N3AS – iTHEMS Meeting on
Quantum Information Science in Multimessenger Astrophysics
June 16–18, 2024, RIKEN, Japan

Structure learning ansatz for Lipkin model

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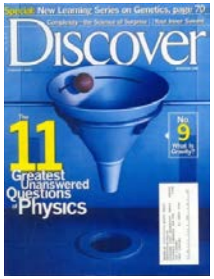
June 16, 2024

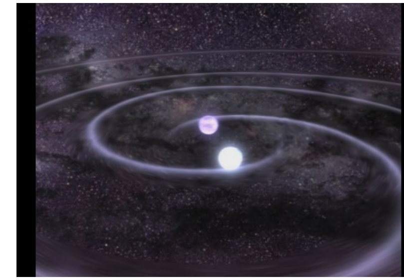
東京大学
THE UNIVERSITY OF TOKYO

r-process nucleosynthesis & nuclear *β* decays

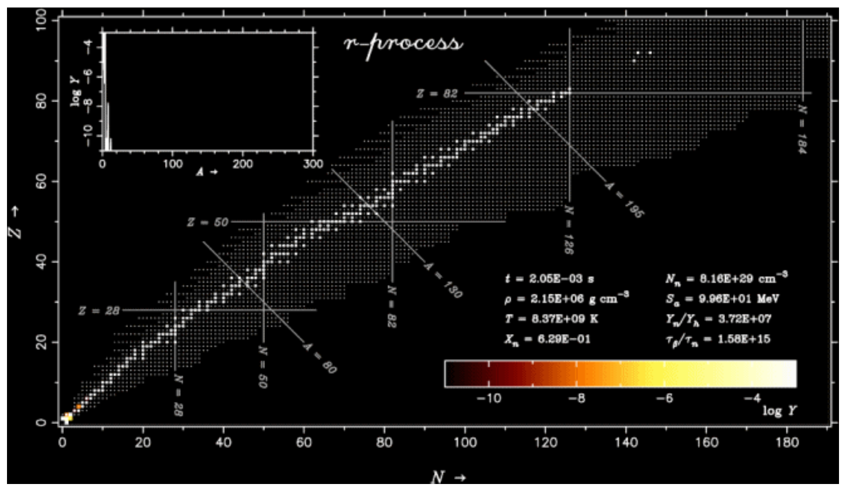
The 11 greatest unanswered questions of physics



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



Rapid neutron-capture process (*r*-process)

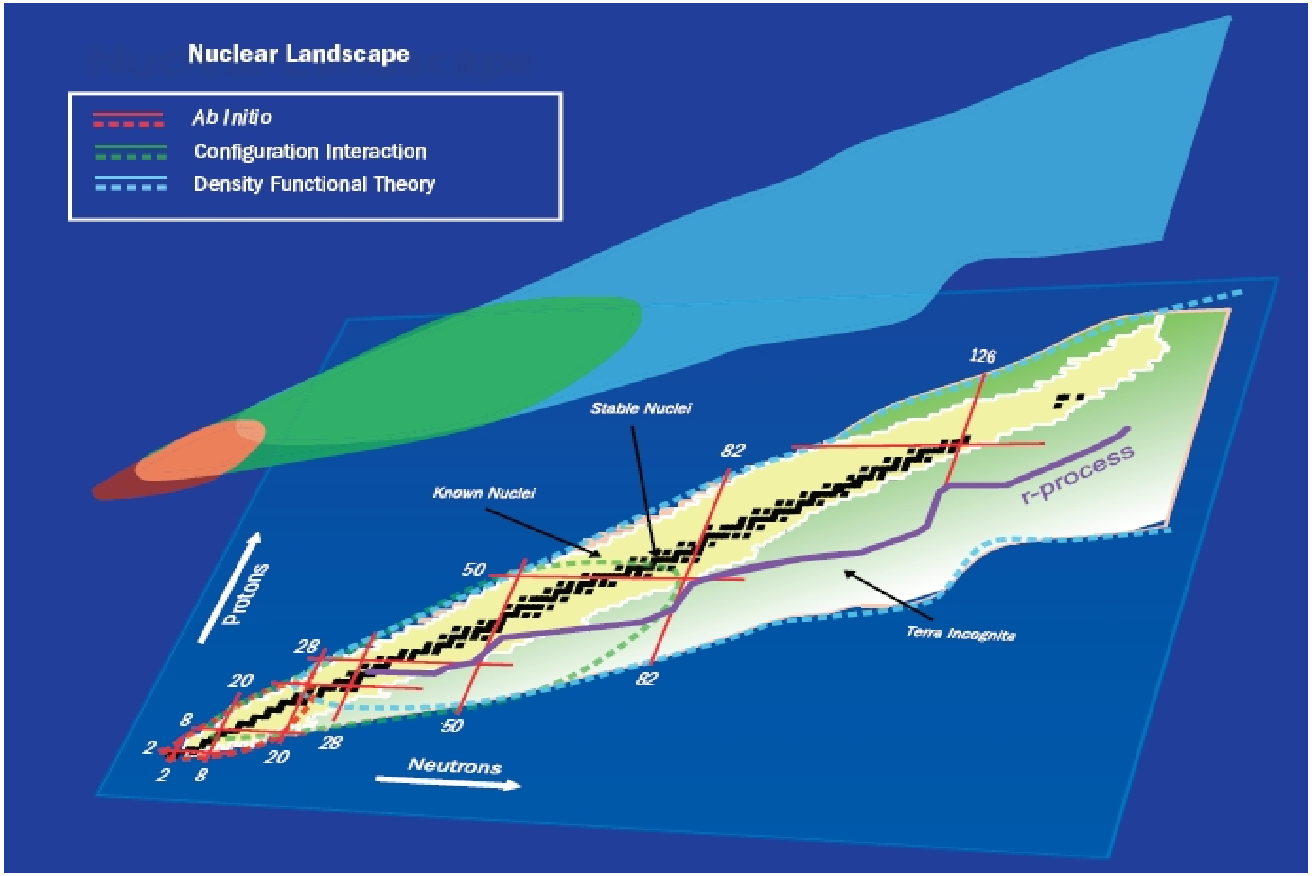


Courtesy of S. Wanajo

- Nuclear masses ➔ **path** of *r*-process
- *β*-decay rates ➔ **timescale** of *r*-process
- *β*-delayed *n*-emission branchings ➔ **final abundance pattern** of *r*-process

Key exp. @ RIKEN

State-of-the-art nuclear methodologies

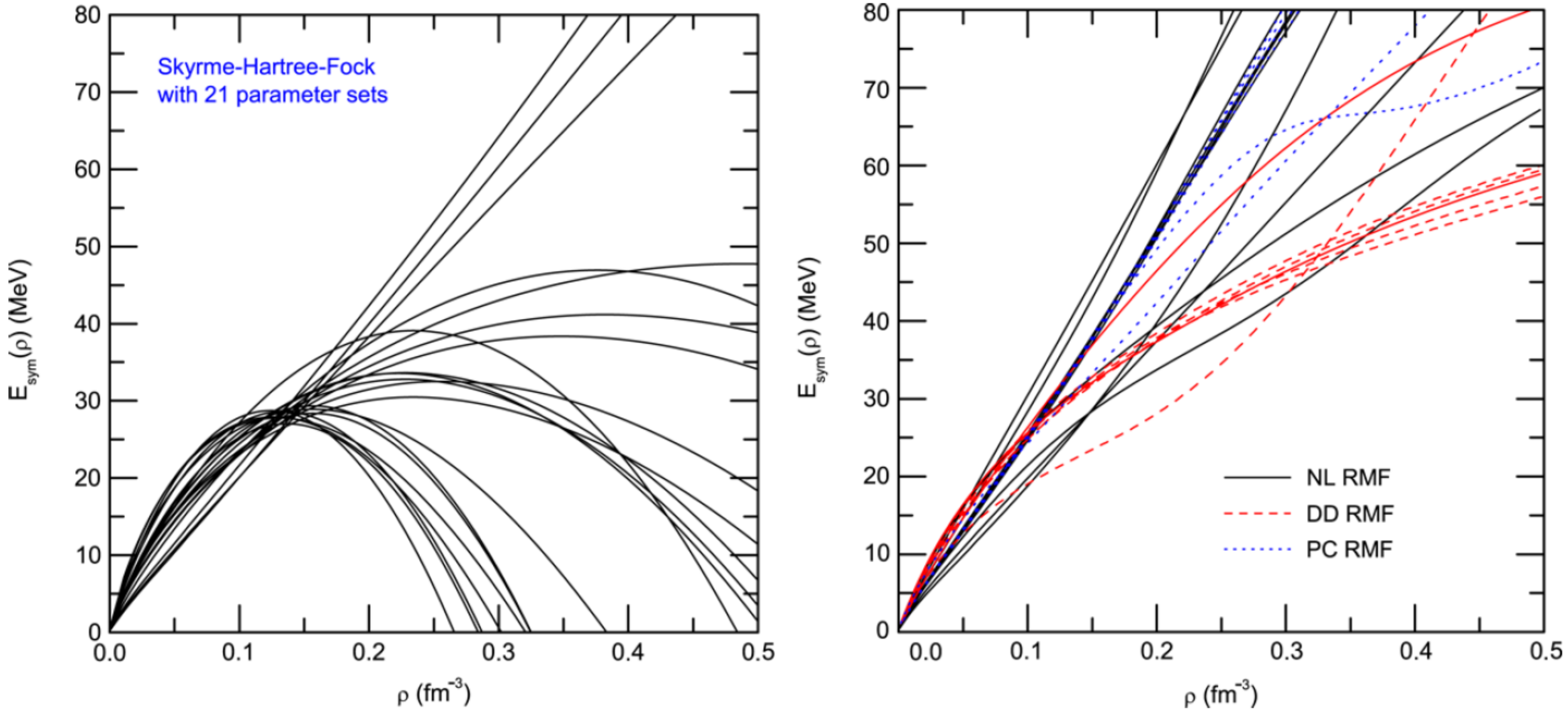


http://www.unedf.org/

- Density functional theory (DFT) aims at understanding <u>both ground-state and excited-state properties</u> of <u>thousands of</u> nuclei in a consistent and predictive way.

Phenomenological energy density functionals

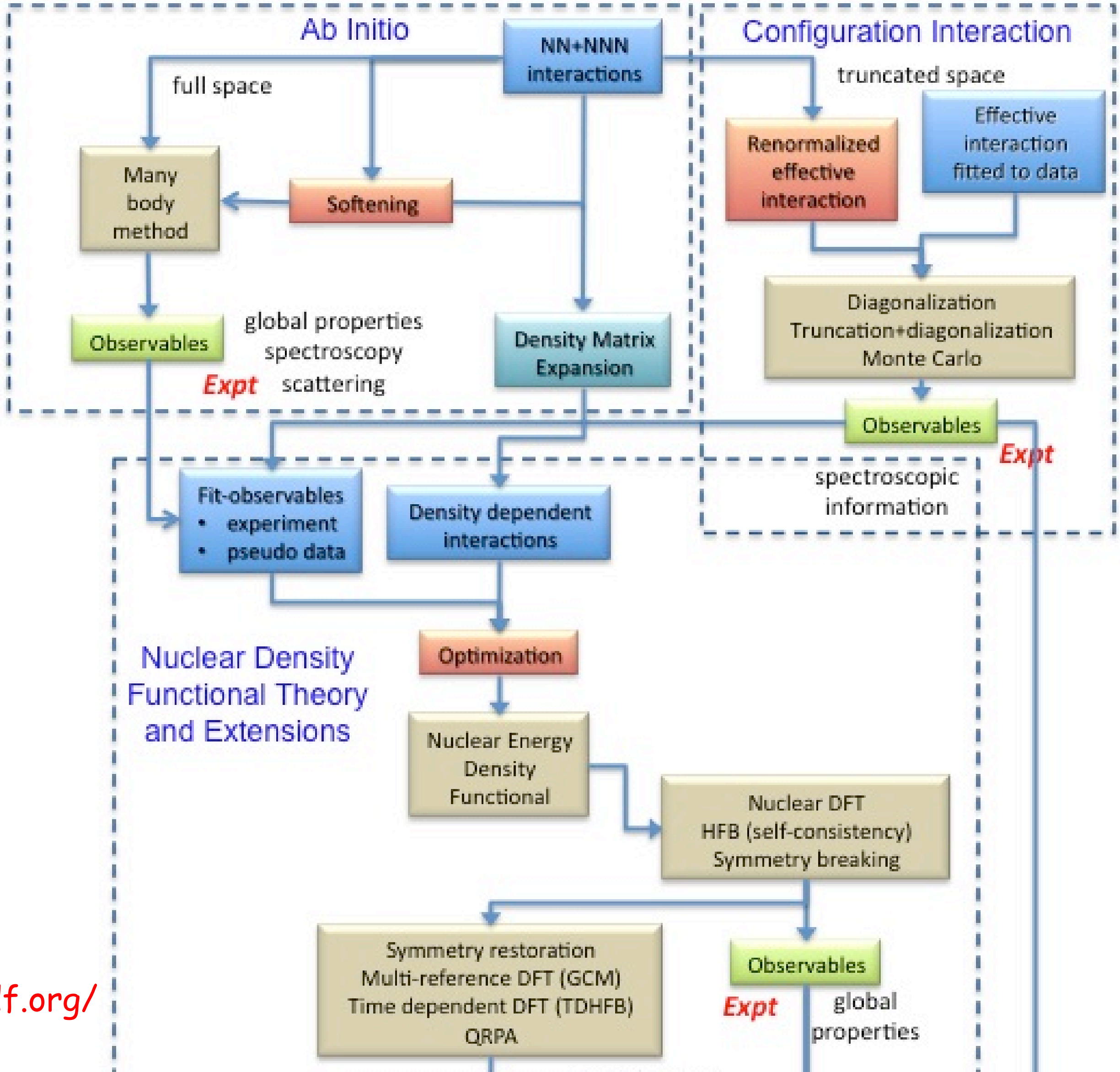
- *Predictions* of phenomenological EDF (~10 years ago)



Li, Chen, Ko, *Phys. Rep.* **464**, 113 (2008)

Possible strategies (I)

- UNEDF



http://www.unedf.org/

A recent review

Progress in Particle and Nuclear Physics 109 (2019) 103713

Contents lists available at ScienceDirect

Progress in Particle and Nuclear Physics

journal homepage: www.elsevier.com/locate/ppnp

Review

Towards an *ab initio* covariant density functional theory for nuclear structure

Shihang Shen [a,b,c], Haozhao Liang [d,e], Wen Hui Long [f,g], Jie Meng [a,h,i,*], Peter Ring [a,j]

53 pages
with 26 figs and 436 references

A dream for new-generation DFT

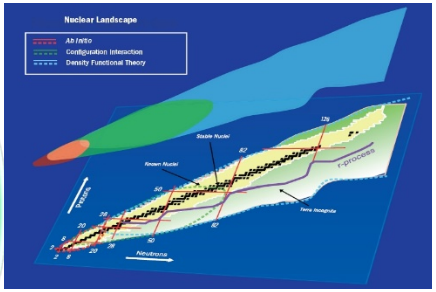
quantum-field-theory oriented DFT

EDF from
effective action
$F_{HK}[\rho] \sim \Gamma[\rho]/\beta$
(Legendre transform)

non-perturbative nature by
renormalization group
$\partial_k \Gamma_k[\rho] = \mathrm{Tr}\{\ldots\}$
(flow eq.)

theoretical uncertainties from **EFT**
$\Gamma^{(2)}, \Gamma^{(3)}, \Gamma^{(4)} \ldots$
(power counting)

Interdisciplinary:
(lattice) QCD
hadron
cold atom
condensed matter
quantum chemistry
……



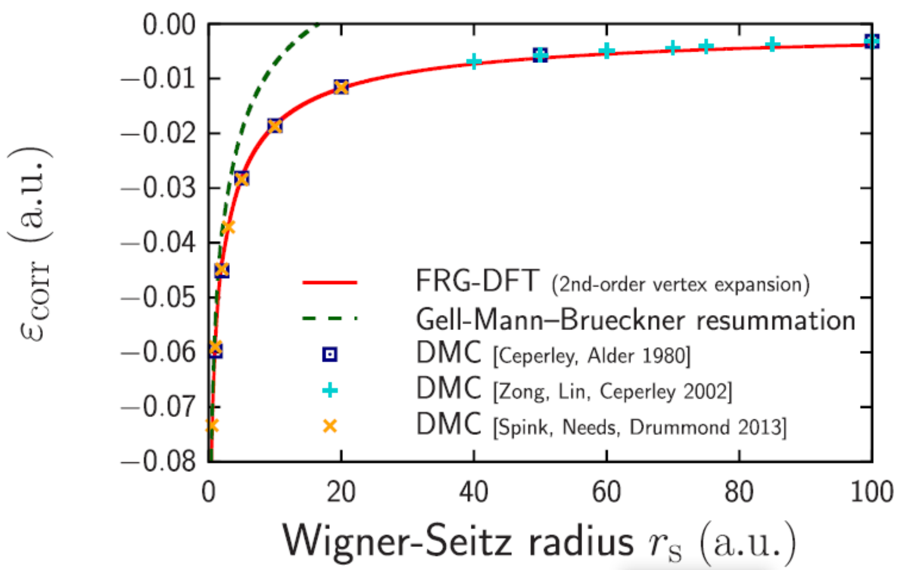
cf. http://www.unedf.org/

IUPAP Young Scientist Prize
@ INPC2016, Australia

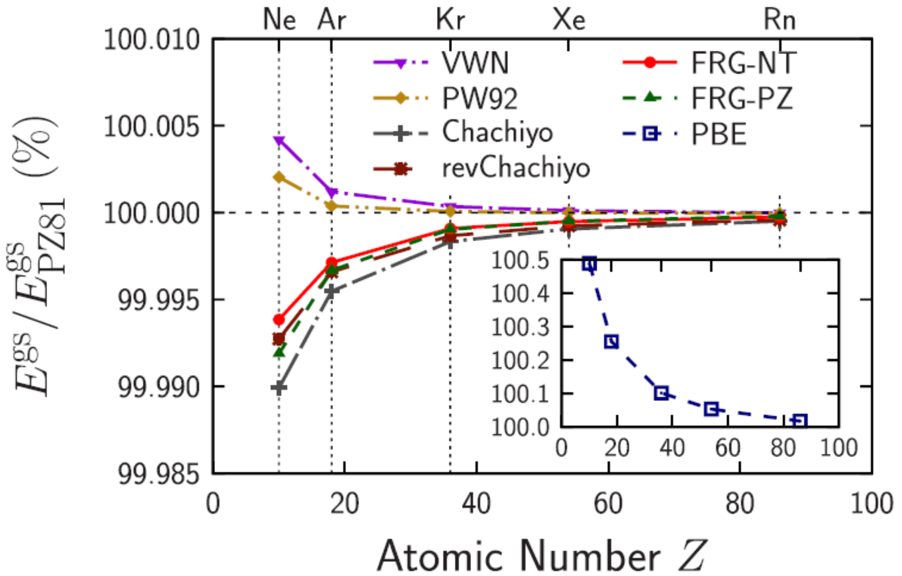
also cf.
Schwenk & Polonyi, arXiv:0403011 [nucl-th]
Kutzelnigg, JMS 768, 163 (2006)
Drut, Furnstahl, Platter, PPNP 64, 120 (2010)
Braun, JPG 39, 033001 (2012)
Metzner et al., RMP 84, 299 (2012)
Drews & Weise, PPNP 93, 69 (2017)
……

Progress in 3D electron systems

- Correlation energy of 3D electron gas



- Ground-state energies of Ne, Ar, Kr, Xe, and Rn atoms



Yokota & Naito, *Phys. Rev. Research* **3**, L012015 (2021).

$$F_{HK}[\rho] = \underline{T_0[\rho] + E_H[\rho] + E_x^{LDA}[\rho] + E_c^{LDA}[\rho]} + E_{xc}^{GGA}[\rho, |\nabla\rho|] + E_{xc}^{Meta-GGA}[\rho, |\nabla\rho|, \nabla^2\rho, \tau] + \cdots$$

ongoing

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*
[4]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
[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 quantum programming

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

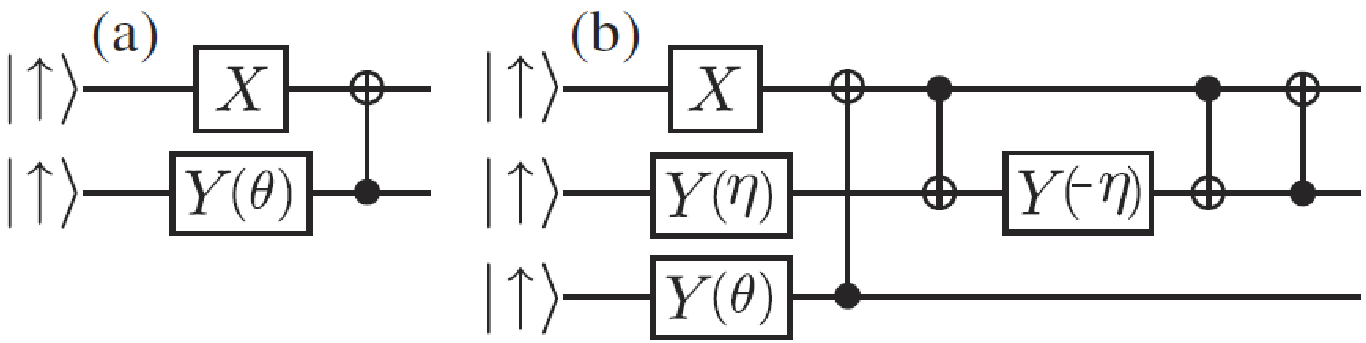
➢ **Variational wave function**

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

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

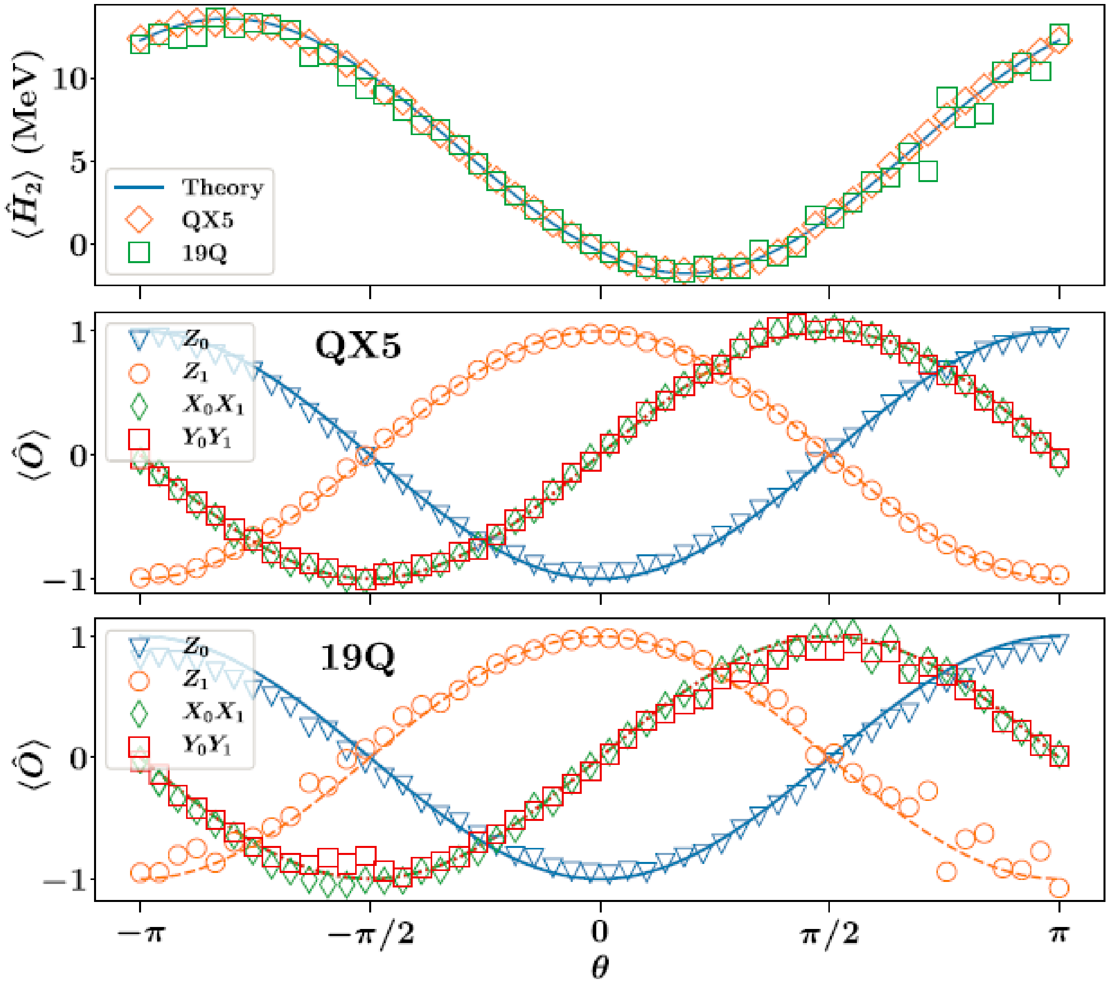
➢ **Computing architectures**

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



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

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

$E_2^{\mathrm{QX5}} = -1.80 \pm 0.05$ MeV
$E_2^{\mathrm{19Q}} = -1.72 \pm 0.03$ MeV
thus
$E_2 = -1.74 \pm 0.03$ MeV

- Experimentally determined energies for H_2

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

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

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

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)

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

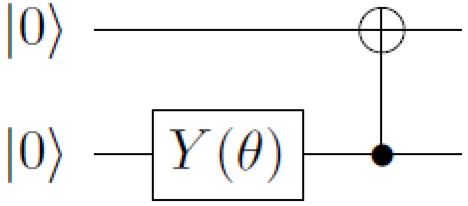
- **Qubit representation of Lipkin Hamiltonian ($W = 0$)**

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

- 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.

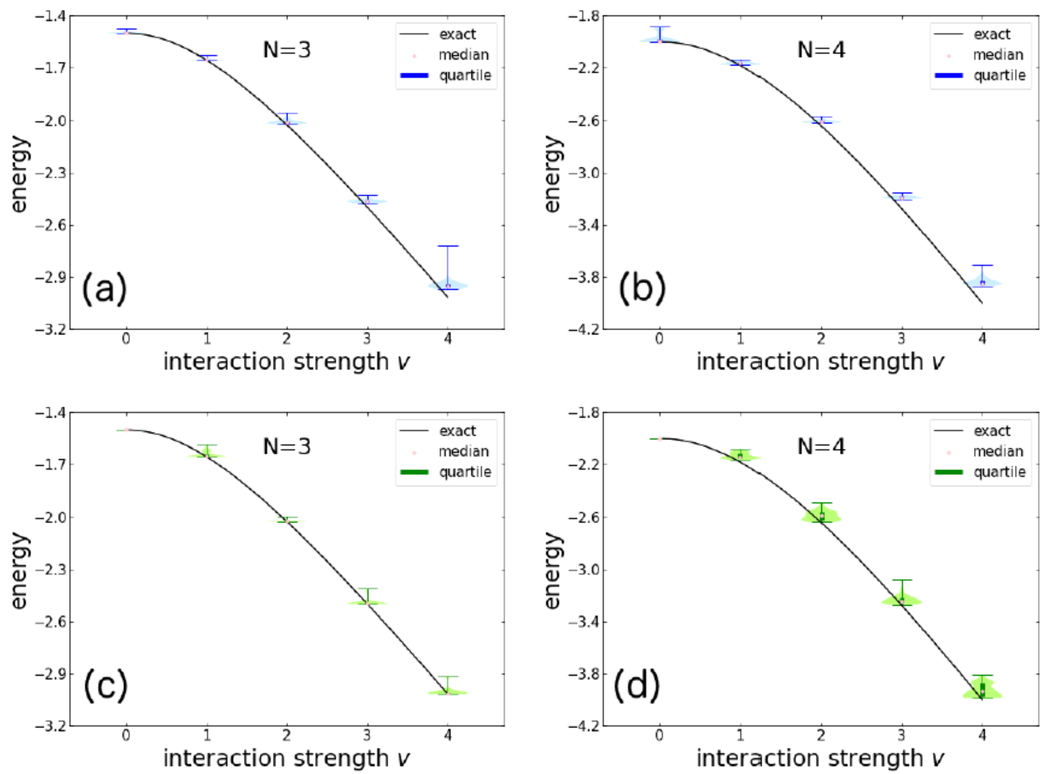
UCC and structure learning ansatz

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



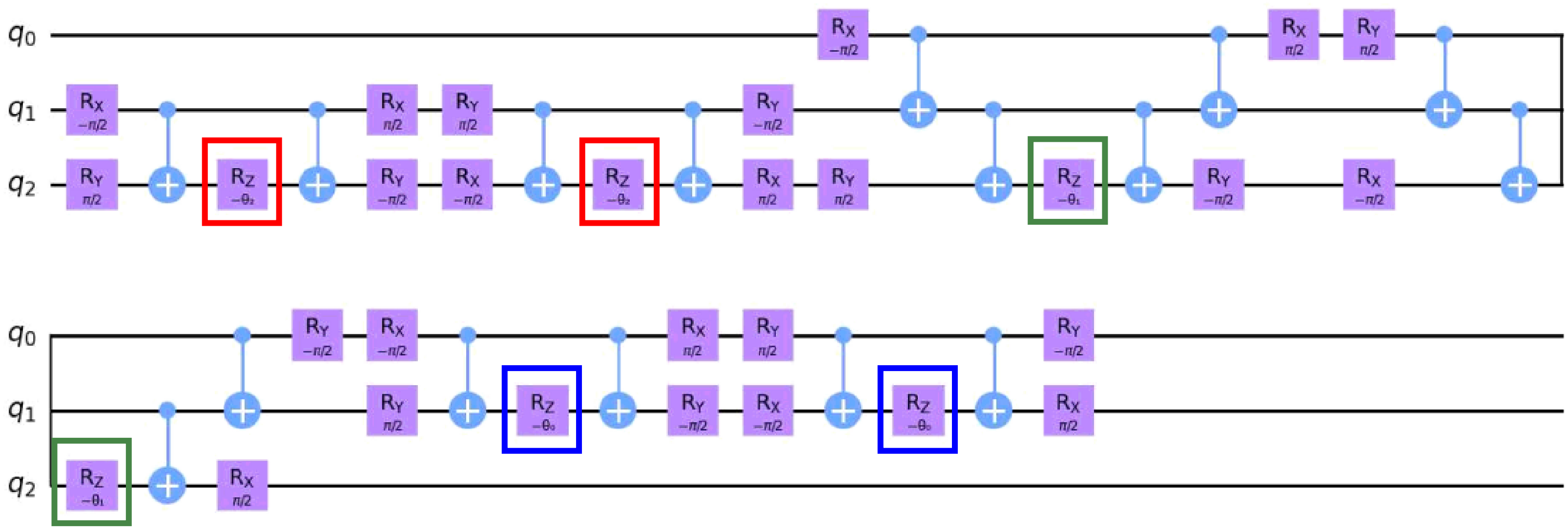
UCC ansatz

- **Trial wave functions**

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

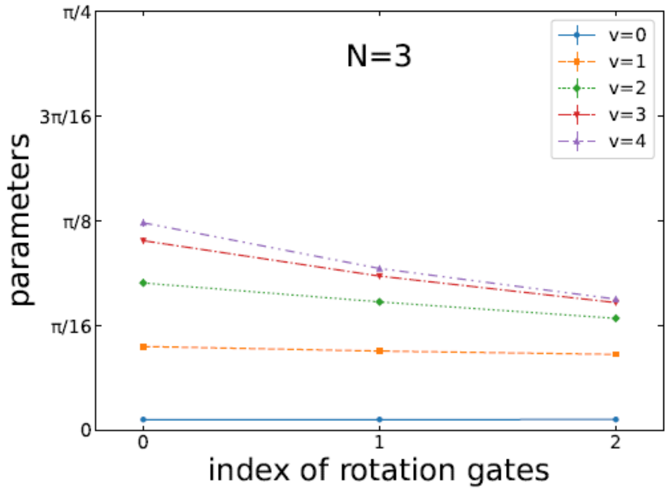
$$U(\theta) \equiv \exp\left[\sum_{ij} \theta_{ij}(a_i^\dagger a_j^\dagger - a_j a_i)\right]$$
$$\mapsto \exp\left\{ i \sum_{ij} \theta_{ij} \frac{(-1)^{j-i-1}}{2} \left[X_i \left(\prod_{k=i+1}^{j-1} Z_k \right) Y_j + Y_i \left(\prod_{k=i+1}^{j-1} Z_k \right) X_j \right] \right\},$$

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

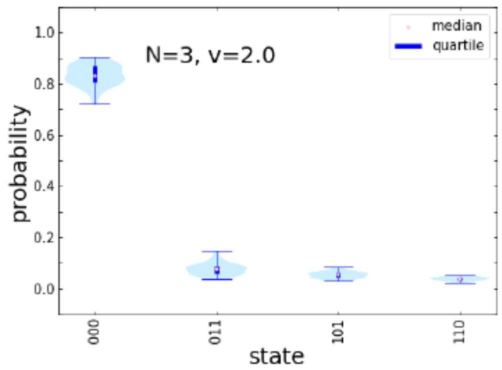


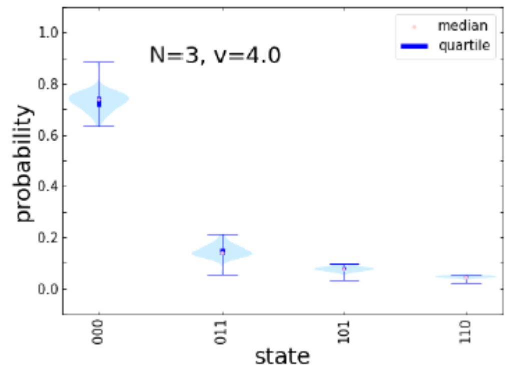
UCC ansatz (N=3)

- Parameters

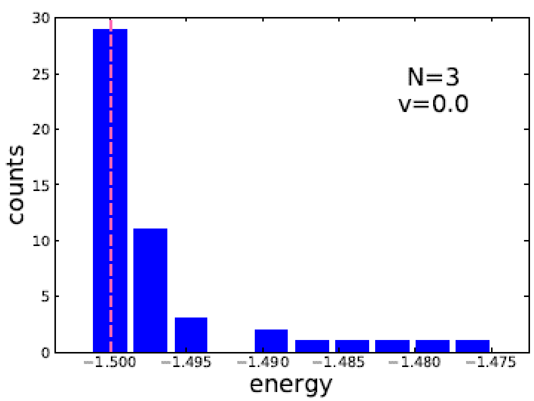


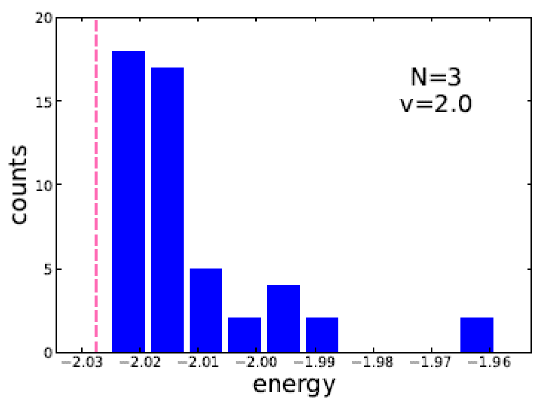
- State probabilities

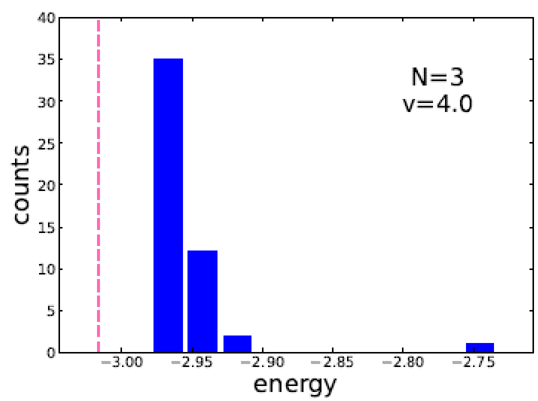




- Ground-state energies



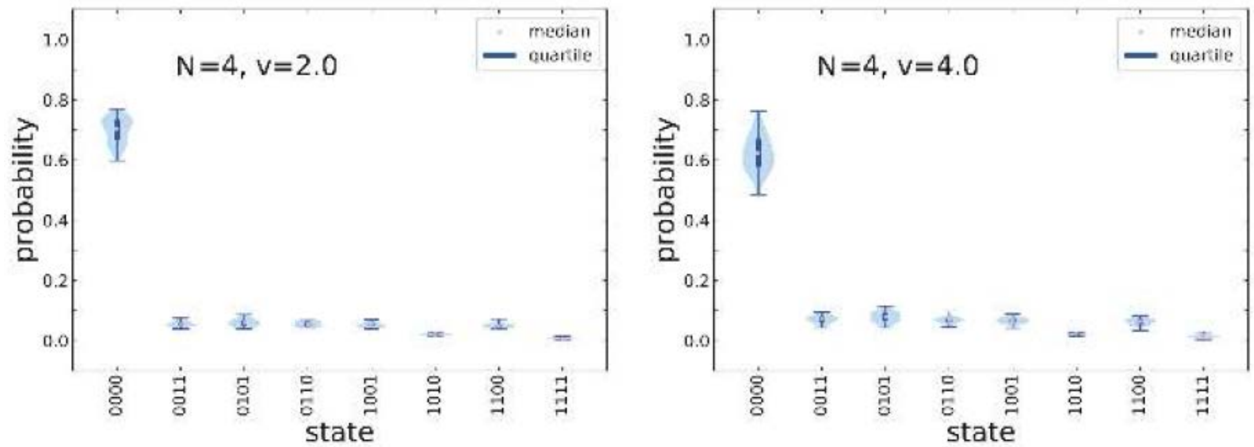




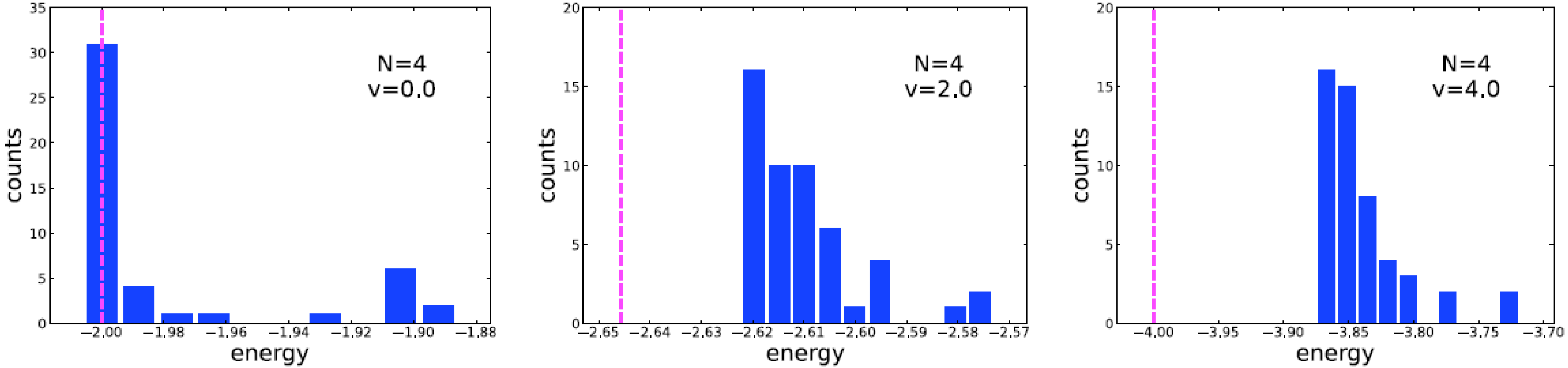
Chikaoka and HZL, *Chin. Phys. C* **46**, 024106 (2022)

UCC ansatz (N=4)

- 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.

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

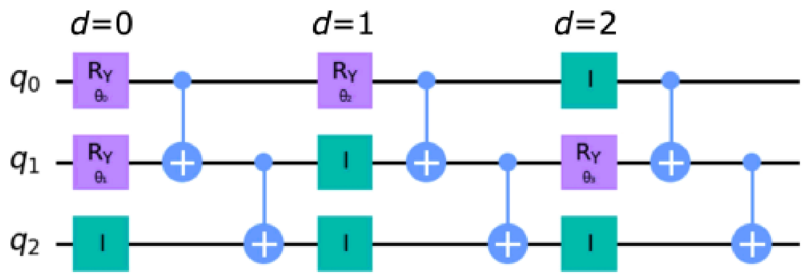
    $\theta_d \leftarrow \theta^*_{d,H_d}$, where θ^*_{d,H_d} is the optimized parameter with the selected gate H_d

  end for

until stopping criterion is met

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

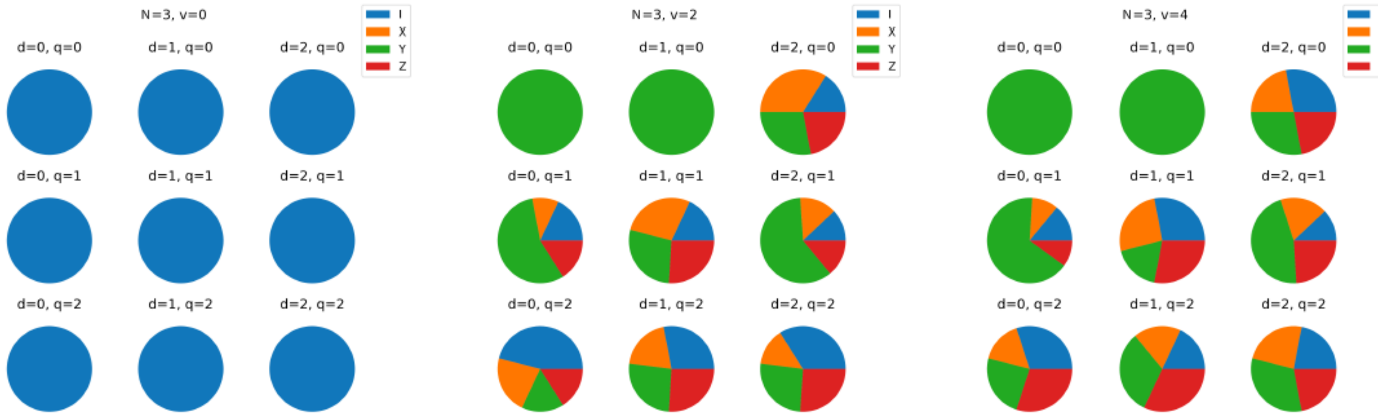
- Quantum circuit ($N = 3$)
(an example)



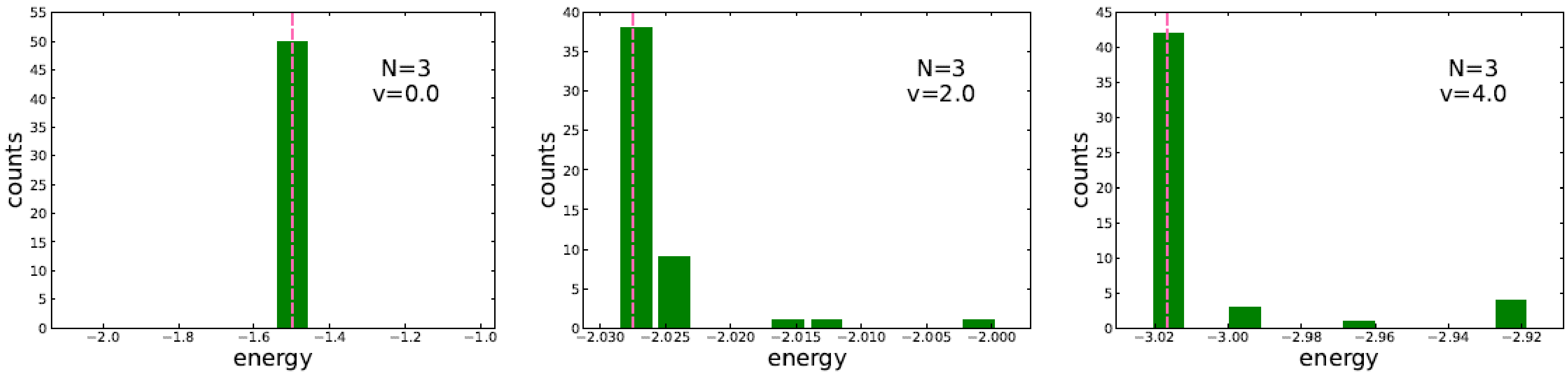
Structure learning ansatz (N=3)

- Rotating axes

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



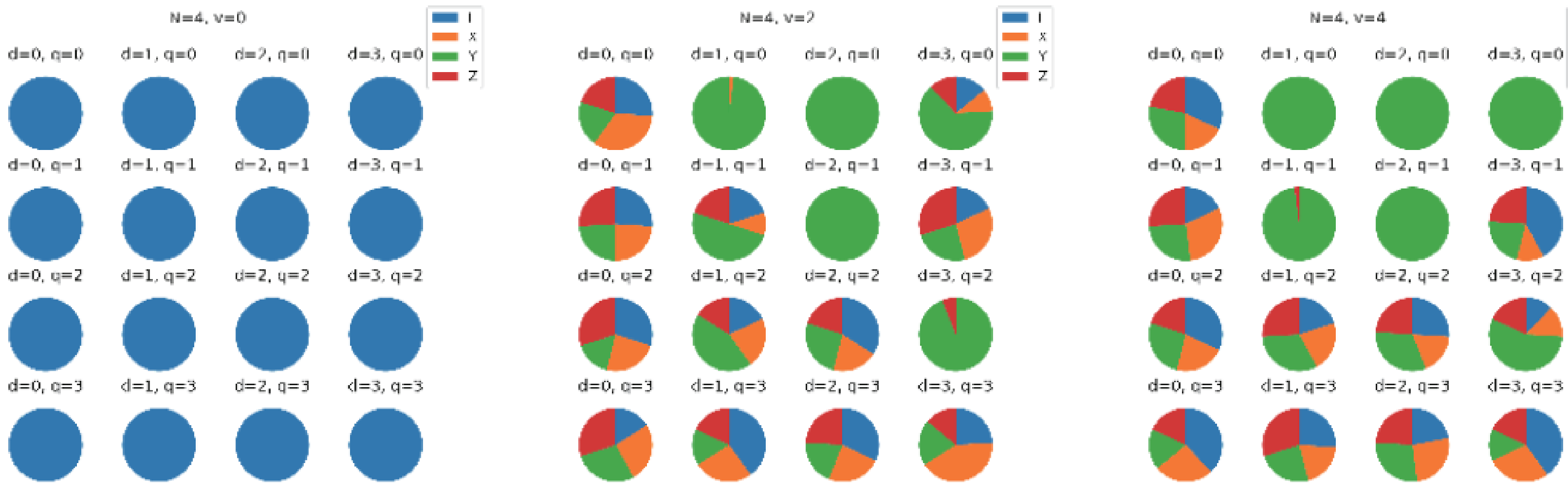
- Ground-state energies



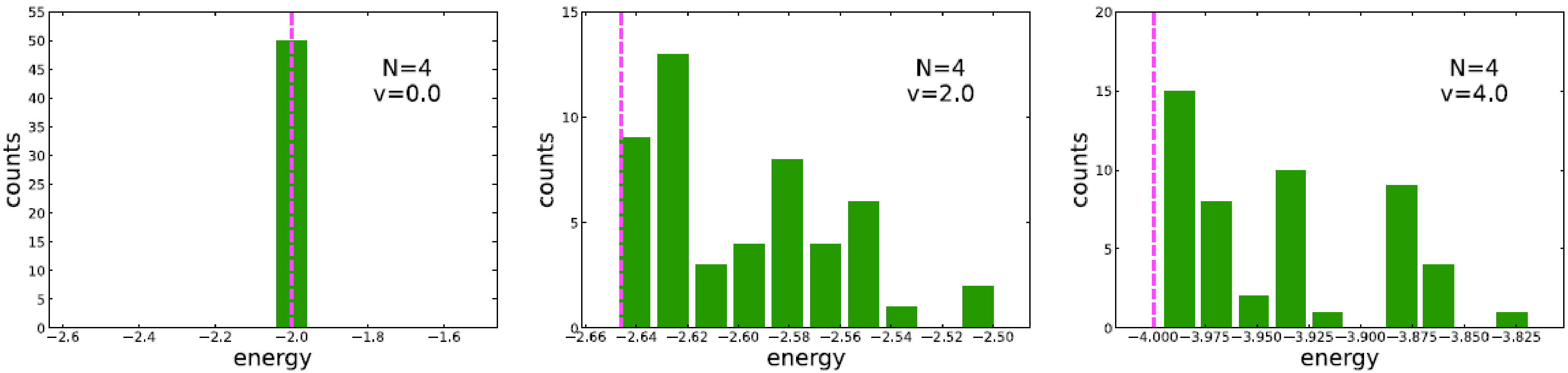
Structure learning ansatz (N=4)

- Rotating axes

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

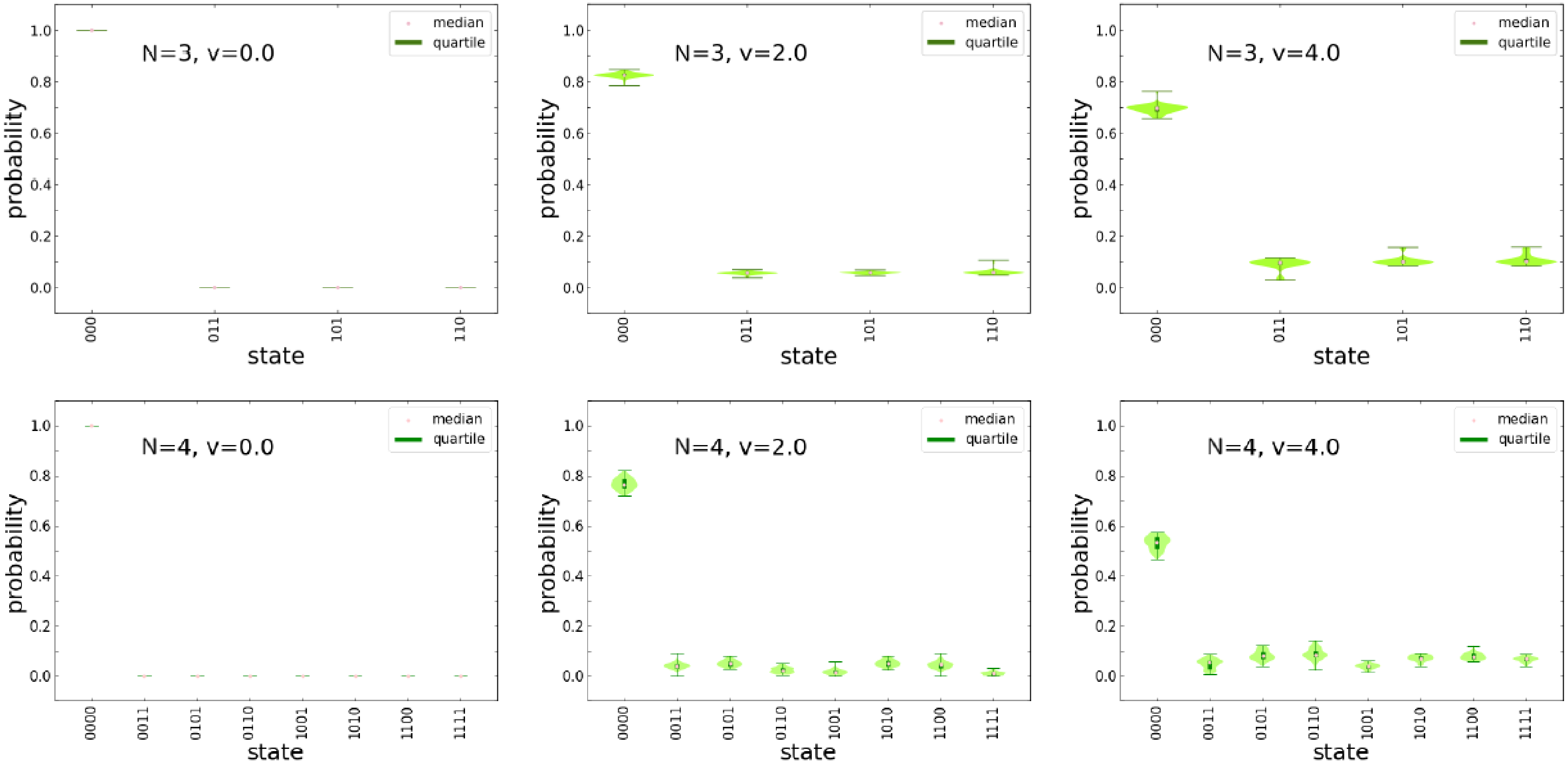


- Ground-state energies



Structure learning ansatz

- State probabilities



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

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

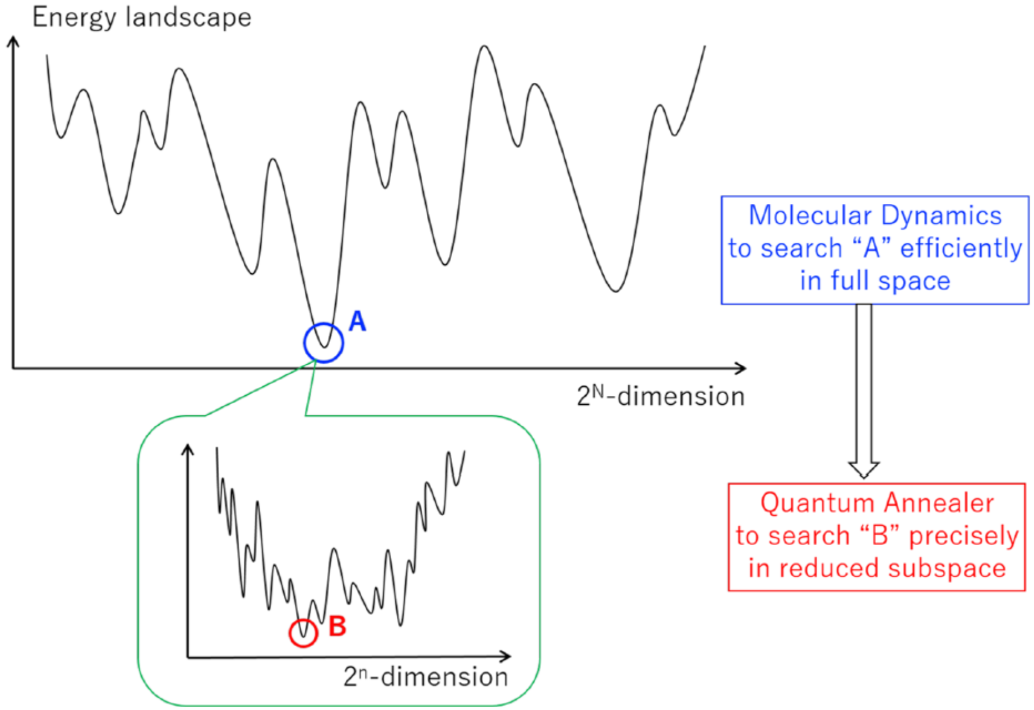


Figure 1. Concept of hybrid quantum annealing via molecular dynamics.

Quantum computing for nuclear physics

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

Solving the Lipkin model using quantum computers with two qubits only with a hybrid quantum-classical technique based on the generator coordinate method

Yann Beaujeault-Taudière and Denis Lacroix
Phys. Rev. C **109**, 024327 – Published 27 February 2024

Quantum simulation approach to implementing nuclear density functional theory via imaginary time evolution

Yang Hong Li, Jim Al-Khalili, and Paul Stevenson
Phys. Rev. C **109**, 044322 – Published 18 April 2024

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/