NUCLEAR PHYSICS APPLICATIONS **OF QUANTUM SIMULATION**

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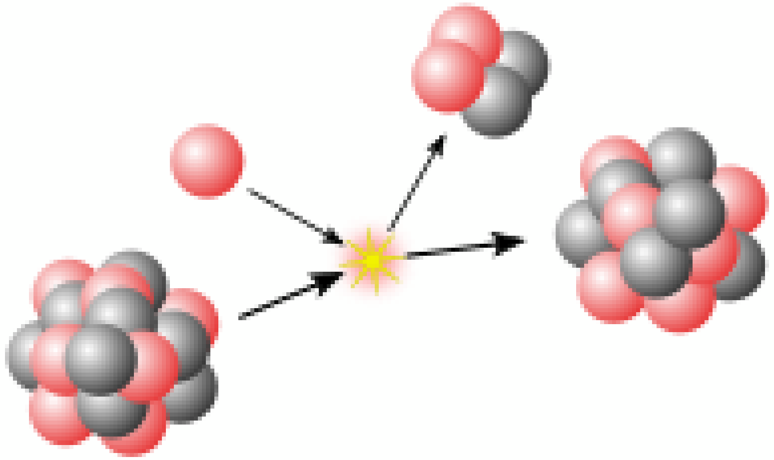
NUCLEI AS A SYSTEM OF SPIN-1/2 FERMIONS

The atomic nucleus is a system of interacting protons and neutrons: each a spin-1/2 fermion

Protons and neutrons themselves can be considered as two states of isospin-1/2 nucleon

Both nuclear spin and isospin can be mapped to qubit 2-dimensional Hilbert space



$^{15}N + p \rightarrow {}^{12}C + {}^{4}He + 4.96$ MeV
Part of CNO cycle. Pic from Wikipedia

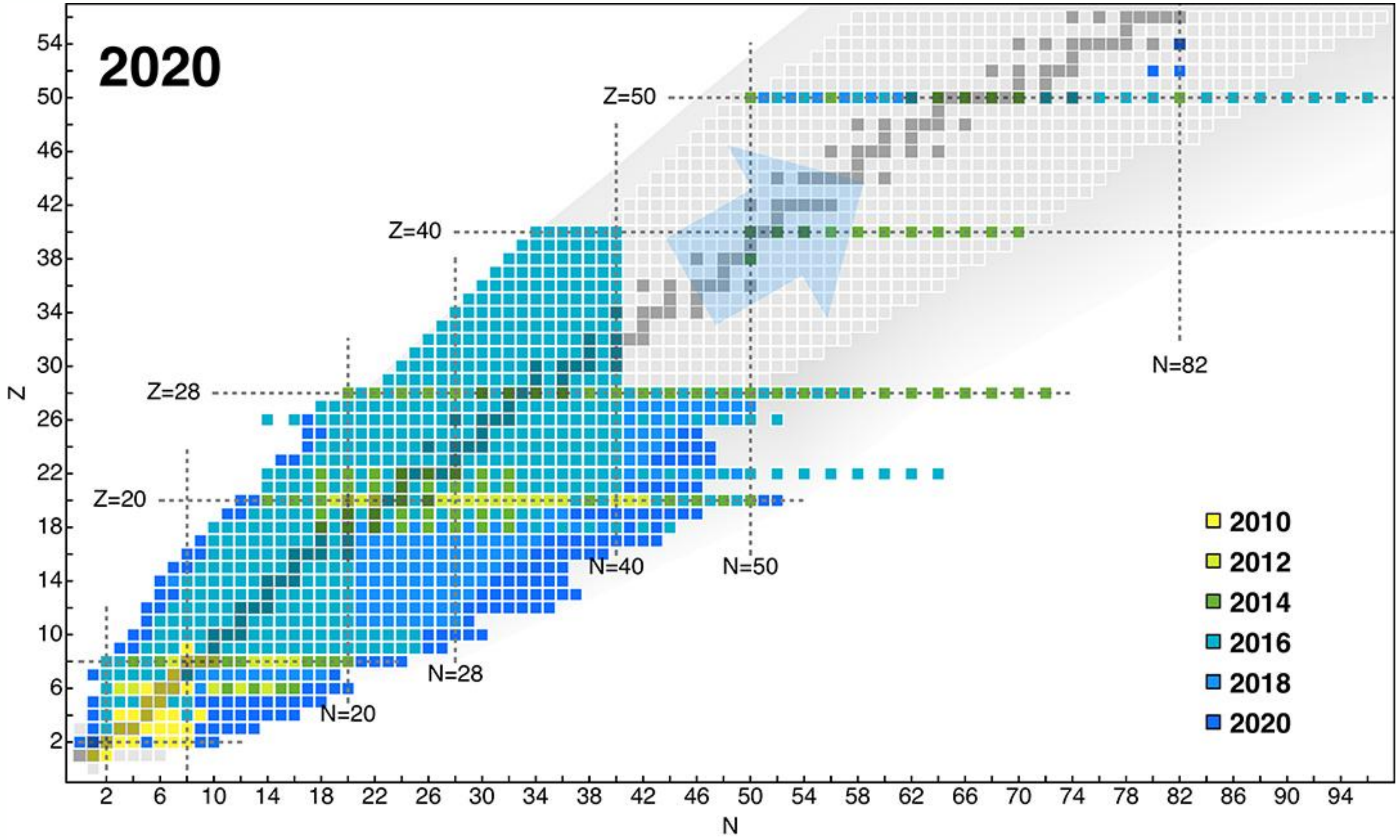
Nuclei are subject to strong nuclear, weak nuclear and electromagnetic forces: combination of very short range, and longer-range interactions; nuclear force has (at least) 3-body parts; particular symmetries exhibited (and broken); radioactive decay

Complex systems of interacting particles showing emergent behaviour, existing in close proximity to the continuum

Each nucleus has its own structure, and reactions between nuclei & other probes are of interest

“EXACT” SOLUTIONS

- Many-body Schrödinger equation becomes difficult to solve when number of nucleons gets large:
  - Hilbert space grows exponentially
  - Approximation methods to simplify many-body theory and/or complex interactions usually used
  - Wave functions entangled- take care with approx. methods
- So-called “ab initio” methods are closest to exact solutions – much progress with HPC but limited to lower parts of nuclear chart

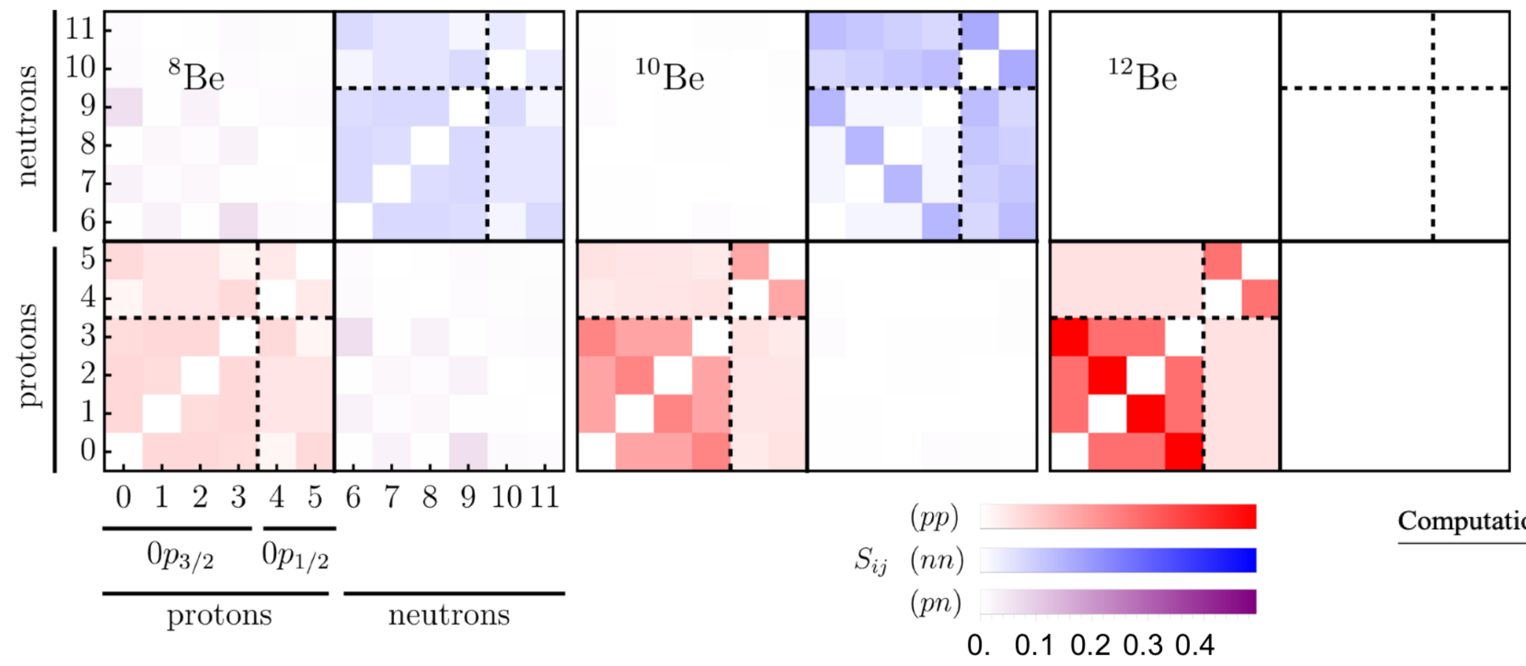


From H. Hergert, *Frontiers in Physics 8 (2020) 00379; showing some structure calculation with 2-body forces*

ENTANGLEMENT

A. Pérez-Obiol[1,a], S. Masot-Llima[1,b], A. M. Romero[2,3,c], J. Menéndez[2,3,d], A. Rios[2,3,e], A. García-Sáez[1,4,f], B. Juliá-Díaz[2,3,g]

240 Page 8 of 15 Eur. Phys. J. A (2023) 59:240



Computational Science & Discovery **1** (2008) 015008 D J Dean *et al*

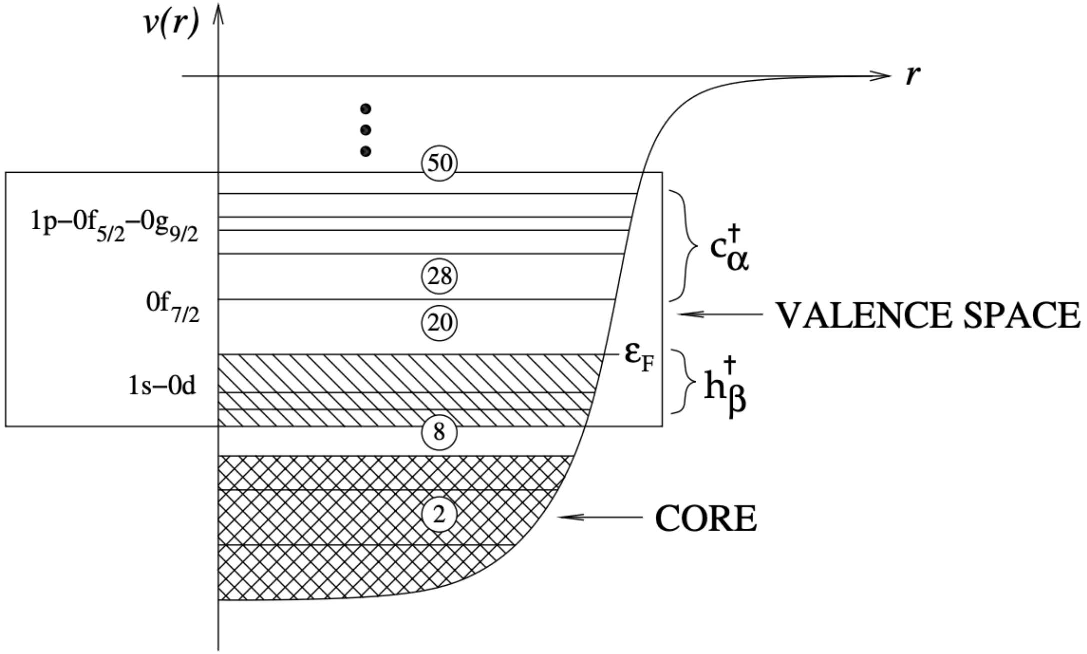
Table 1. Shell-model dimensions (single-particle product selected light nuclei.

Nucleus	Four major shells	Seven major shells
^{4}He	4×10^4	9×10^6
^{8}B	4×10^8	5×10^{13}
^{12}C	6×10^{11}	4×10^{19}
^{16}O	3×10^{14}	9×10^{24}

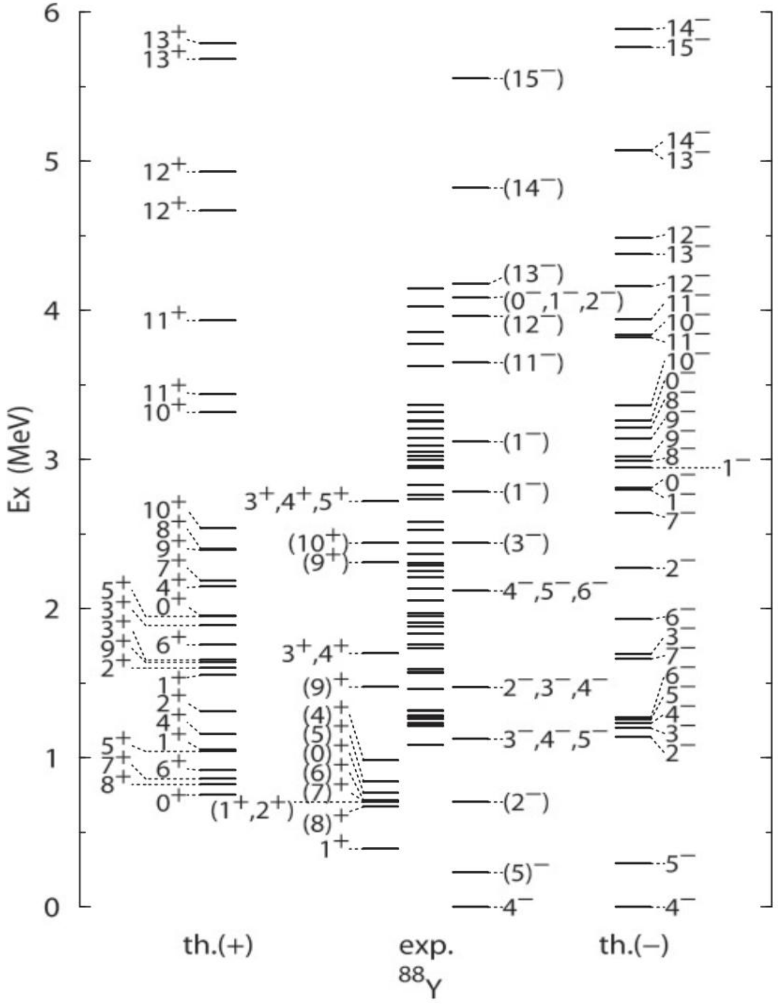
Growth of Hilbert Space

SHELL-MODEL

The archetype of many-body theories. Aka “configuration interaction”. Mayer + Jensen Nobel Prize 1963



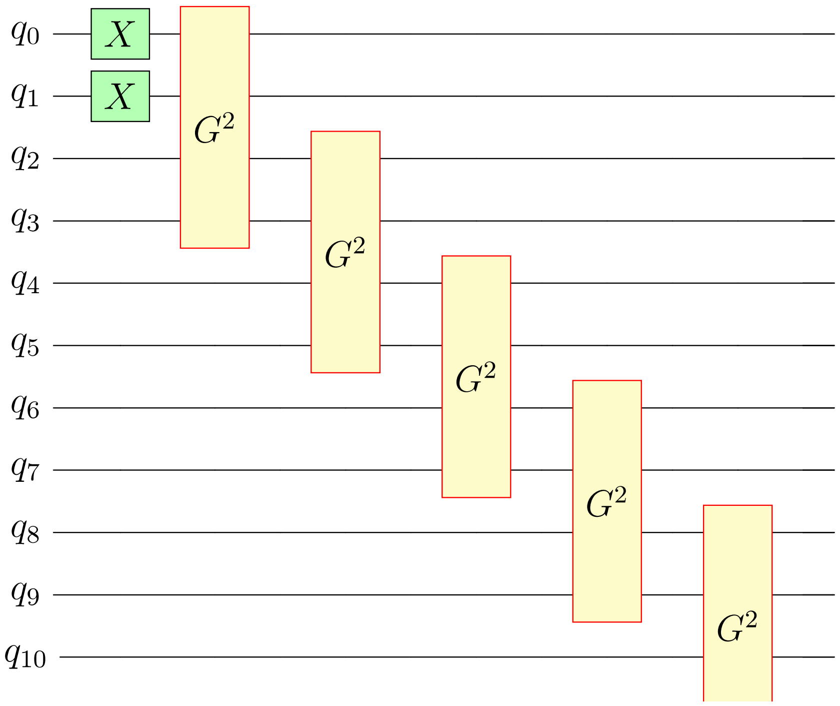
Suhonon, *From Nucleons to Nucleus, Springer Verlag*



Honma et al Phys. Rev. C80, 064323 (2009)

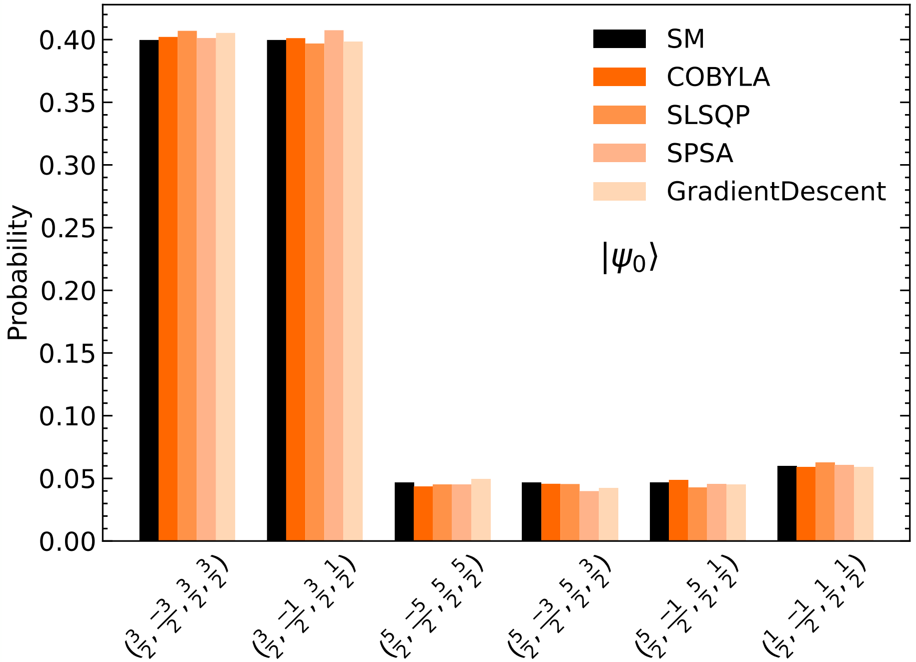
SHELL MODEL: NI-58

"Shell-model study of ^{58}Ni using quantum computing algorithm", Bharti Bhoy and Paul Stevenson, [New Journal of Physics 26, 075001 (2024)](), [arxiv:2402.15577]()



Quantum-classical hybrid VQE with tailored ansatz

JW transformation in "m-scheme"



State	No. parameters	2-qubit	1-qubit	Depth
G.S.	5	70	72	96
1^{st} e.s.	7	82	78	108
2^{nd} e.s.	1	4	4	7

Qubit(α)	0	1	2	3	4	5	6	7	8	9	10	11
n	1	1	1	1	0	0	0	0	0	0	1	1
l	1	1	1	1	3	3	3	3	3	3	1	1
j	3/2	3/2	3/2	3/2	5/2	5/2	5/2	5/2	5/2	5/2	1/2	1/2
m_α	$-3/2$	$3/2$	$-1/2$	$1/2$	$-5/2$	$5/2$	$-3/2$	$3/2$	$-1/2$	$1/2$	$-1/2$	$1/2$

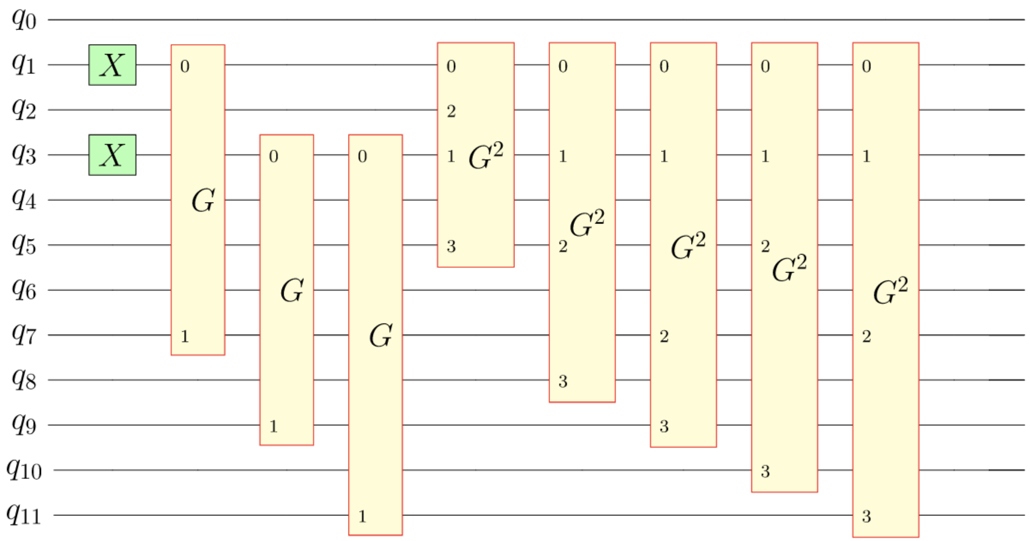
Cf Perez-Obiol et al., Scientific Reports 13, 12291 (2023)

^{42}Ca	9	10^{-8}	116 (304)

~1000 gates

EXCITED STATES

Ansatz using domain knowledge / symmetry, but optimizer has difficulty finding global minimum



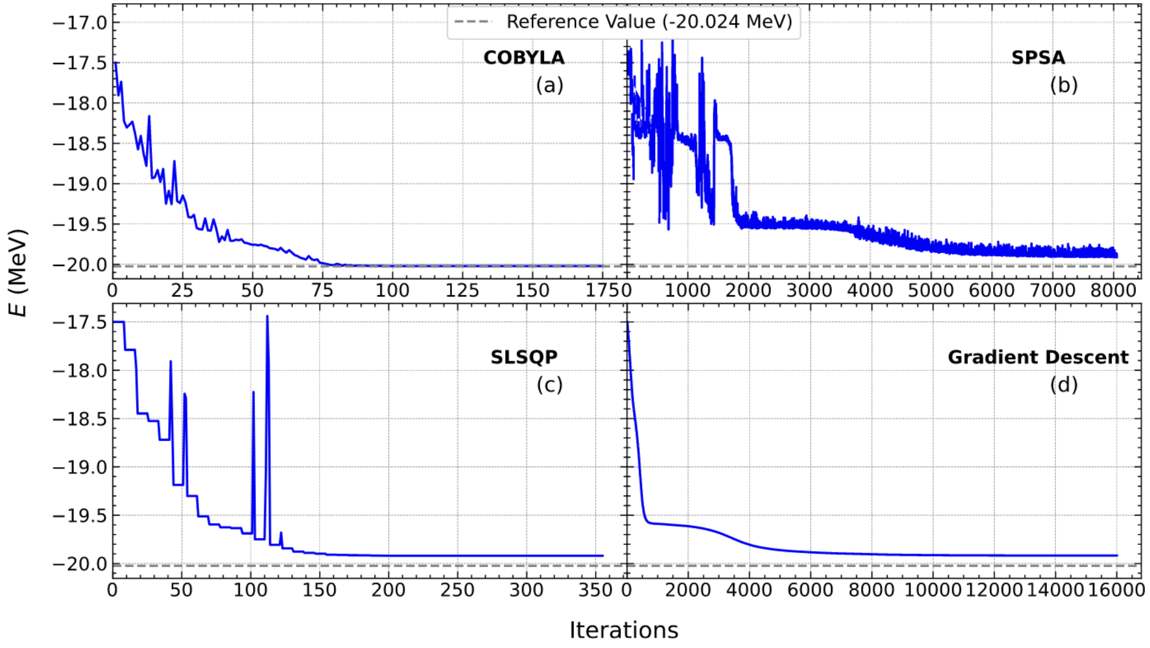


Figure 6. Different optimizers convergence results for 12 Qubit 2^+ ground state.

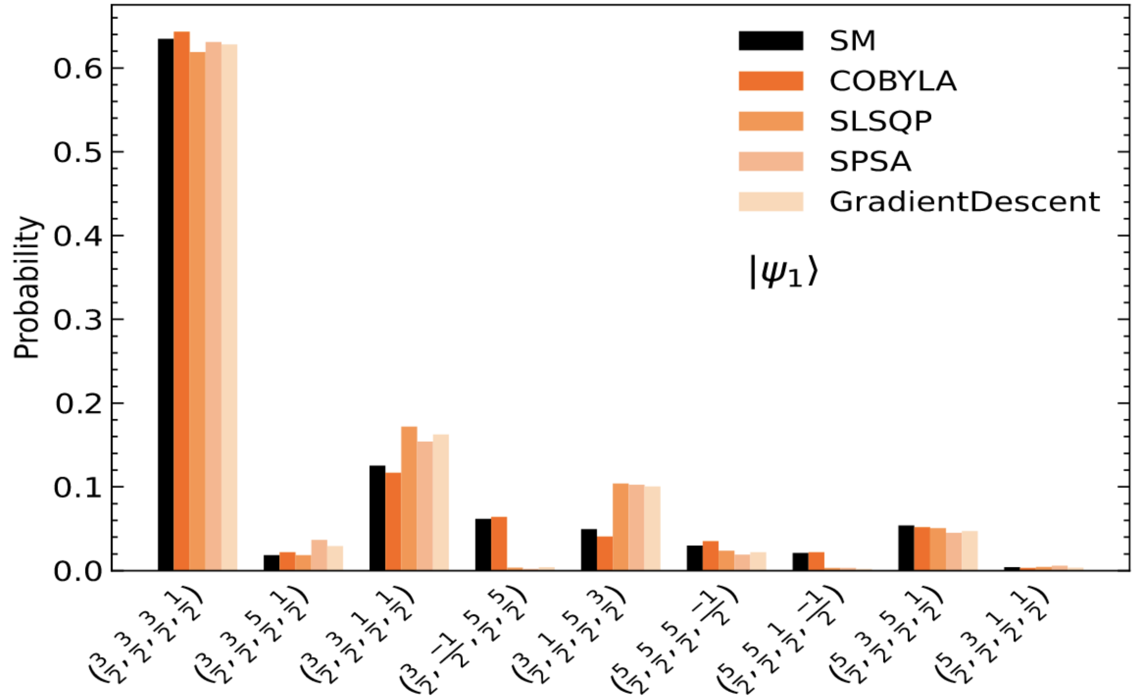


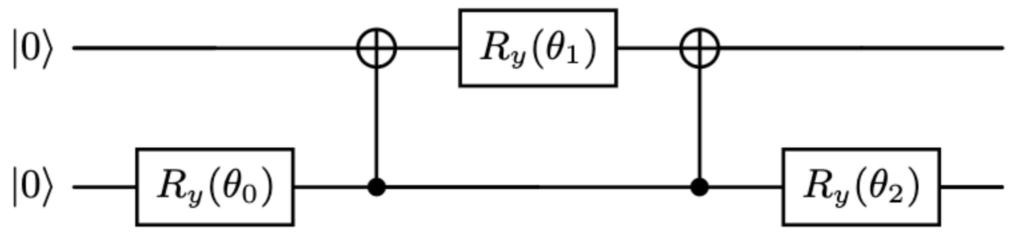
Figure 7. Components of the first excited state wave-function with different optimizers in comparison with the shell model (SM). The x-axis labels represent $(j_1, m_{\alpha_1}, j_2, m_{\alpha_2})$ and $(m_{\alpha_1} + m_{\alpha_2}) = 2$.

VARIANCE MINIMIZATION AS ALTERNATIVE VQA

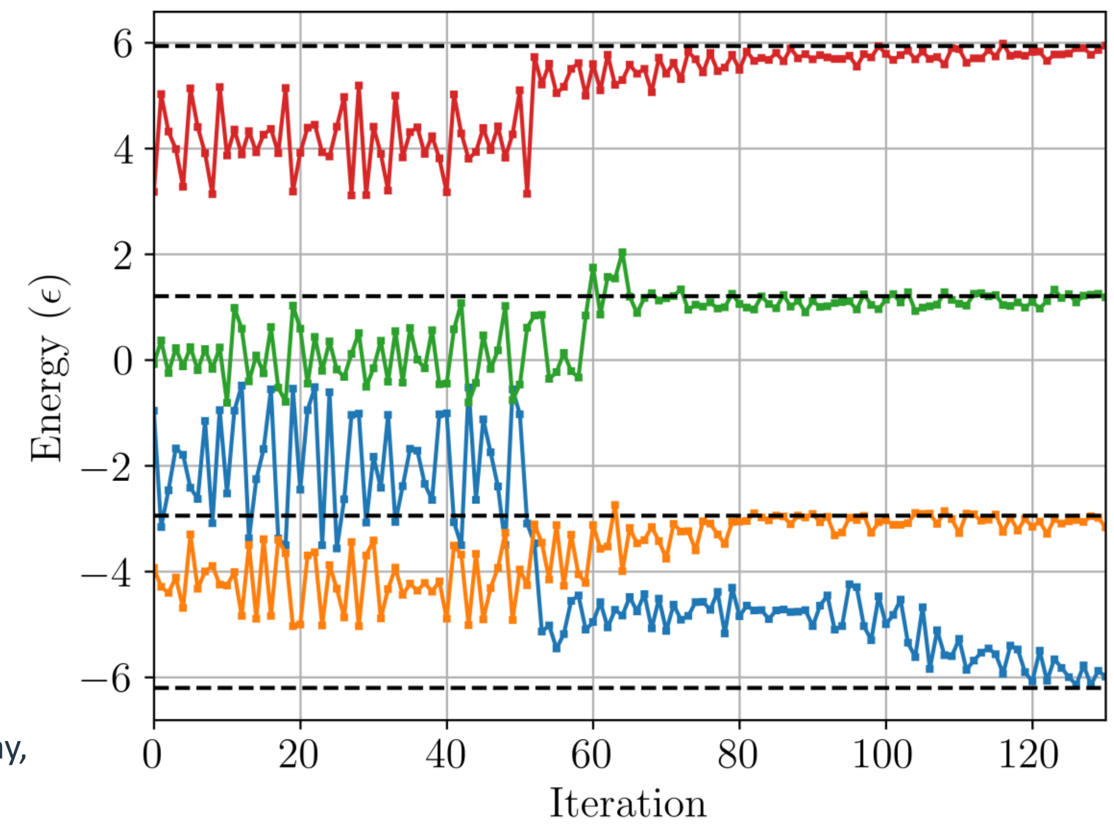
Variational Quantum Eigensolvers are a workhorse quantum computing method for current noisy quantum computers. Classical optimizer asks quantum computer to evaluate some expectation values of Pauli-decomposed Hamiltonian.

Simple extension: Minimize variance, not energy:

$$\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2.$$



IBM_Nairobi real QC results



LMG model

"*Quantum Computing Calculations for Nuclear Structure and Nuclear Data*", Isaac Hobday, Paul. D. Stevenson, and James Benstead, Proc. SPIE 12133, Quantum Technologies 2022, 121330J (2022) arxiv: 2205.05576

"*Variance minimisation on a quantum computer of the Lipkin-Meshkov-Glick model with three particles*", Isaac Hobday, Paul Stevenson, and James Benstead, EPJ Web of Conferences 284, 16002 (2023) arxiv: 2209.07820

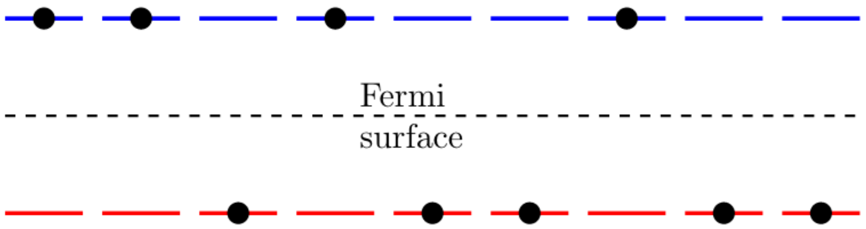
"*Variance Minimisation of the Lipkin-Meshkov-Glick Model on a Quantum Computer*", I. Hobday, P. Stevenson, and J. Benstead, submitted to Phys Rev C, arxiv:2403.08625

VARIANCE-VARIATIONAL-QITE

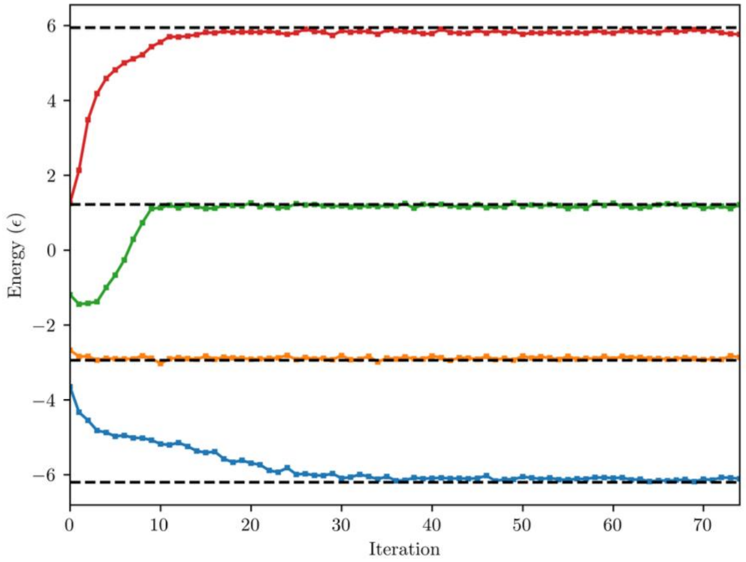
I. Hobday, PhD thesis, University of Surrey (2025)
LMG toy shell model (Lipkin, Meshkov, Glick, Nucl. Phys. 62, 188 (1965)

Based on “VarQITE” for ground states, Xiao Yuan et al., Quantum 3, 191 (2019)

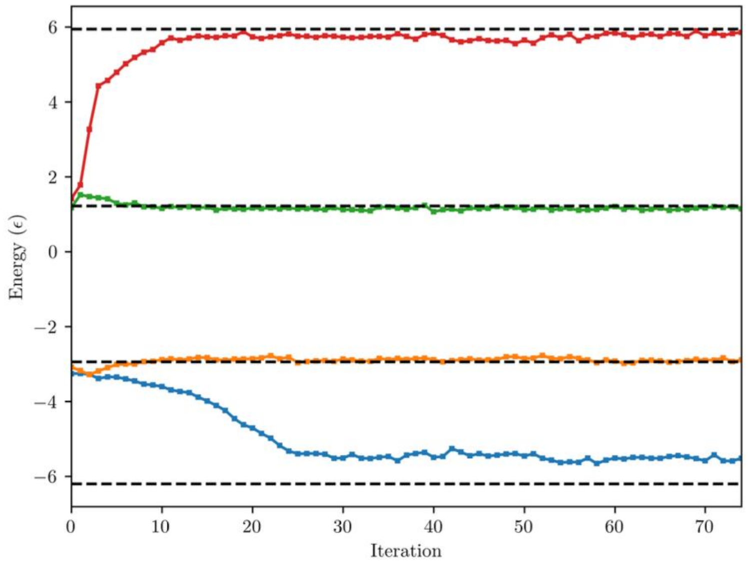
$$H = \tfrac{1}{2}\varepsilon \sum_{p\sigma} \sigma a^{\dagger}_{p\sigma} a_{p\sigma} + \tfrac{1}{2}V \sum_{pp'\sigma} a^{\dagger}_{p\sigma} a^{\dagger}_{p'\sigma} a_{p'-\sigma} a_{p-\sigma}$$



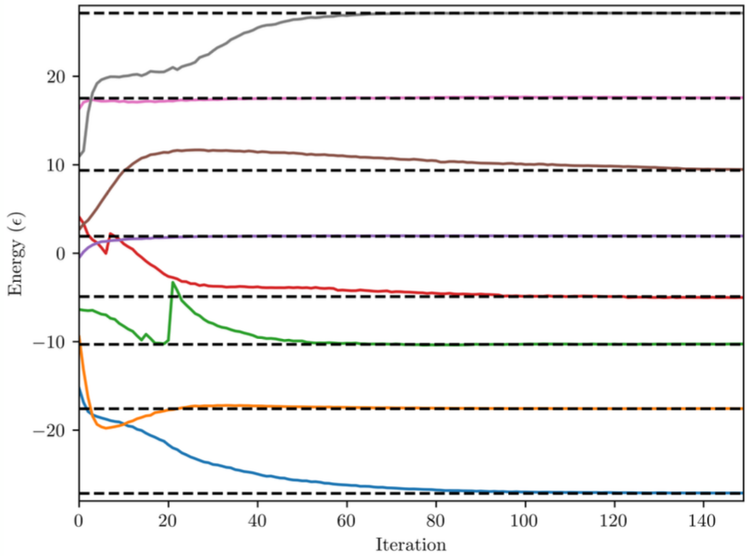
N=7 simulated IBM_Nairobi noise model



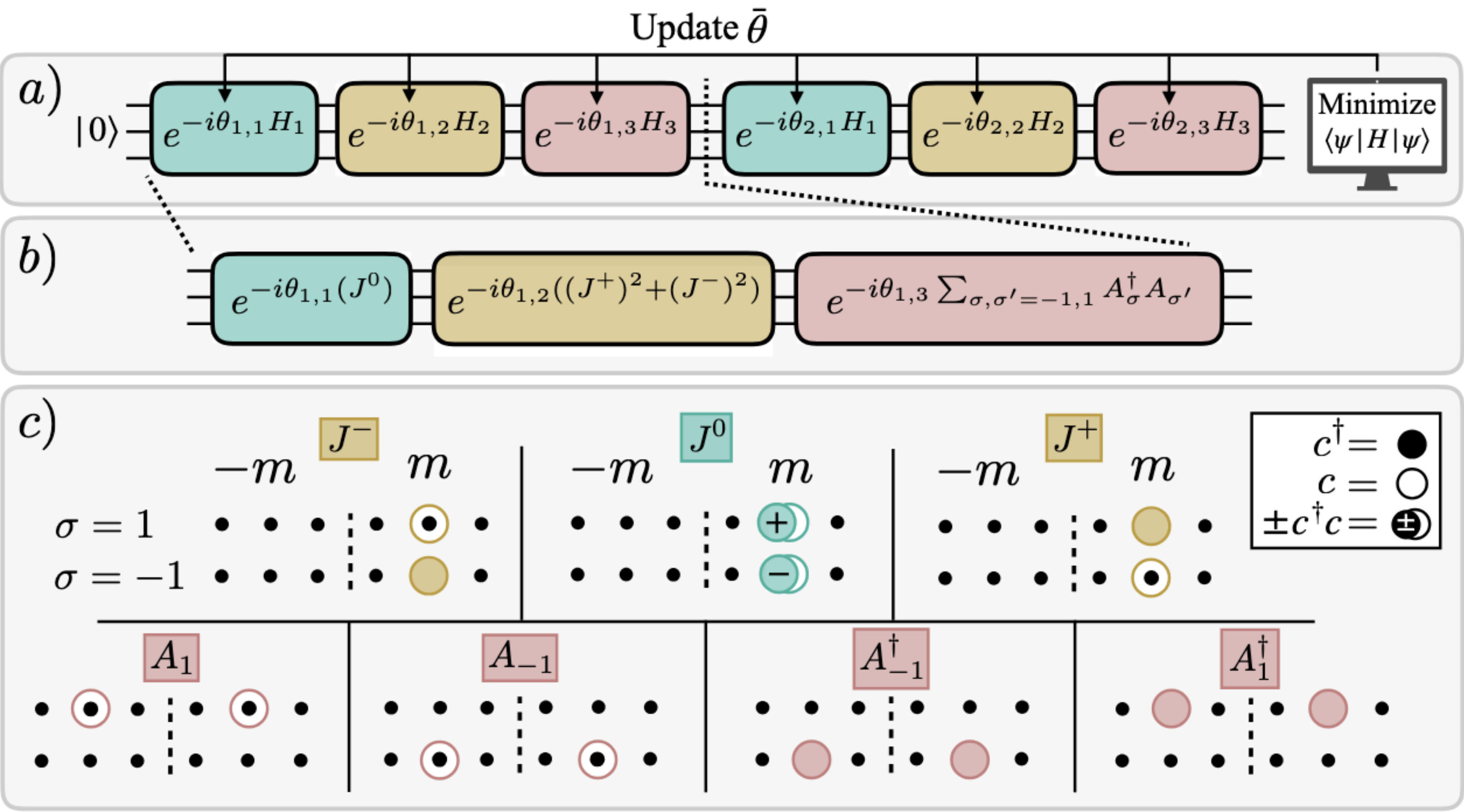
N=7 real IBM_Nairobi calculations



N=15 noiseless simulation

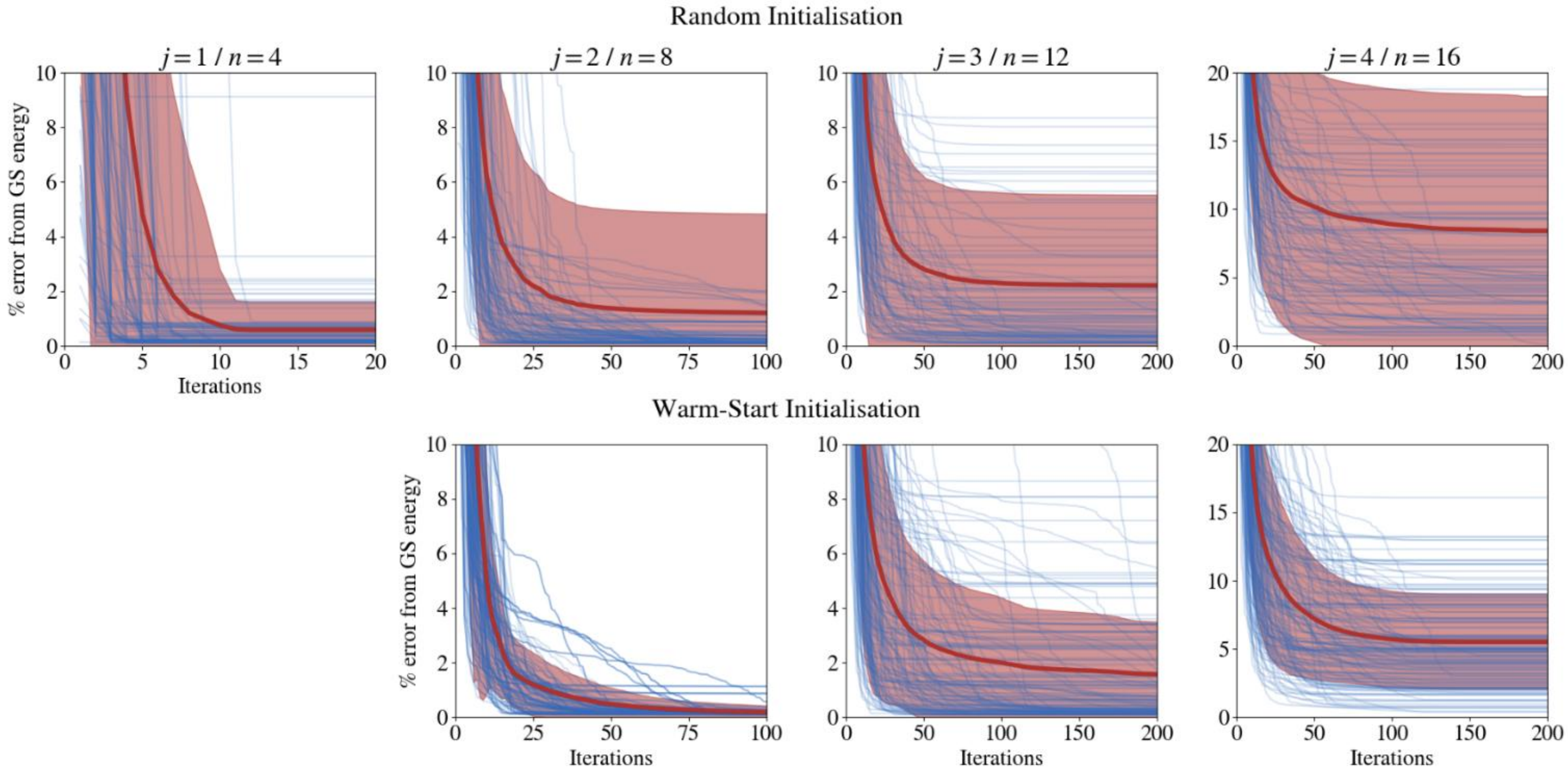


HVA – HAMILTONIAN VARIATIONAL ANSATZ



Joe Gibbs, Paul Stevenson, and Zoë Holmes, *to be published in Quantum Machine Intelligence*, arxiv:2402.10277

VQE WITH HVA: RANDOM VS WARM START



Joe Gibbs, Paul Stevenson, and Zoë Holmes, *to be published in Quantum Machine Intelligence*, arxiv:2402.10277

CONCLUSION / ACKNOWLEDGEMENTS

Other work includes solution of nuclear density functional theory equations via quantum imaginary time / general method for solving nonlinear coupled Schrödinger equations:

- Yang Hong Li, Jim Al-Khalili, and Paul Stevenson, Phys. Rev. C 109, 044322 (2024)
- Yang Hong Li, Jim Al-Khalili and Paul Stevenson, Eur. Phys. J. Spec. Top., *in press* (2024) doi: .1140/epjs/s11734-024-01384-z

Tensor networks methods for expressing nuclear wave functions: Joe Gibbs

Long(er) term goal: nuclear reactions

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AWE: James Benstead, Joe Gibbs
EPFL: Zoë Holmes

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STFC, AWE, SEPnet for PhD funding

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(QUANTUM) IMAGINARY TIME EVOLUTION (Q)ITE

Yang Hong Li, Jim Al-Khalili, and Paul Stevenson, Phys. Rev. C 109, 044322 (2024) arxiv:2402.01623
Yang Hong Li, Jim Al-Khalili, and Paul Stevenson, Eur. Phys. J. Spec. Top., *in press* (2024) arxiv:2402.01623

Formal solution to time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t) = H\Psi(\boldsymbol{r},t)$$

leads to

$$\Psi(\boldsymbol{r},t) = \mathcal{T}\exp\left(-\int_0^t \frac{iHt'}{\hbar}\right)\Psi$$

Practical implementation using small t

$$\Psi(\boldsymbol{r},t+\Delta t) = \exp\left(-\frac{iH\Delta t}{\hbar}\right)$$

Real-time evolution: Describes dynam
structure & reactions

Substitution $t \to -i\tau$ = imaginary time.

Why do this?
As τ increases, high energy components are

RESEARCH

Science 369, 1084 (2020)

QUANTUM COMPUTING

Hartree-Fock on a superconducting qubit quantum computer

Google AI Quantum and Collaborators*†

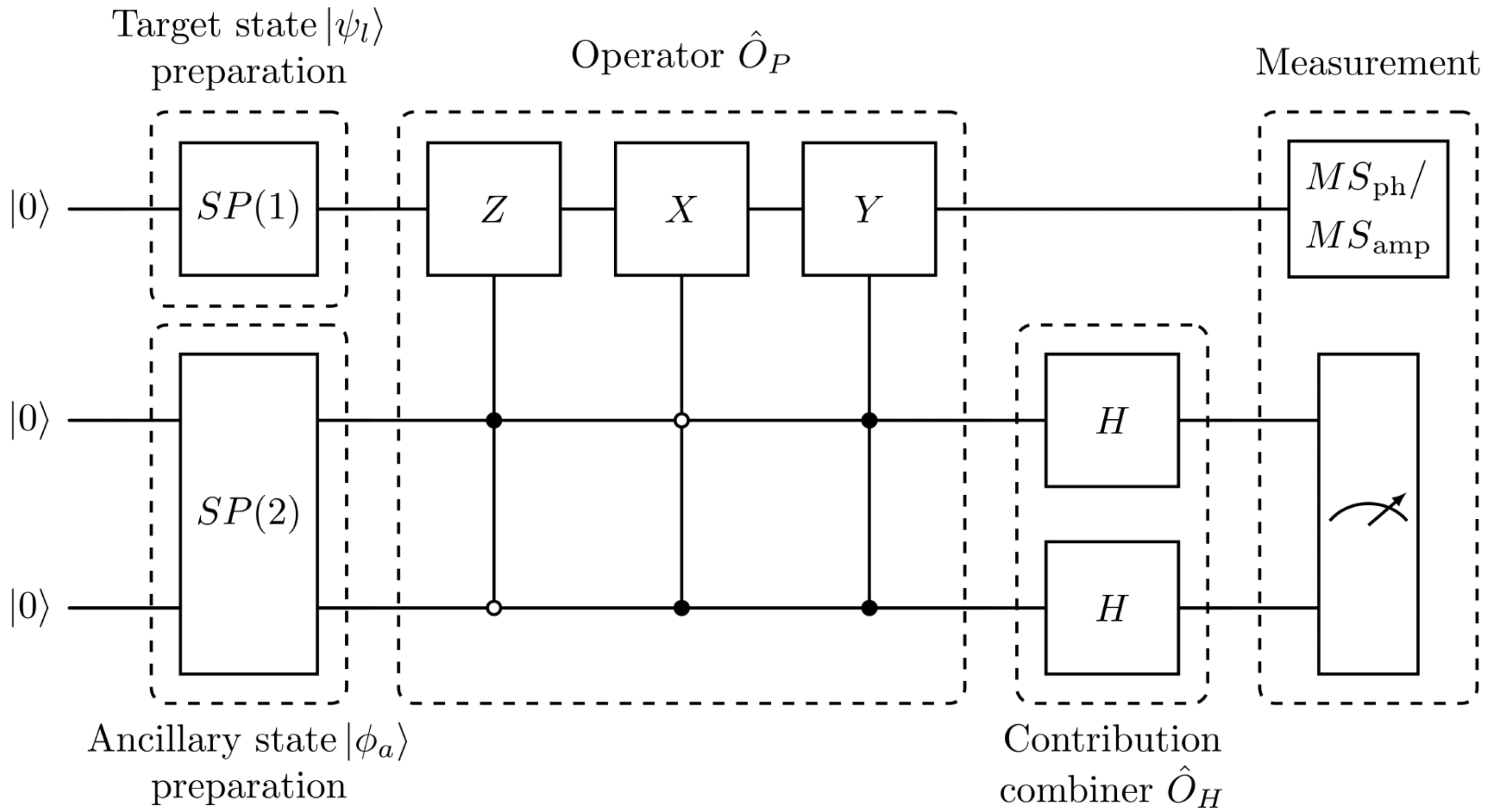
QITE CIRCUIT

Circuit for one iteration of imaginary time evolution for smallest possible model space: Expansion of unknown state (“target state”) in two oscillator basis states.

Ancillary qubits apply QITE operator

Post-selection on ancillary qubits requires them to be all zero for qualifying result in target qubit.

NB this is for a single orbital

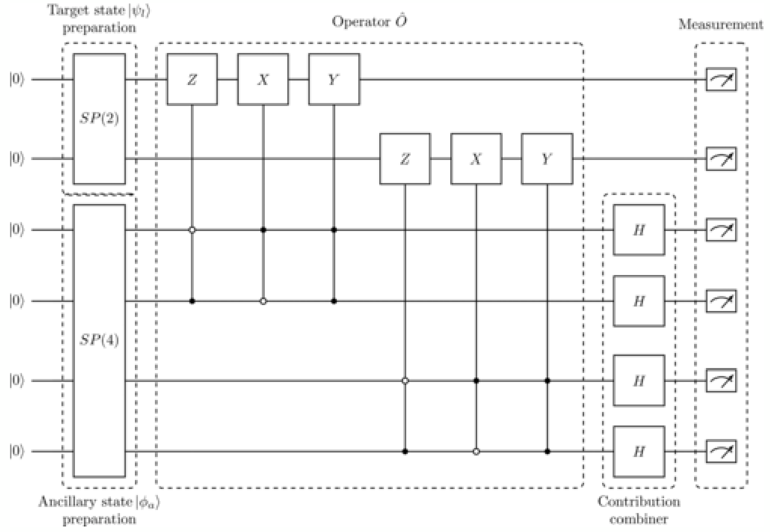


HE-4 WITH SIMPLIFIED SKYRME FORCE

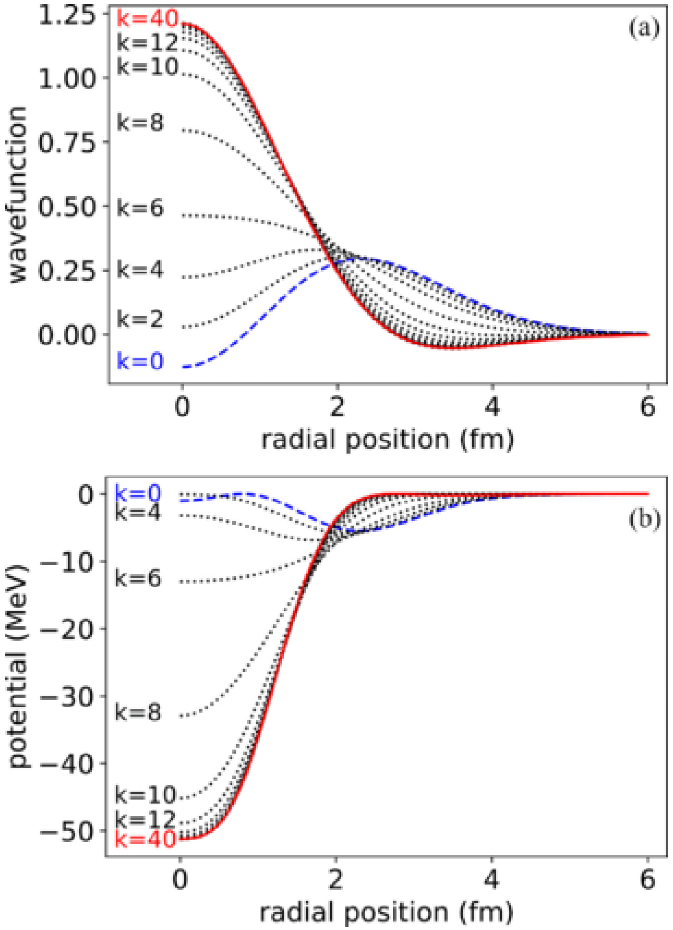
For simplicity and to test the model: a previously-used simplified $t_0 + t_3$ Skyrme interaction for ^{4}He where we are solving for only one single particle state

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{3t_0}{4\pi r^2}|u_{00}|^2 + \frac{3t_3}{16\pi^2 r^4}|u_{00}|^4\right) u_{00} = \varepsilon_{00} u_{00},$$

(very poor) starting “guess” $$u_{00}^{(0)} = \frac{1}{\sqrt{2}}\mathscr{R}_0^{\frac{1}{b},\frac{3}{2}} + \frac{1}{\sqrt{2}}\mathscr{R}_1^{\frac{1}{b},\frac{3}{2}}.$$



Can scale up:
N=2 qubits -> 2^N=4 expansion coefficients; 2N=4 ancillary qubits to represent operators



Quantum simulation (shot-based, noiseless)

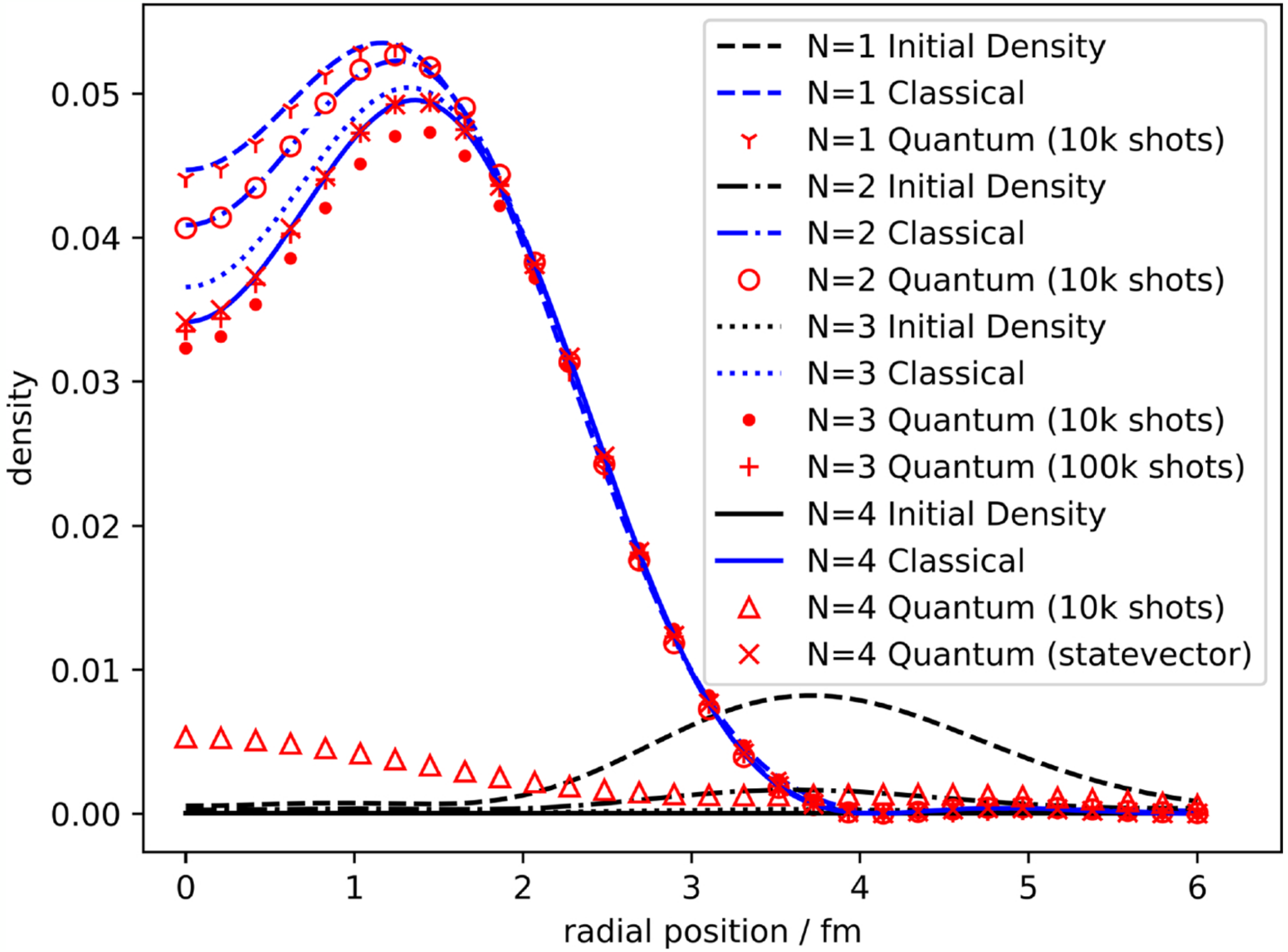
O - 1 6

For simple force with ^{16}O, we have two unknown wave functions to solve for: Now the HF equation are coupled nonlinear differential equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right]u_{00}=\varepsilon_{00}u_{00},$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\frac{\hbar^2}{mr^2}+V(r)\right]u_{01}=\varepsilon_{01}u_{01},$$

$$\begin{aligned}V(r)=&\frac{3}{4}t_0\rho(r)+\frac{3}{16}t_3\rho^2(r)\\=&\frac{3t_0}{4\pi r^2}\left(|u_{00}|^2+3|u_{01}|^2\right)+\frac{3t_3}{16\pi^2r^4}\left(|u_{00}|^2+3|u_{01}|^2\right)^2.\end{aligned}$$



We have O(N) complexity in the circuit, compared with at least $O(2^N)$ for higher depth but lower-qubit count methods. *But* we also have post-selection problem with exponentially bad scaling. We are working on some ideas here.