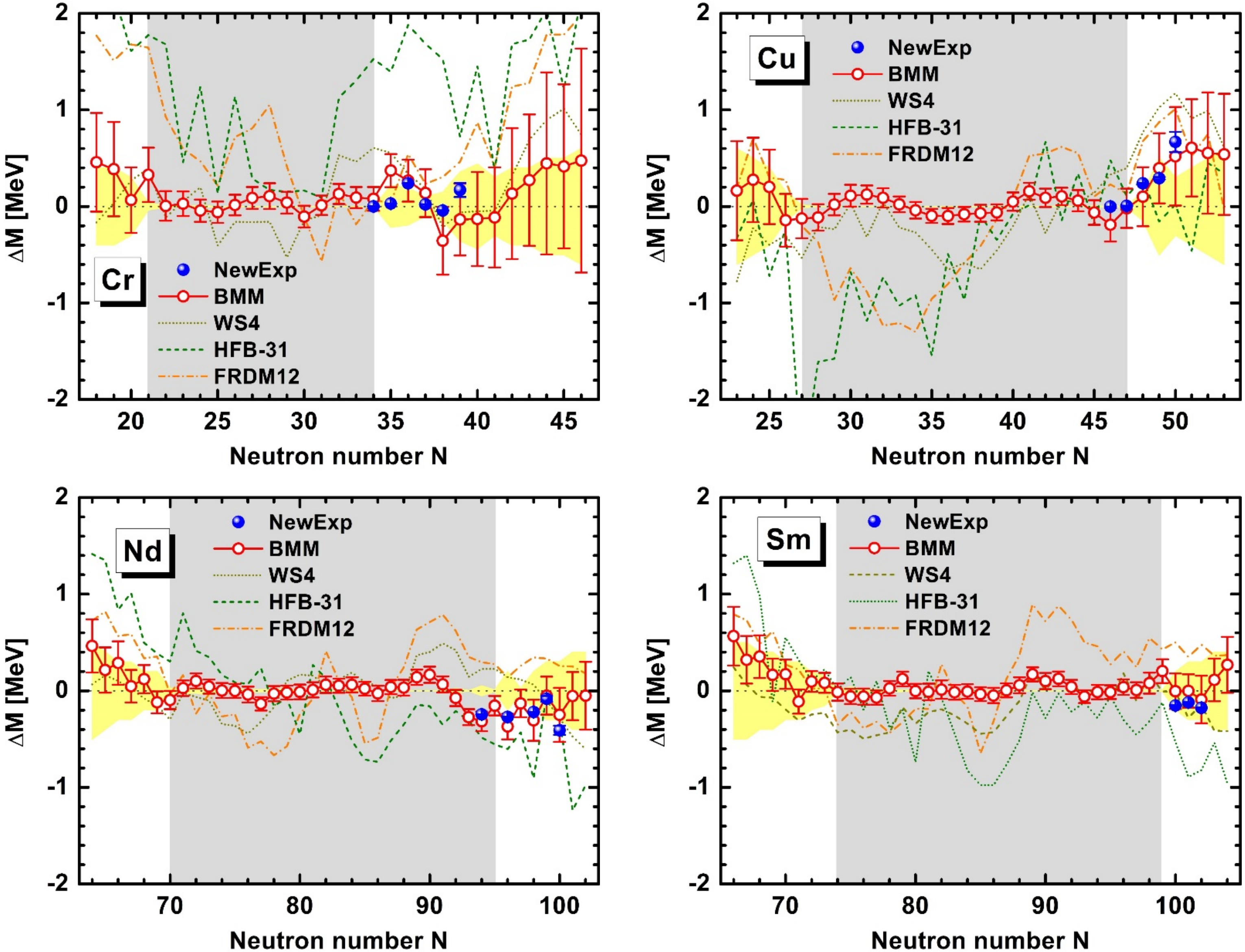


Fig: Left panel: E_{mic} of BMM with the training data from T_{set} of AME16. Right panel: mass differences between the experimental data and BNN predictions.

Model	M	S_n	S_{2n}	S_p	S_{2p}	S_D	Q_β
BMM	**0.084**	**0.078**	**0.105**	**0.083**	**0.111**	**0.096**	**0.099**
HFB31	0.559	0.451	0.456	0.489	0.496	0.566	0.557
FRDM12	0.576	0.340	0.442	0.341	0.420	0.411	0.450
WS4	0.285	0.254	0.261	0.261	0.300	0.324	0.327

- The first nuclear mass model with accuracy within **100 keV** is constructed. Its accuracies to S_* and Q_* are also much higher than other mass models.

BMM extrapolations



Niu and HZL, *PRC* **106**, L021303 (2022)

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- **Nuclear inputs with Bayesian approaches**
  - Nuclear Masses
  - Nuclear β-decay half-lives

Skyrme HFB+pnQRPA

PHYSICAL REVIEW C **106**, 024306 (2022)

Calculation of β-decay half-lives within a Skyrme-Hartree-Fock-Bogoliubov energy density functional with the proton-neutron quasiparticle random-phase approximation and isoscalar pairing strengths optimized by a Bayesian method

Futoshi Minato (湊 太志),[1,*] Zhongming Niu (牛中明),[2,†] and Haozhao Liang (梁豪兆)[3,4,‡]

- Skyrme HFB+pnQRPA (**SkO'**) with a finite-range pairing force

- Isovector (***T* = 1**) pairing (**Gogny D1S**)

$$V_{pp}^{(1)}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \sum_{i=1}^{2}\Big(W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau\Big) e^{-r_{12}^2/\mu_i^2},$$

- Isosclar (***T* = 0**) pairing (**two-Gaussian**)

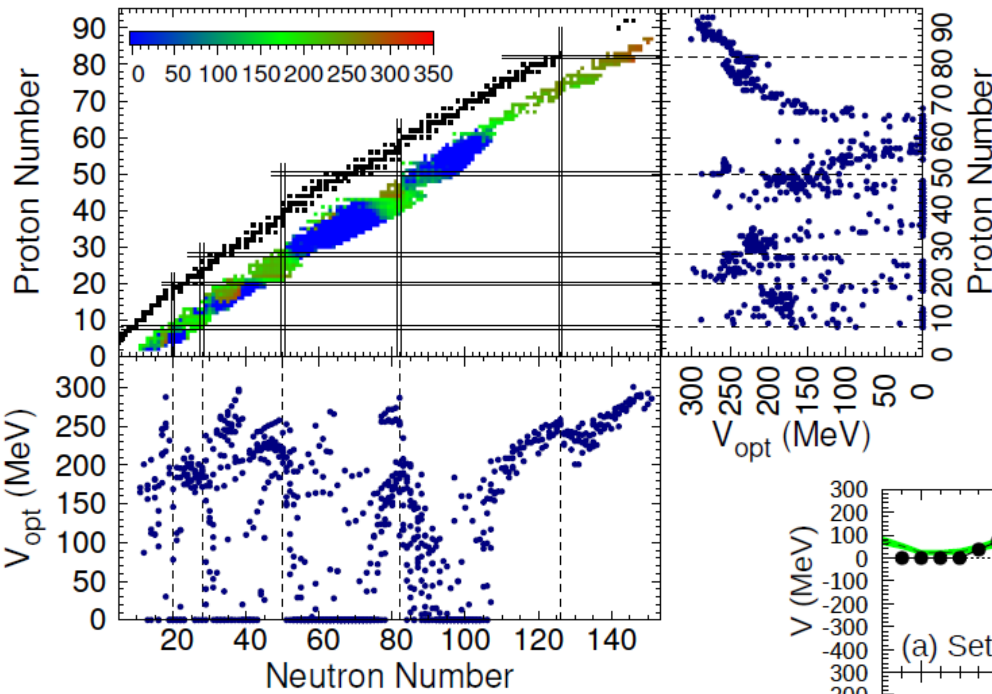
$$V_{pp}^{(0)}(\boldsymbol{r}_1,\boldsymbol{r}_2) = -V \sum_{i=1,2} g_i \exp\left(-\frac{r_{12}^2}{\mu_i'^2}\right)\hat{\Pi}_{S=1,T=0},$$

with $g_1 = 1$, $g_2 = -2$, $\mu_1 = 1.2$ fm, $\mu_2 = 0.7$ fm

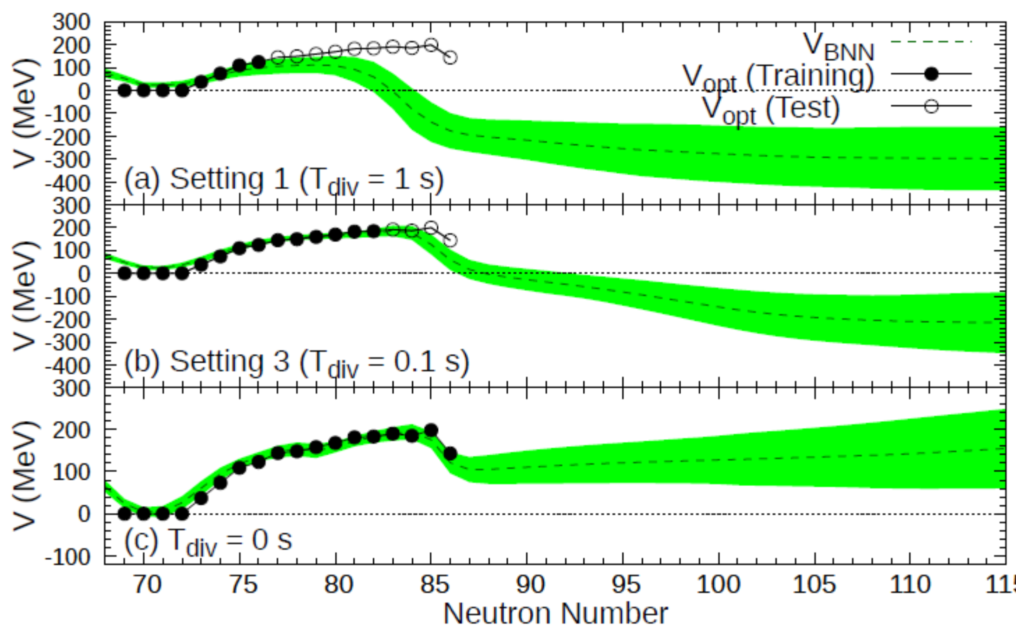
- **Both allowed and first-forbidden transitions** ➔ *β*-decay half-lives

Strengths of isoscalar pairing

★ Optimized isoscalar pairing strengths V_{opt} determined to reproduce $T_{1/2}$ of NUBASE2016



★ Isoscalar pairing strengths in **Cd** isotopes estimated by BNN (V_{BNN})

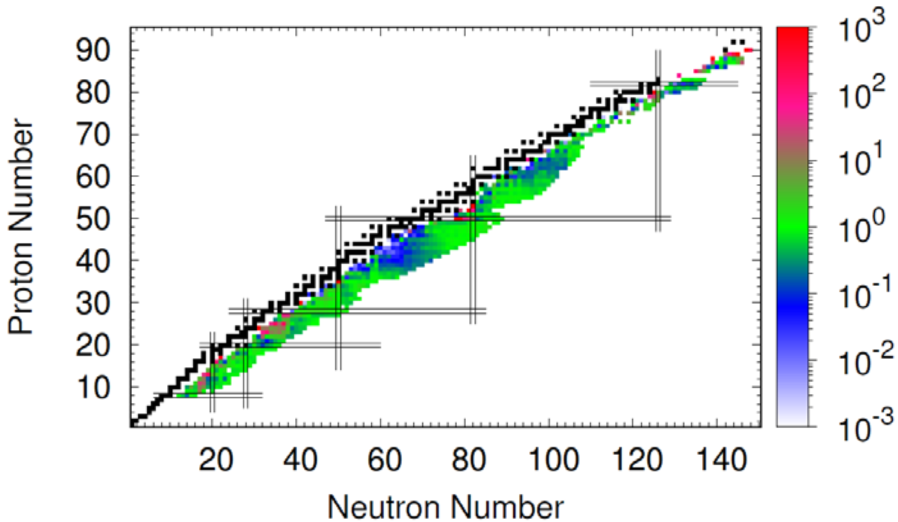


Minato, Niu, HZL, *PRC* **106**, 024306 (2022)

cf. Niu, Niu, HZL, Long, Niksic, Vretenar, Meng, *PLB* **723**, 172 (2013)

Predictions of nuclear half-lives

★ Ratios between calculated and experimental half-lives



- mean deviation

$$\bar{r} = \frac{1}{N}\sum_i^N r_i, \quad r_i = \log_{10}\left(\frac{T_{\mathrm{calc},i}}{T_{\mathrm{exp},i}}\right),$$

- standard deviation

$$s = \sqrt{\frac{1}{N}\sum_i^N r_i^2}.$$

★ The results of this work, D3C*, and pnFAM

	This work		D3C*		*pn*FAM	
	$\bar{r}$	s	$\bar{r}$	s	$\bar{r}$	s
E-E	−0.009	0.294	−0.001	0.475	−0.039	0.428
E-O	−0.020	0.301	0.019	0.544	−0.055	0.428
O-E	0.043	0.406	0.153	0.608	−0.014	0.338
O-O	0.106	0.552	0.378	1.154	0.120	0.557

Minato, Niu, HZL,
PRC **106**, 024306 (2022)

D3C*: Marketin, Huther, and Martinez-Pinedo, PRC 93, 025805 (2016)
pnFAM: Ney, Engel, Li, and Schunck, PRC 102, 034326 (2020)

Machine learning

Machine Learning for physics?

- We learn what we need ……
- We learn what we have less control ……
- We learn what we are guaranteed ……
  e.g., Imoto's talk & works by Akashi, Sugino, et al.

Or

We build physics (space and time) in neural networks …

e.g., Koji Hashimoto's talk

Contents

- **Quantum computing for nuclear structure properties?**
  - Computations with quantum circuits
  - Computations with quantum annealing

A pioneering work: QC for atomic nuclei

PHYSICAL REVIEW LETTERS **120**, 210501 (2018)

Editors' Suggestion | Featured in Physics

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,[1] A. J. McCaskey,[2] G. Hagen,[3,4] G. R. Jansen,[5,3] T. D. Morris,[4,3] T. Papenbrock,[4,3,*] R. C. Pooser,[1,4] D. J. Dean,[3] and P. Lougovski[1,†]

[1]*Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[2]*Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[3]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
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[5]*National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

Physics

by Stefano Gandolfi*

VIEWPOINT

Cloud Quantum Computing Tackles Simple Nucleus

Researchers perform a quantum computation of the binding energy of the deuteron using a web connection to remote quantum devices.

Model setup and main results

Dumitrescu et al., *PRL* **120**, 210501 (2018)

- **Deuteron Hamiltonian** (discrete variable representation in HO basis)

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^{\dagger} a_n .$$

where $\langle n'|T|n\rangle = \frac{\hbar\omega}{2}\Big[(2n+3/2)\delta_n^{n'} - \sqrt{n(n+1/2)}\delta_n^{n'+1} - \sqrt{(n+1)(n+3/2)}\delta_n^{n'-1}\Big],$

$$\langle n'|V|n\rangle = V_0 \delta_n^0 \delta_n^{n'} .$$

$V_0 = -5.68658111$ MeV

$\hbar\omega = 7$ MeV

- **Results**

E from exact diagonalization				
N	E_N	$O(e^{-2kL})$	$O(kLe^{-4kL})$	$O(e^{-4kL})$
2	-1.749	-2.39	-2.19	
3	-2.046	-2.33	-2.20	-2.21
E from quantum computing				
N	E_N	$O(e^{-2kL})$	$O(kLe^{-4kL})$	$O(e^{-4kL})$
2	$-1.74(3)$	$-2.38(4)$	$-2.18(3)$	
3	$-2.08(3)$	$-2.35(2)$	$-2.21(3)$	$-2.28(3)$

$E_{\text{exact}} = -2.22$ MeV

Introduction (by Gandolfi)

Gandolfi, *Physics* **11**, 51 (2018)

- The **qubits** come in a variety of physical implementations, with some represented by the **spin up or down of atoms** and others by **two excited states in a superconducting circuit**, for exmple.

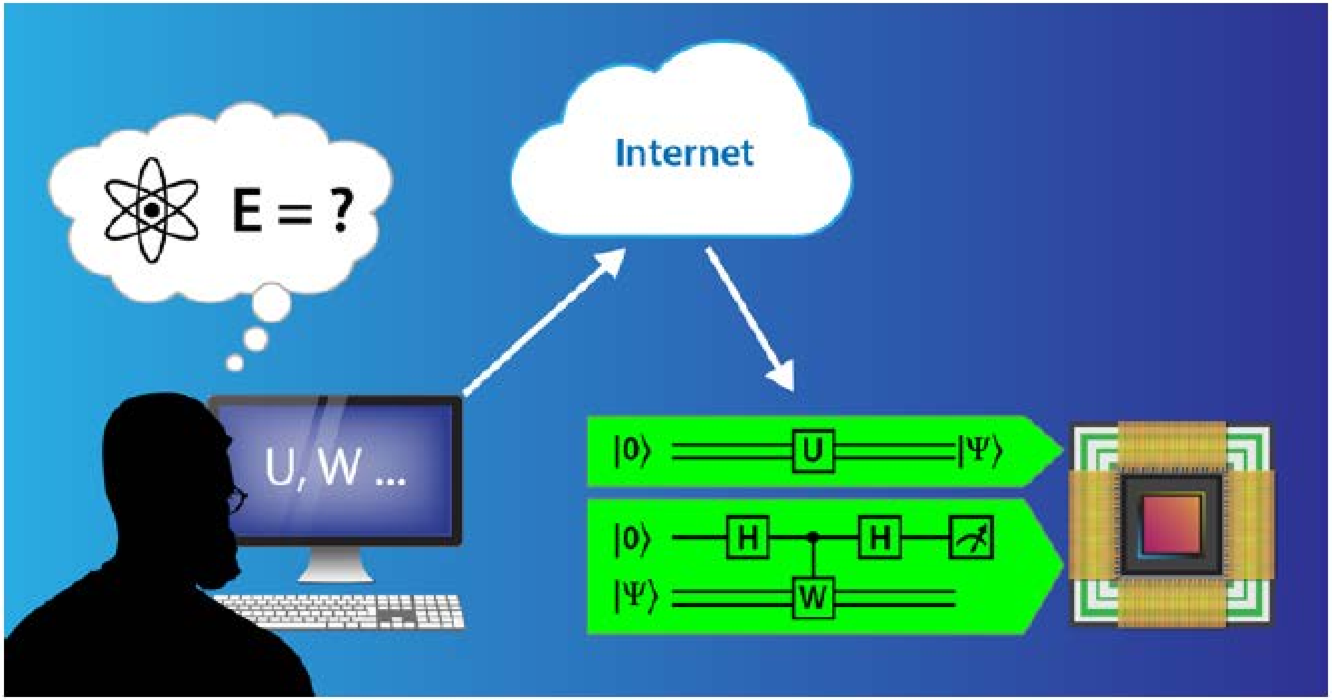
- In general, problem solving using quantum computers involves **three main blocks**:

I. formulate the problem to be solved **in terms of unitary matrices**

II. rewrite those matrices **in terms of gates** that can be realized on a given quantum computer

III. implement and try to improve the <u>efficiency</u> of (II), <u>reducing the number of gates</u> as much as possible

Introduction (by Gandolfi)



$E = \langle\Psi|\hat{H}|\Psi\rangle$ with $|\Psi\rangle = U|0\rangle$ and $W = \hat{H}$

- At the end of these operations, the ancilla qubit is measured, **returning either zero or one**.

- This measurement, however, is sampling just one possibility out of many, so it is necessary to **repeat** the measurement many times and **take the average**.

Gandolfi, *Physics* **11**, 51 (2018)

Model setup and quantum programming

Dumitrescu et al., *PRL* **120**, 210501 (2018)

- **Deuteron Hamiltonian** (discrete variable representation in HO basis)

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^{\dagger} a_n.$$

where $\langle n'|T|n\rangle = \frac{\hbar\omega}{2}\Big[(2n+3/2)\delta_n^{n'} - \sqrt{n(n+1/2)}\delta_n^{n'+1} - \sqrt{(n+1)(n+3/2)}\delta_n^{n'-1}\Big],$

$$\langle n'|V|n\rangle = V_0 \delta_n^0 \delta_n^{n'}.$$

$V_0 = -5.68658111$ MeV

$\hbar\omega = 7$ MeV

- Quantum computers manipulate qubits by operations based on **Pauli matrices**

$$a_n^{\dagger} \rightarrow \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n - iY_n),$$

$$a_n \rightarrow \frac{1}{2}\left[\prod_{j=0}^{n-1} -Z_j\right](X_n + iY_n).$$

$$H_2 = 5.906\,709 I + 0.218\,291 Z_0 - 6.125 Z_1 - 2.143\,304(X_0X_1 + Y_0Y_1),$$

$$H_3 = H_2 + 9.625(I - Z_2) - 3.913\,119(X_1X_2 + Y_1Y_2).$$

Model setup and quantum programming

Dumitrescu et al., *PRL* **120**, 210501 (2018)

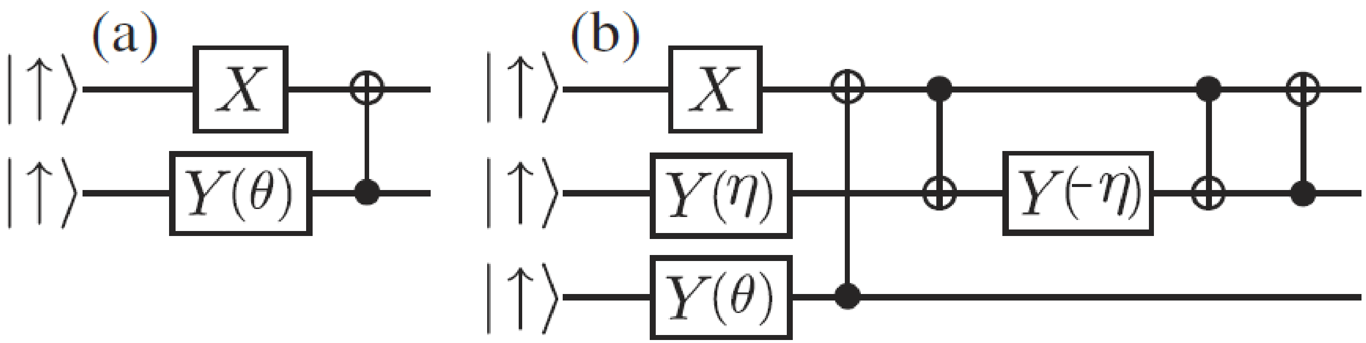
- **Variational wave function**

$$U(\theta) \equiv e^{\theta(a_0^\dagger a_1 - a_1^\dagger a_0)} = e^{i(\theta/2)(X_0 Y_1 - X_1 Y_0)},$$

$$U(\eta,\theta) \equiv e^{\eta(a_0^\dagger a_1 - a_1^\dagger a_0) + \theta(a_0^\dagger a_2 - a_2^\dagger a_0)} \approx e^{i(\eta/2)(X_0 Y_1 - X_1 Y_0)} e^{i(\theta/2)(X_0 Z_1 Y_2 - X_2 Z_1 Y_0)}.$$

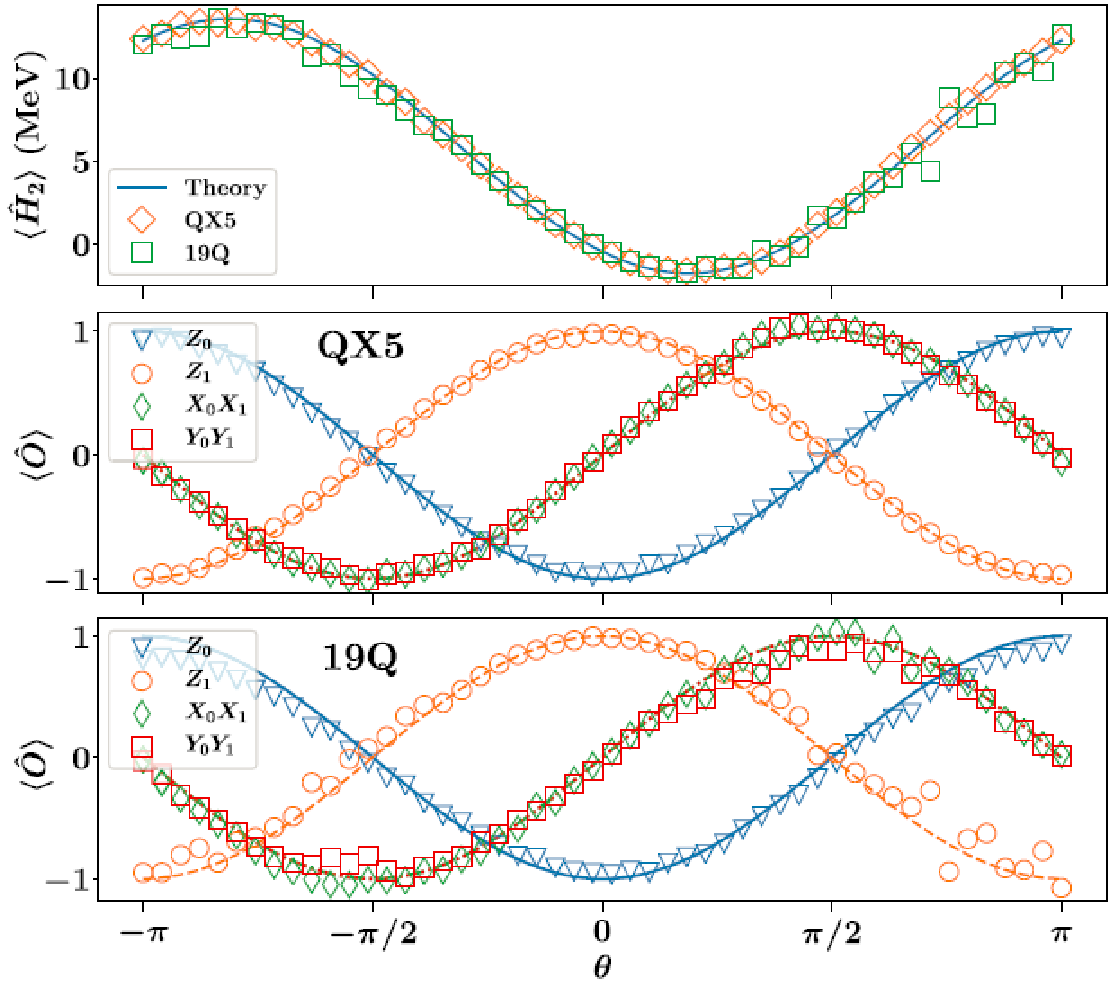
- **Computing architectures**

https://en.wikipedia.org/wiki/Quantum_logic_gate
https://algassert.com/quirk



- **QX5** and **19Q** chips: with a single qubit **connected to up to three neighbors**
- It works here 🡰 **only requires up to two connections** for each qubit

Results



$$H_2 = 5.906\,709 I + 0.218\,291 Z_0 - 6.125 Z_1 - 2.143\,304 (X_0 X_1 + Y_0 Y_1),$$

$$U(\theta) \equiv e^{\theta(a_0^\dagger a_1 - a_1^\dagger a_0)} = e^{i(\theta/2)(X_0 Y_1 - X_1 Y_0)},$$

$E_2^{QX5} = -1.80 \pm 0.05$ MeV

$E_2^{19Q} = -1.72 \pm 0.03$ MeV

thus

$E_2 = -1.74 \pm 0.03$ MeV

- Experimentally determined energies for H_2

Dumitrescu et al., *PRL* **120**, 210501 (2018)

Lipkin model

- **Lipkin Hamiltonian**

$$H = \frac{1}{2}\varepsilon \sum_{p\sigma} \sigma a^{\dagger}_{p,\sigma} a_{p,\sigma} + \frac{1}{2} V \sum_{pp'\sigma} a^{\dagger}_{p,\sigma} a^{\dagger}_{p',\sigma} a_{p',-\sigma} a_{p,-\sigma} + \frac{1}{2} W \sum_{pp'\sigma} a^{\dagger}_{p,\sigma} a^{\dagger}_{p',-\sigma} a_{p',\sigma} a_{p,-\sigma} \, ,$$

VALIDITY OF MANY-BODY APPROXIMATION METHODS FOR A SOLVABLE MODEL

(I). Exact Solutions and Perturbation Theory

VALIDITY OF MANY-BODY APPROXIMATION METHODS FOR A SOLVABLE MODEL

(II). Linearization Procedures

VALIDITY OF MANY-BODY APPROXIMATION METHODS FOR A SOLVABLE MODEL

(III). Diagram Summations

VALIDITY OF MANY-BODY APPROXIMATION METHODS FOR A SOLVABLE MODEL

(IV). The Deformed Hartree-Fock Solution

D. AGASSI and H. J. LIPKIN

The Weizmann Institute of Science, Rehovoth, Israel

and

N. MESHKOV

Catholic University of America, Washington, D.C. †

Lipkin model

- **Quasi-spin formulation**

$$J_+ = \sum_p a^\dagger_{p,+1} a_{p,-1}\,, \qquad J_- = \sum_p a^\dagger_{p,-1} a_{p,+1}\,, \qquad J_z = \frac{1}{2}\sum_{p\sigma} \sigma a^\dagger_{p,\sigma} a_{p,\sigma}\,.$$

- Hamiltonian

$$H = \varepsilon J_z + \frac{1}{2} V (J_+^2 + J_-^2) + \frac{1}{2} W (J_+ J_- + J_- J_+)\,.$$

- Exact solutions (***N* = 2, 3, 4, 6, 8** with ***W* = 0**)

  - for $N = 2$:

$$\frac{E}{\varepsilon} = 0\,, \pm \left[1 + \left(\frac{V}{\varepsilon}\right)^2\right]^{\frac{1}{2}}\,,$$

  - for $N = 3$:

$$\frac{E}{\varepsilon} = \pm \left\{\frac{1}{2} \pm \left[1 + 3\left(\frac{V}{\varepsilon}\right)^2\right]^{\frac{1}{2}}\right\}\,,$$

  - for $N = 4$:

$$\frac{E}{\varepsilon} = 0\,, \pm 2\left[1 + 3\left(\frac{V}{\varepsilon}\right)^2\right]^{\frac{1}{2}}\,,$$

$$\frac{E}{\varepsilon} = \pm \left[1 + 9\left(\frac{V}{\varepsilon}\right)^2\right]^{\frac{1}{2}}\,,$$

Lipkin, Meshkov, Glick, *Nucl. Phys.* **62**, 188 (1965)

Lipkin model

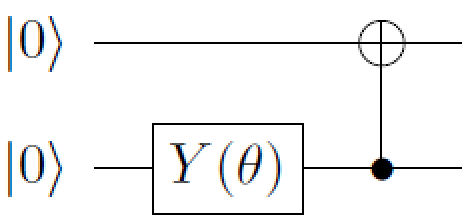
- **Qubit representation of Lipkin Hamiltonian** (***W* = 0**)

$$H = -\frac{1}{2}\varepsilon \sum_{i=1}^{N} Z_i + \frac{1}{4} V \sum_{i,j=1}^{N} \left(X_i X_j - Y_i Y_j \right).$$

- Trial wave functions (***N* = 2**)

$$|\psi\rangle = U(\theta)|00\rangle = \cos\frac{\theta}{2}|00\rangle + \sin\frac{\theta}{2}|11\rangle.$$

- Quantum circuit (***N* = 2**)



- Number of parameters, ***O*(2*^N*)**, is needed for a complete expression of the trial wave functions.

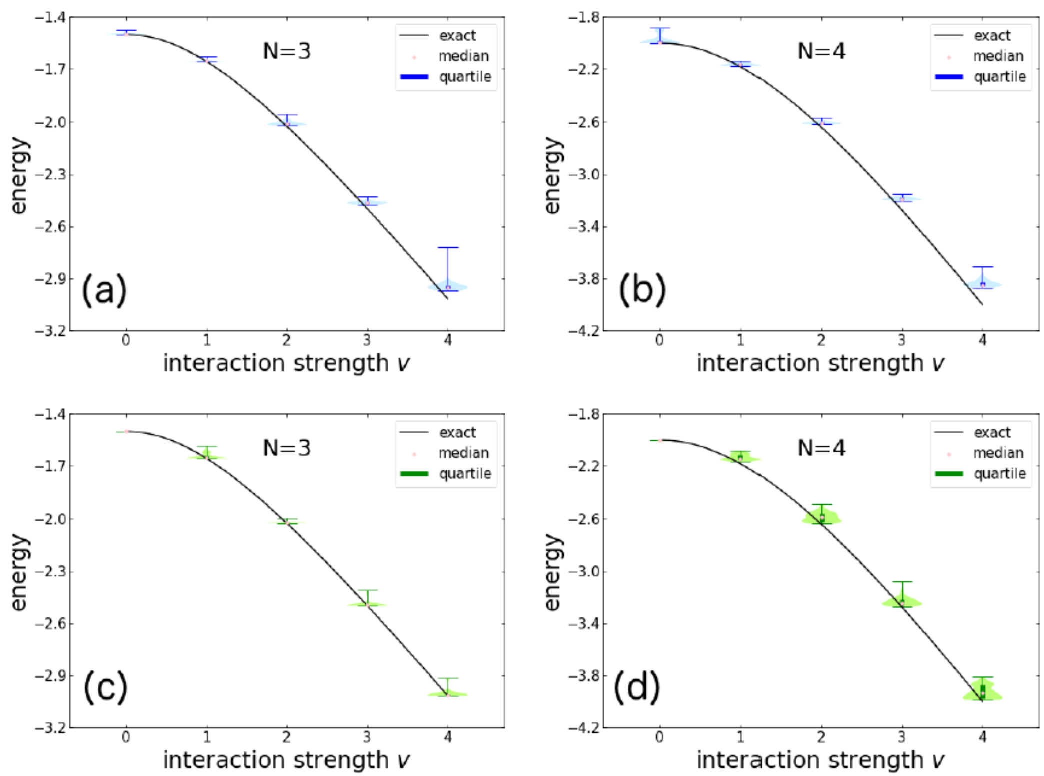
UCC and structure learning ansatz

Chinese Physics C Vol. 46, No. 2 (2022) 024106

Quantum computing for the Lipkin model with unitary coupled cluster and structure learning ansatz*

Asahi Chikaoka(近岡旭)[1,2] Haozhao Liang(梁豪兆)[1,2†]

[1]Department of Physics, Graduate School of Science, The University of Tokyo, Tokyo 113-0033, Japan
[2]RIKEN Nishina Center, Wako 351-0198, Japan



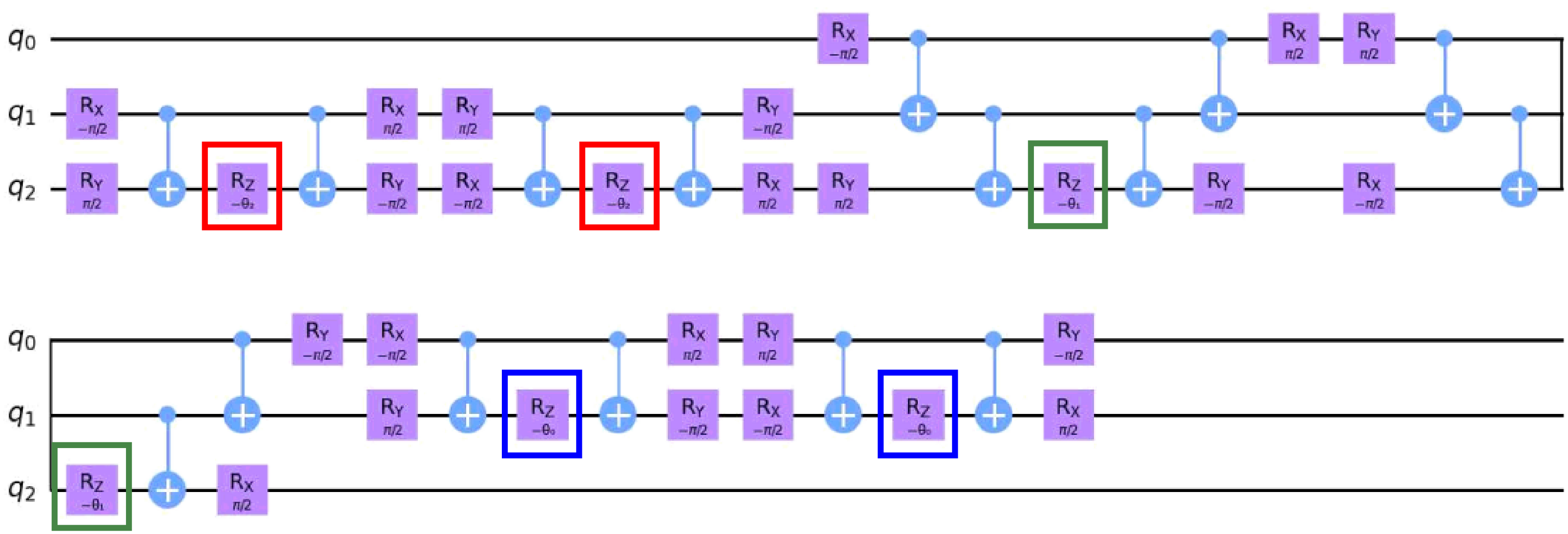
UCC ansatz

- **Trial wave functions**

Chikaoka and HZL, *Chin. Phys. C* **46**, 024106 (2022)

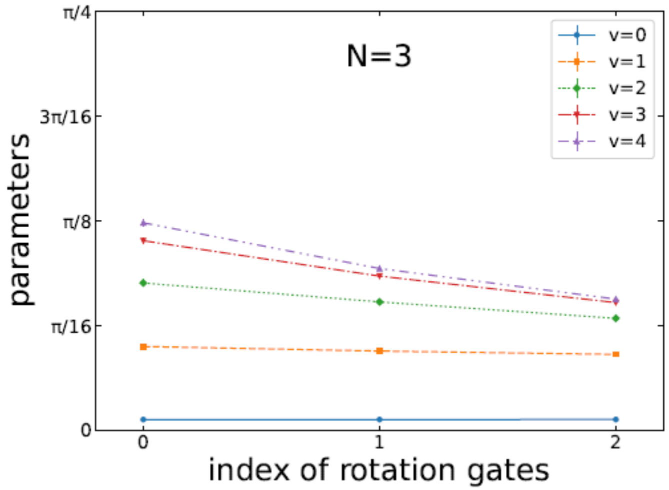
$$U(\theta) \equiv \exp\left[\sum_{ij} \theta_{ij}(a_i^\dagger a_j^\dagger - a_j a_i)\right]$$
$$\mapsto \exp\left\{ i \sum_{ij} \theta_{ij} \frac{(-1)^{j-i-1}}{2} \left[X_i \left(\prod_{k=i+1}^{j-1} Z_k \right) Y_j + Y_i \left(\prod_{k=i+1}^{j-1} Z_k \right) X_j \right] \right\},$$

- Quantum circuit (N = 3)

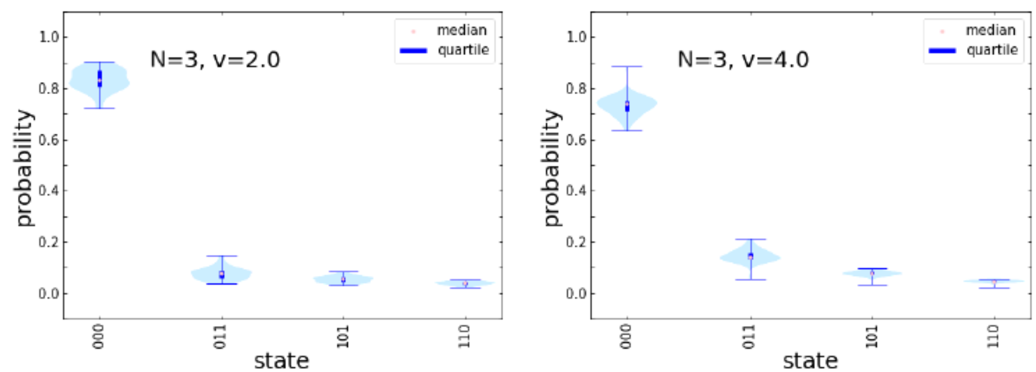


UCC ansatz

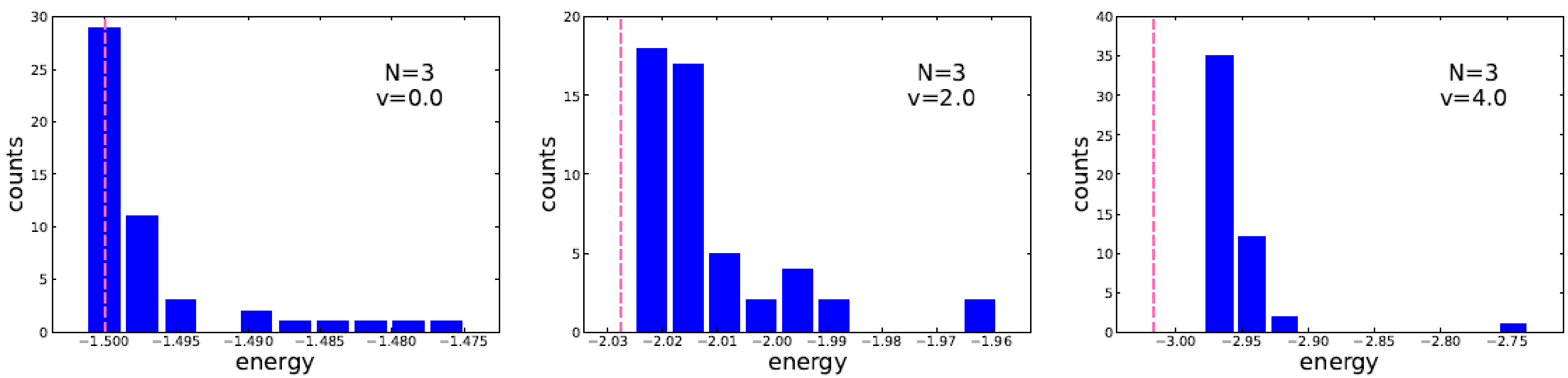
- Parameters



- State probabilities



- Ground-state energies



Chikaoka and HZL, *Chin. Phys. C* **46**, 024106 (2022)

Structure learning ansatz

- **Trial wave functions**

Chikaoka and HZL, *Chin. Phys. C* **46**, 024106 (2022)

Algorithm 1 Rotoselect

Input: Function calculating expectation values with respect to each quantum circuit U: $\langle M(U) \rangle$. Here, M represents a Hermitian operator. The quantum circuit U with the maximum value of the depth, D, is composed of rotation gates at the depth d, $U_d(\theta_d, H_d) = H_d(\theta_d)$ (e.g., $R_X(\theta_d) = \exp[-i\frac{\theta_d}{2}X]$), and the CNOTs. Here, θ_d is a parameter at the depth d and H_d is the element of the set of the rotation operators $\{I, R_X, R_Y, R_Z\}$. Axes of rotation gates, i.e. I, R_X, R_Y, or R_Z, are chosen in order to minimize the expectation value.

Output: Optimized quantum circuit $U_{\rm opt}$. Here, $U_{\rm opt}$ is optimized with respect to θ_d and H_d.

Initialize $\theta_d \in (\pi, \pi]$ and $H_d \in \{I, R_X, R_Y, R_Z\}$ for $d = 1, \cdots, D$ heuristically or at random. (In practice, initialize all $\theta_d = 0$ and all $H_d = I$.)

repeat

  for $d = 1, \cdots, D$ **do**

    Compute $\theta^*_{d,P}$ for $P \in \{I, R_X, R_Y, R_Z\}$ using SMO method, where $\theta^*_{d,P}$ is the optimized parameter with the selected gate P.

    $H_d \leftarrow \arg\min_P \langle M(U) \rangle|_{U_d(\theta_d, H_d) = U_d(\theta^*_d, P)}$

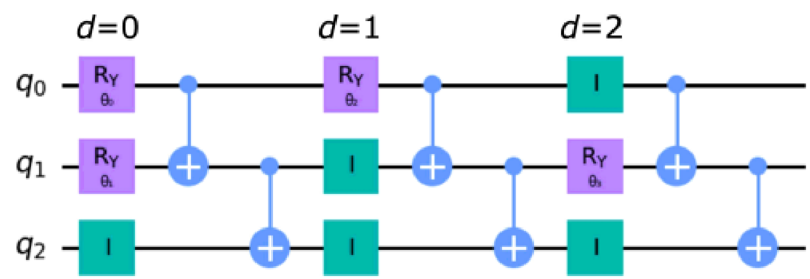
    $\theta_d \leftarrow \theta^*_{d,H_d}$, where θ^*_{d,H_d} is the optimized parameter with the selected gate H_d

  end for

until stopping criterion is met

return optimized quantum circuit $U_{\rm opt}$

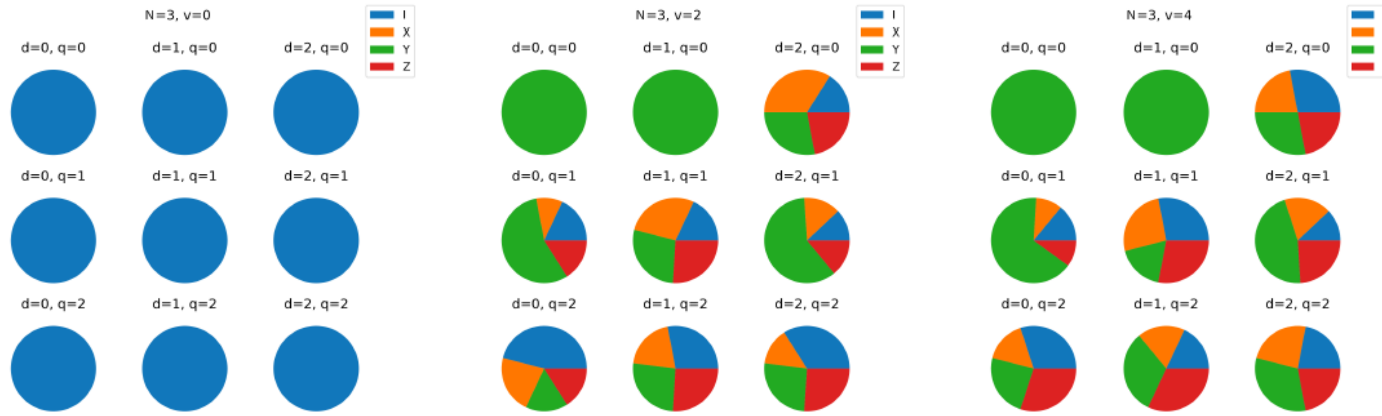
- Quantum circuit (***N* = 3**)
  (an example)



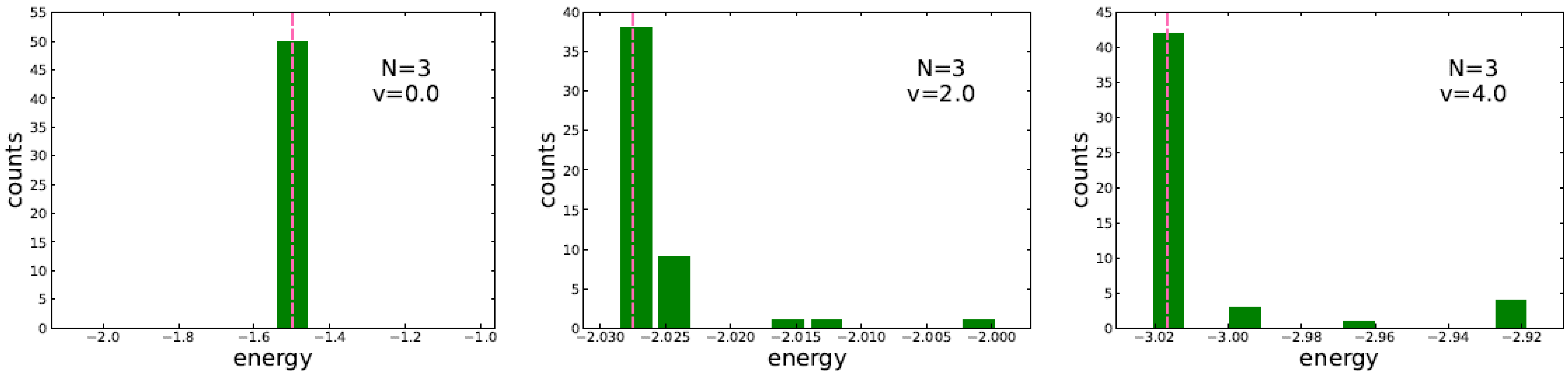
Structure learning ansatz

- Rotating axes

Chikaoka and HZL, *Chin. Phys. C* **46**, 024106 (2022)



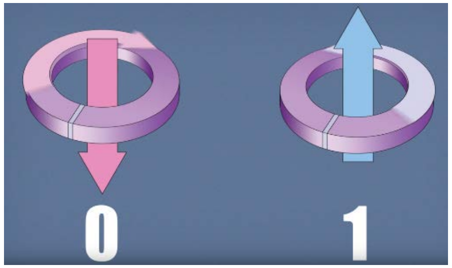
- Ground-state energies

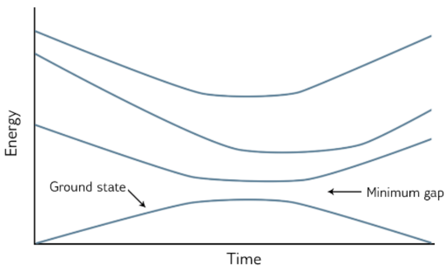


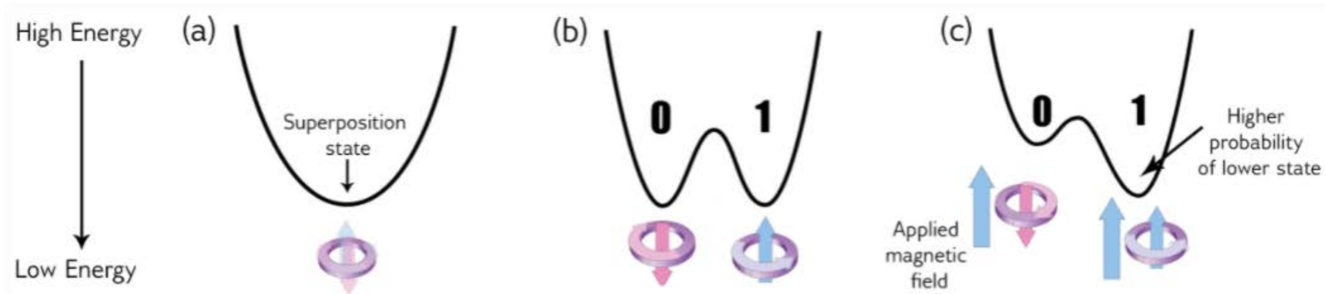
Contents

- **Quantum computing for nuclear structure properties?**
  - Computations with quantum circuits
  - Computations with quantum annealing

Quantum Annealing







Comparison of D-Wave systems [edit]

	D-Wave One	D-Wave Two	D-Wave 2X	D-Wave 2000Q[57][58]	Advantage[59][60]	Advantage 2[61][62]
Release date	May 2011	May 2013	August 2015	January 2017	2020	2023-2024
Topology				Chimera	Pegasus	Zephyr
Code-name	Rainier	Vesuvius	W1K	W2K	Pegasus P16	
Qubits	128	512	1152	2048	5640	7000+ (7440)
Couplers[63]	352	1,472	3,360	6,016	40,484	
Connectivity				6	15	20
Josephson junctions	24,000	?	128,000	128,472[60]	1,030,000	
I/O lines / Control lines	?	192	192	200[64]	?	
Active area				5.5 mm^2	8.4 mm^2	
On-chip memory				22 kB	130 kB	
Operating temperature (K)	?	0.02	0.015	0.015	<0.015	
Power consumption (kW)	?	15.5	25	25	25	
Buyers	Lockheed Martin	• Google/NASA/USRA • Lockheed Martin	• Los Alamos National Laboratory • Google/NASA/USRA • Lockheed Martin	• Temporal Defense Systems • Google/NASA/USRA[65] • Los Alamos National Laboratory	• Lockheed Martin • Los Alamos National Laboratory[66] • Jülich Supercomputing Centre[67][68] (Forschungszentrum Jülich)	

https://docs.dwavesys.com/docs/latest/c_gs_2.html
https://en.wikipedia.org/wiki/D-Wave_Systems#Computer_systems

Hybrid Quantum Annealing (HQA)

scientific reports

Irie, HZL, Doi, Gongyo, Hatsuda, *Sci. Rep.* **11**, 8426 (2021)

OPEN

Hybrid quantum annealing via molecular dynamics

Hirotaka Irie[1,2], Haozhao Liang[3,4], Takumi Doi[2,3], Shinya Gongyo[2,3] & Tetsuo Hatsuda[2]

- Concept of HQA

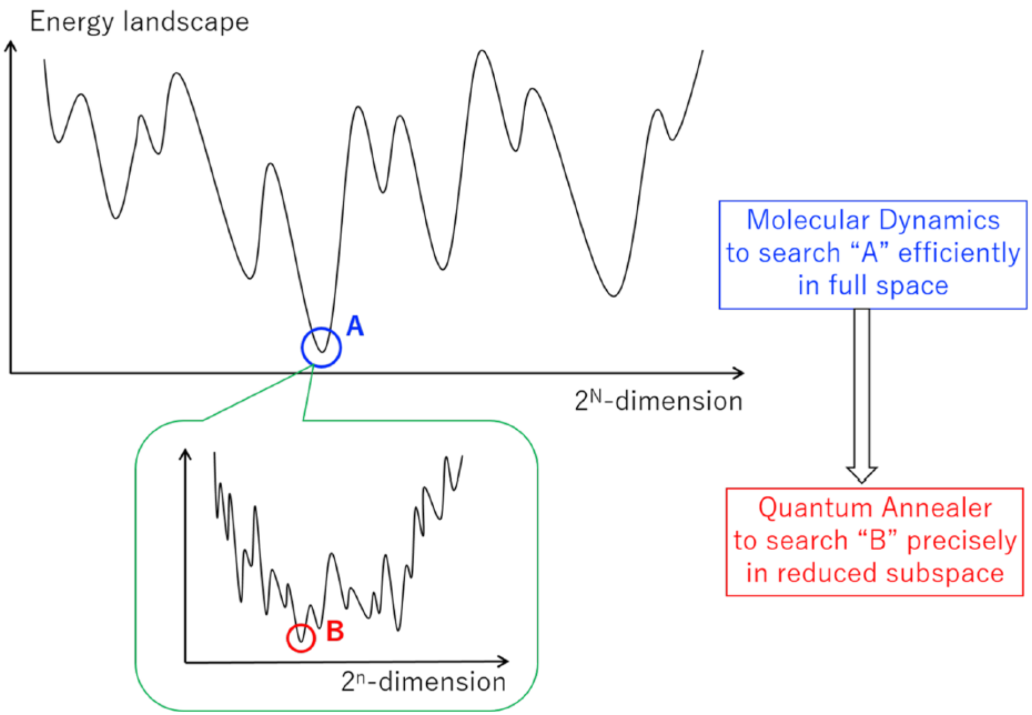


Figure 1. Concept of hybrid quantum annealing via molecular dynamics.

Hybrid Quantum Annealing (HQA)

- Ising Hamiltonian

$$\mathcal{H}_{\text{Ising}}(s) = \frac{1}{2}\sum_{i\neq j}^{N} J_{ij} s_i s_j + \sum_{i=1}^{N} h_i s_i,$$

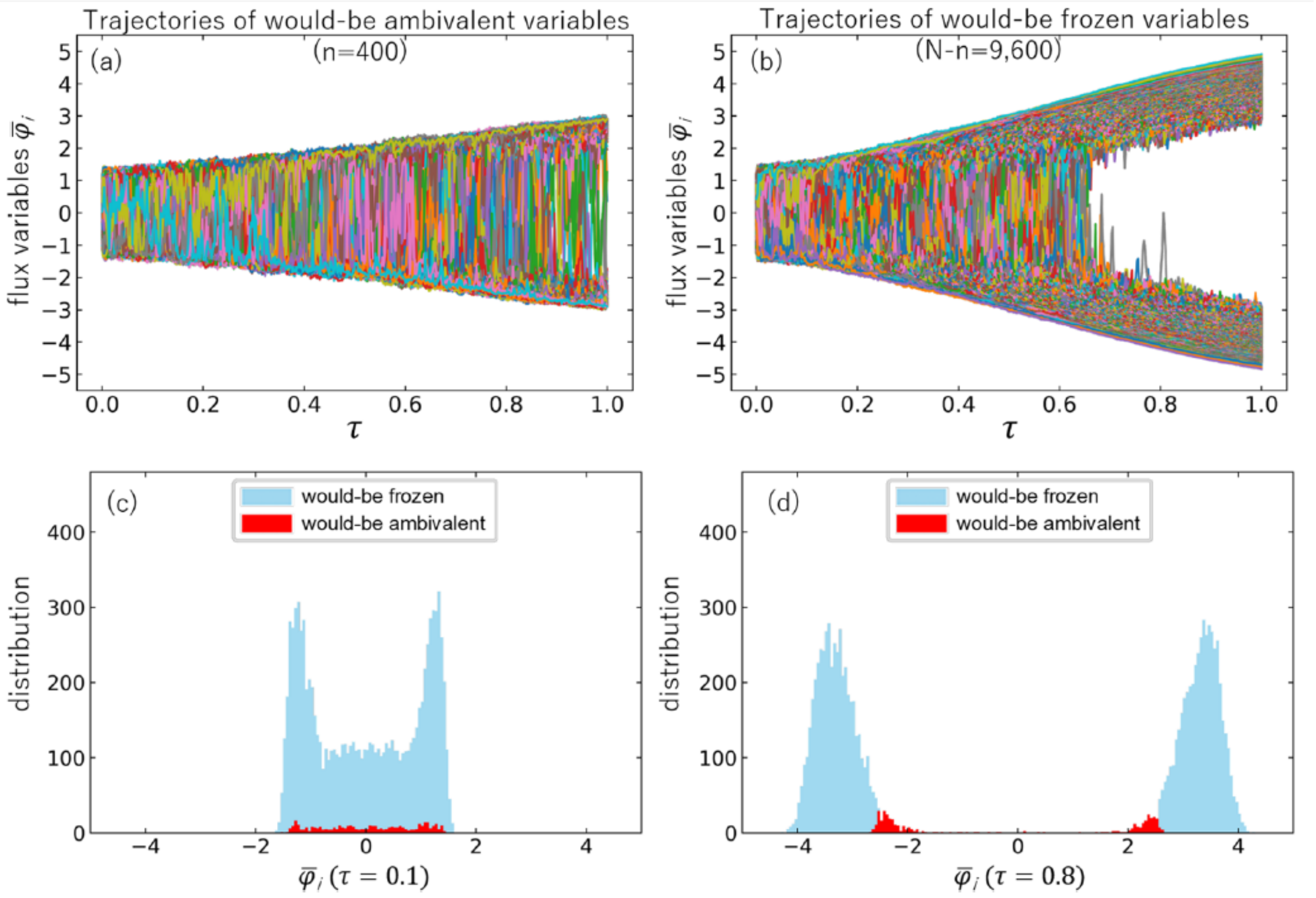
- Hamiltonian for quantum annealing

$$\mathcal{H}_{\text{QA}}(\sigma;\tau) = A(\tau)\left[-\sum_{i=1}^{N}\sigma_i^x\right] + B(\tau)\left[\frac{1}{2}\sum_{i\neq j}^{N} J_{ij}\sigma_i^z\sigma_j^z + \sum_{i=1}^{N} h_i\sigma_i^z\right],$$

Irie, HZL, Doi, Gongyo, Hatsuda, *Sci. Rep.* **11**, 8426 (2021)

Hybrid Quantum Annealing (HQA)

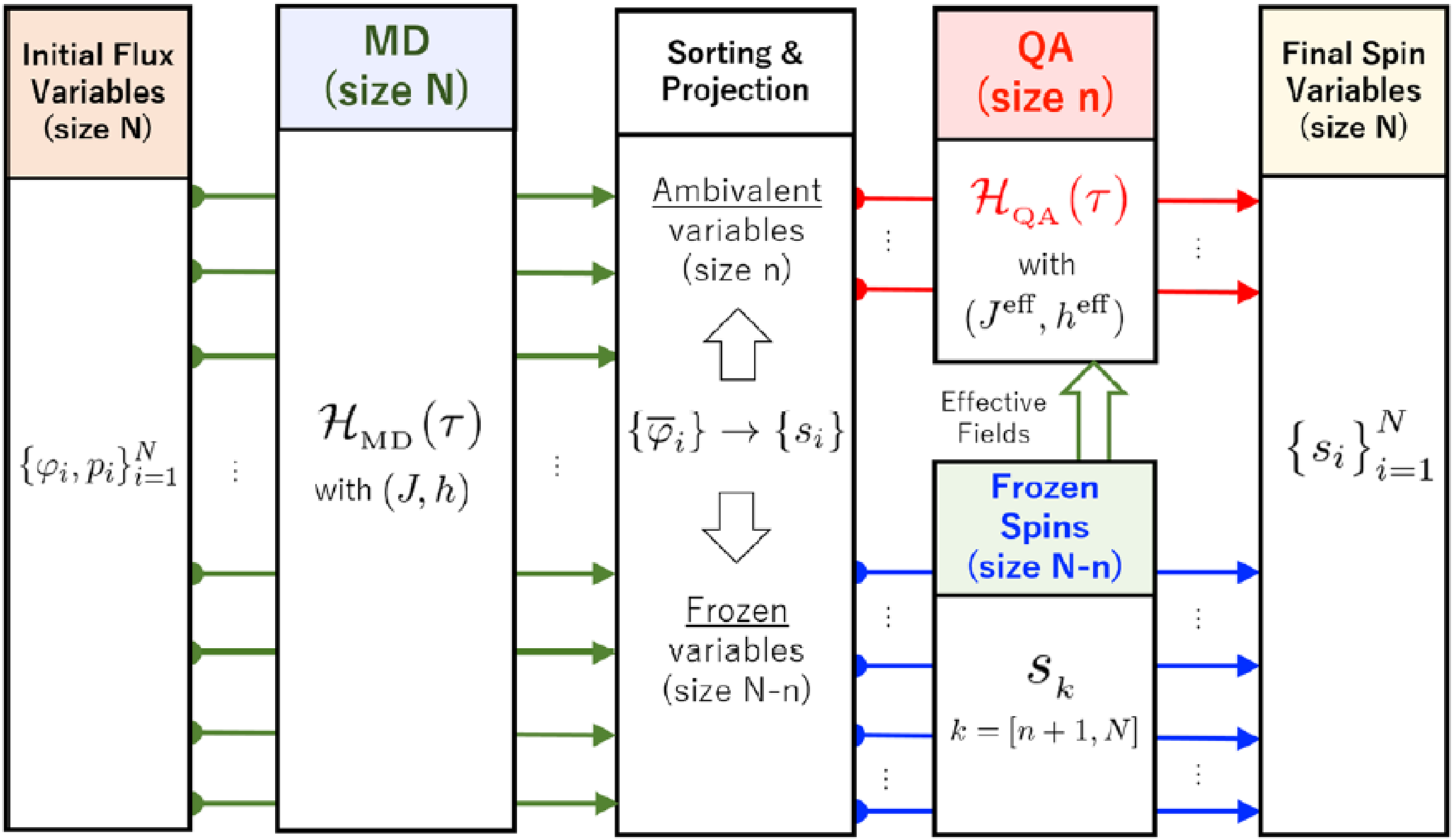
➢ Typical trajectories



Irie, HZL, Doi, Gongyo, Hatsuda, *Sci. Rep.* **11**, 8426 (2021)

Hybrid Quantum Annealing (HQA)

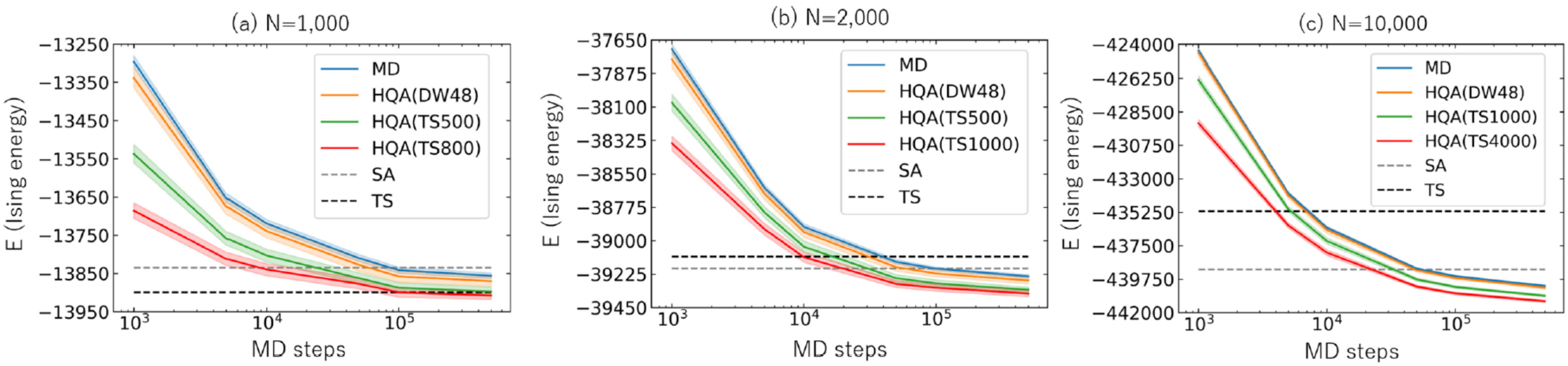
- Flowchart of HQA



Irie, HZL, Doi, Gongyo, Hatsuda, *Sci. Rep.* **11**, 8426 (2021)

Results of Ising spin-glass

- Ground-state energies



Irie, HZL, Doi, Gongyo, Hatsuda, *Sci. Rep.* **11**, 8426 (2021)

Quantum computing for nuclear physics

Physics Letters B 807 (2020) 135536

Projected cooling algorithm for quantum computation

Dean Lee *, Joey Bonitati, Gabriel Given, Caleb Hicks, Ning Li, Bing-Nan Lu, Abudit Rai, Avik Sarkar, Jacob Watkins

Facility for Rare Isotope Beams and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

Lipkin model on a quantum computer

Michael J. Cervia, A. B. Balantekin, S. N. Coppersmith, Calvin W. Johnson, Peter J. Love, C. Poole, K. Robbins, and M. Saffman
Phys. Rev. C **104**, 024305 – Published 3 August 2021

Simulating excited states of the Lipkin model on a quantum computer

Manqoba Q. Hlatshwayo, Yinu Zhang, Herlik Wibowo, Ryan LaRose, Denis Lacroix, and Elena Litvinova
Phys. Rev. C **106**, 024319 – Published 18 August 2022

iTHEMS 理化学研究所 数理創造プログラム
RIKEN Interdisciplinary Theoretical and Mathematical Sciences Program

QCoIn Working Group https://suuri.riken.jp/qcoin-wg/