Quantum Computing for Nuclear Structure

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IoP (HEP/AP/N)P 2024 @ Liverpool

UNIVERSITY OF SURREY

Quantum Computing

Classical computers operate on *bits*: binary digits which can be in the states 0 or 1

Quantum computers have *qubits:* two-level quantum systems of the form $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$

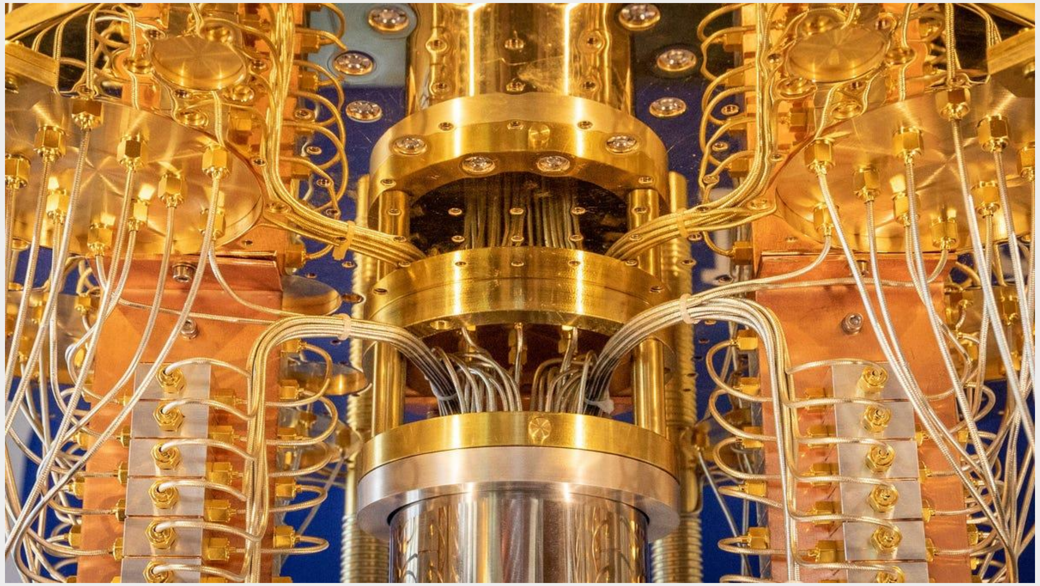
α & β are complex numbers ($\alpha^*\alpha + \beta^*\beta = 1$) – in principle store much more information in these continuous numbers than in discrete bits.

But it is hard to access the information: When you measure the state of a qubit you always get either $|0\rangle$ or $|1\rangle$

2-dimensional Hilbert space from one qubit grows exponentially as more qubits added:

$|0\rangle\otimes|0\rangle\otimes \cdots \otimes|0\rangle = |00\cdots0\rangle$ has Hilbert space dimension 2^n

e.g. can use ~100 qubits to deal with 2^{100}~10^{30} dimensionality



IBM's 53 qubit quantum processor. Image from https://www.cnet.com/tech/computing/ibm-new-53-qubit-quantum-computer-is-its-biggest-yet/

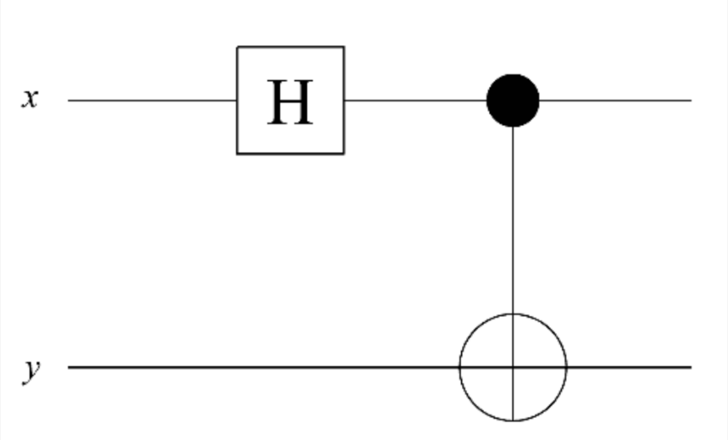
Quantum Computing

… and then there is entanglement

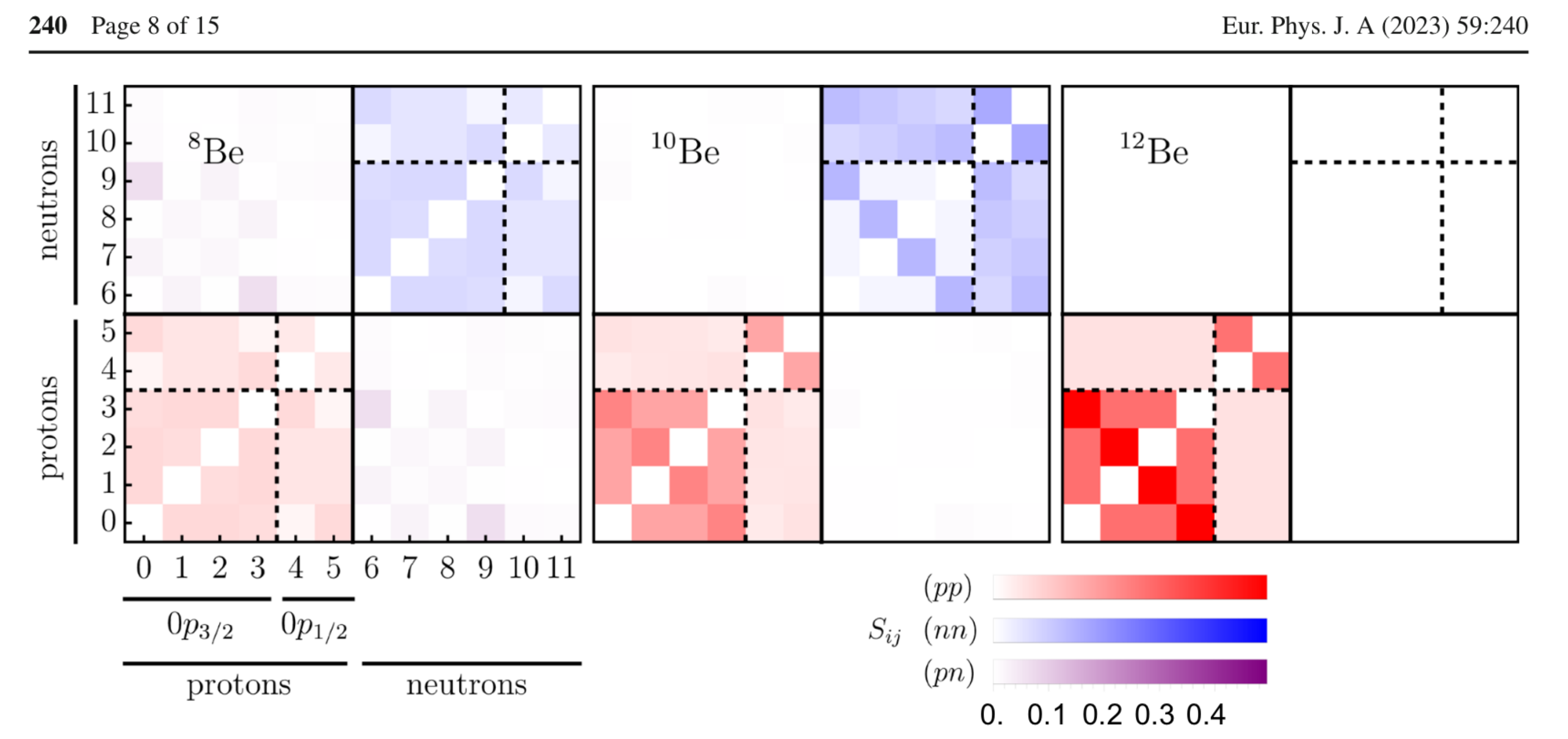
$$|\beta_{00}\rangle = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

A Bell state

…from this quantum circuit



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]



there *is* entanglement in nuclear wave functions

Quantum Simulation

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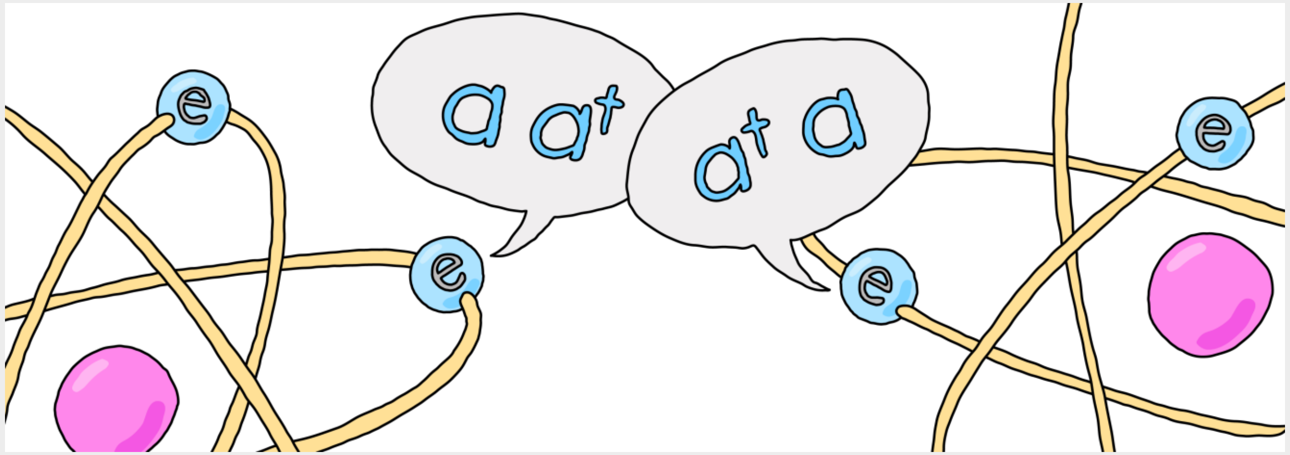
- Qubits are controlled by quantum gates

- Pauli X, Y, Z, I operators span the Hilbert Space of a single qubit. Tensor products extend this to multiple qubits.

- Mappings (e.g. Jordan-Wigner) link fermion creation and annihilation operators to Pauli matrices

- Any interacting fermion system can be simulated on quantum computer

- Fundamentally different to how classical computers do "number-crunching"



cute picture from pennylane.ai

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

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

Jordan-Wigner Transformation
Zeitschrift für Physik 47, 631 (1928)

Nuclear structure on quantum computers

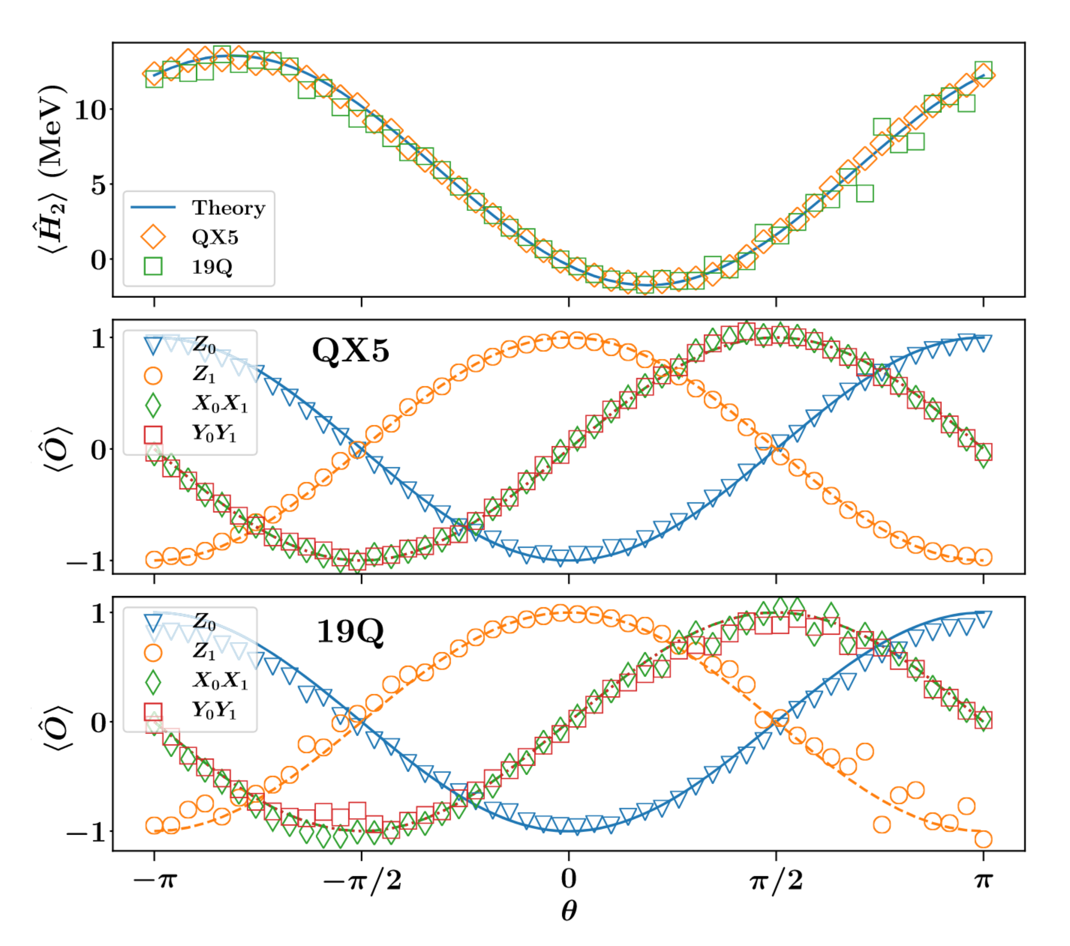
- Goal is, as always in nuclear structure, to solve $H\Psi_n = E_n\Psi_n$.
- H represented as Pauli op
- Ψ guessed / calculated / v … presented by a quantum circuit

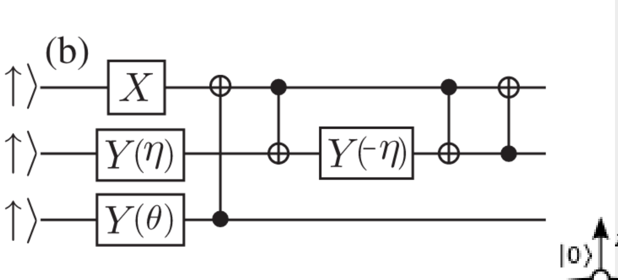
First high-profile nuclear ph
by Dumitrescu et al. PRL**12**

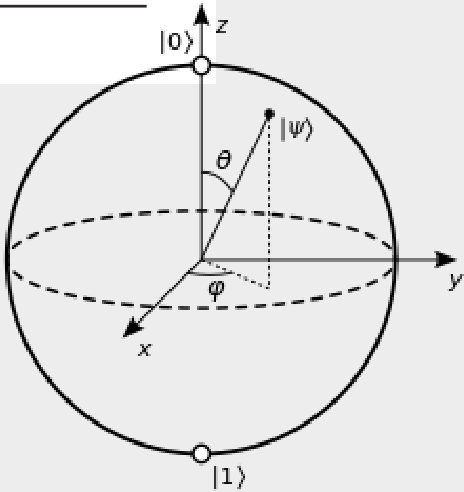
We follow Refs. [26,27] and
representation in the harmonic
Hamiltonian. The deuteron Hami

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T +$$

They looked at N=

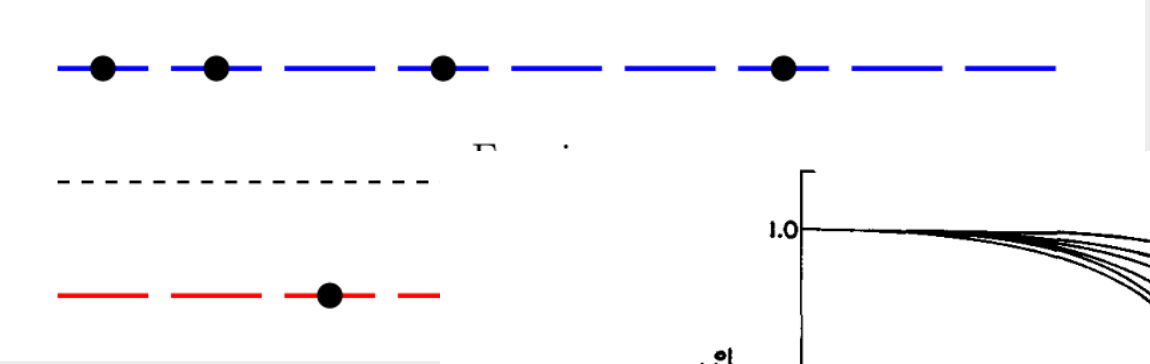






Wave function preparation in 2-level models

Popular test-bed: Lipkin-Meshkov-Glick model as a simplified Shell Model



H. J. LIPKIN,
Weizmann Institute of Science, Rehovoth, Israel
N. MESHKOV and A. J. GLICK †
Weizmann Institute of Science, Rehovoth, Israel
and
University of Maryland, College Park, Maryland ††

65) 188—198;

$\sum_{p'\sigma} a^{\dagger}_{p\sigma} a^{\dagger}_{p'\sigma} a_{p'-\sigma} a_{p-\sigma}$

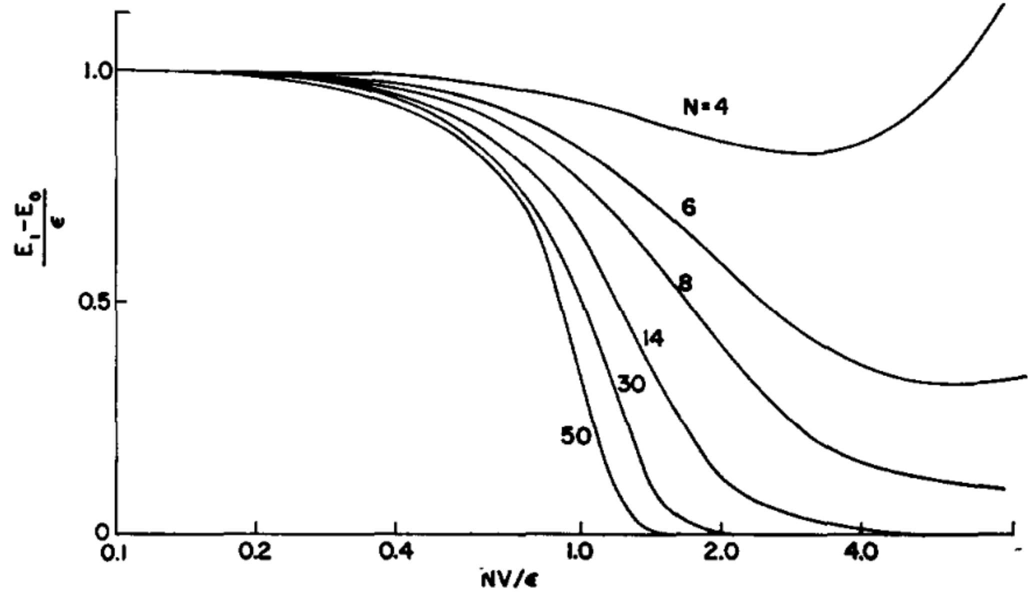
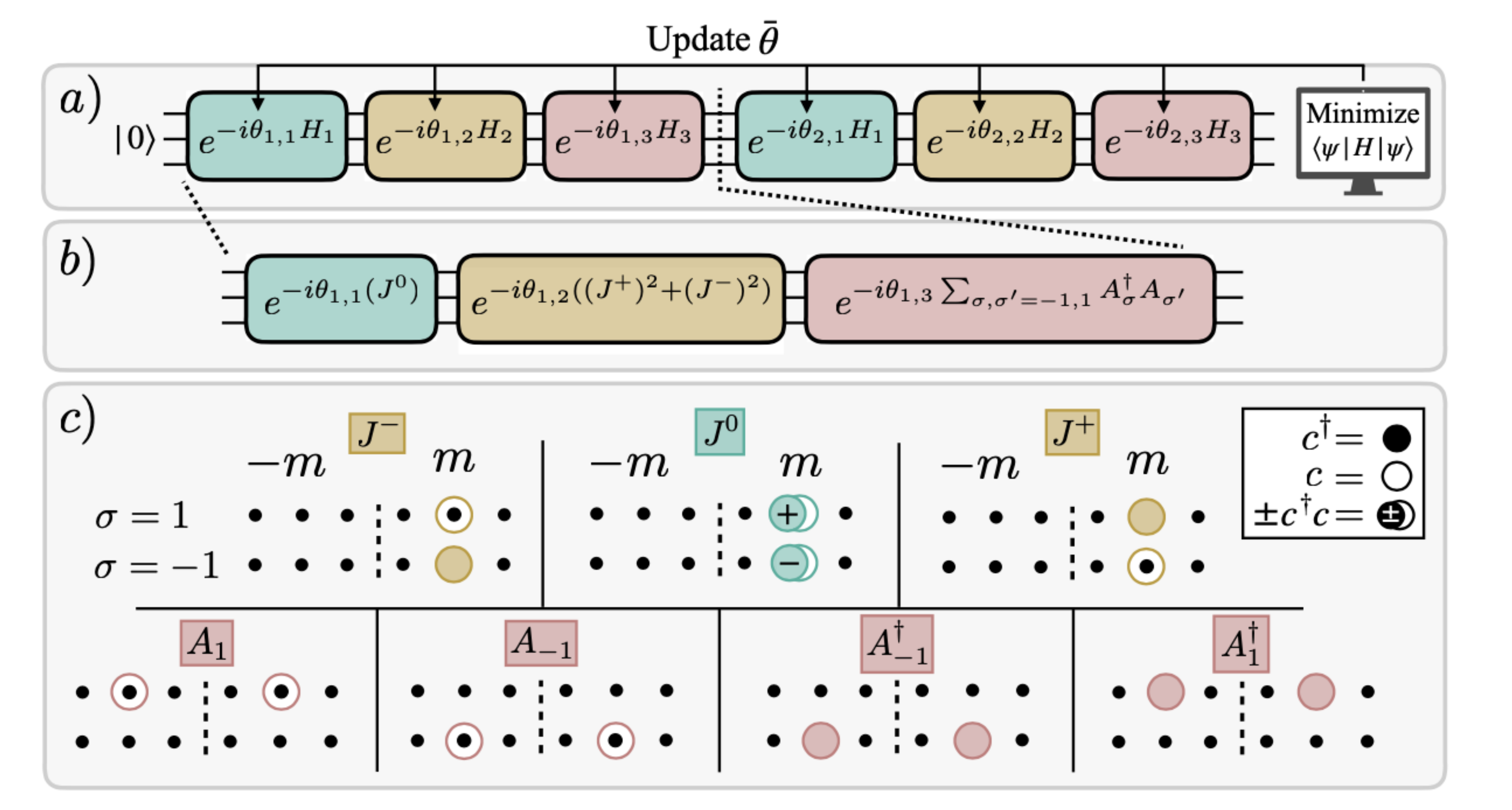


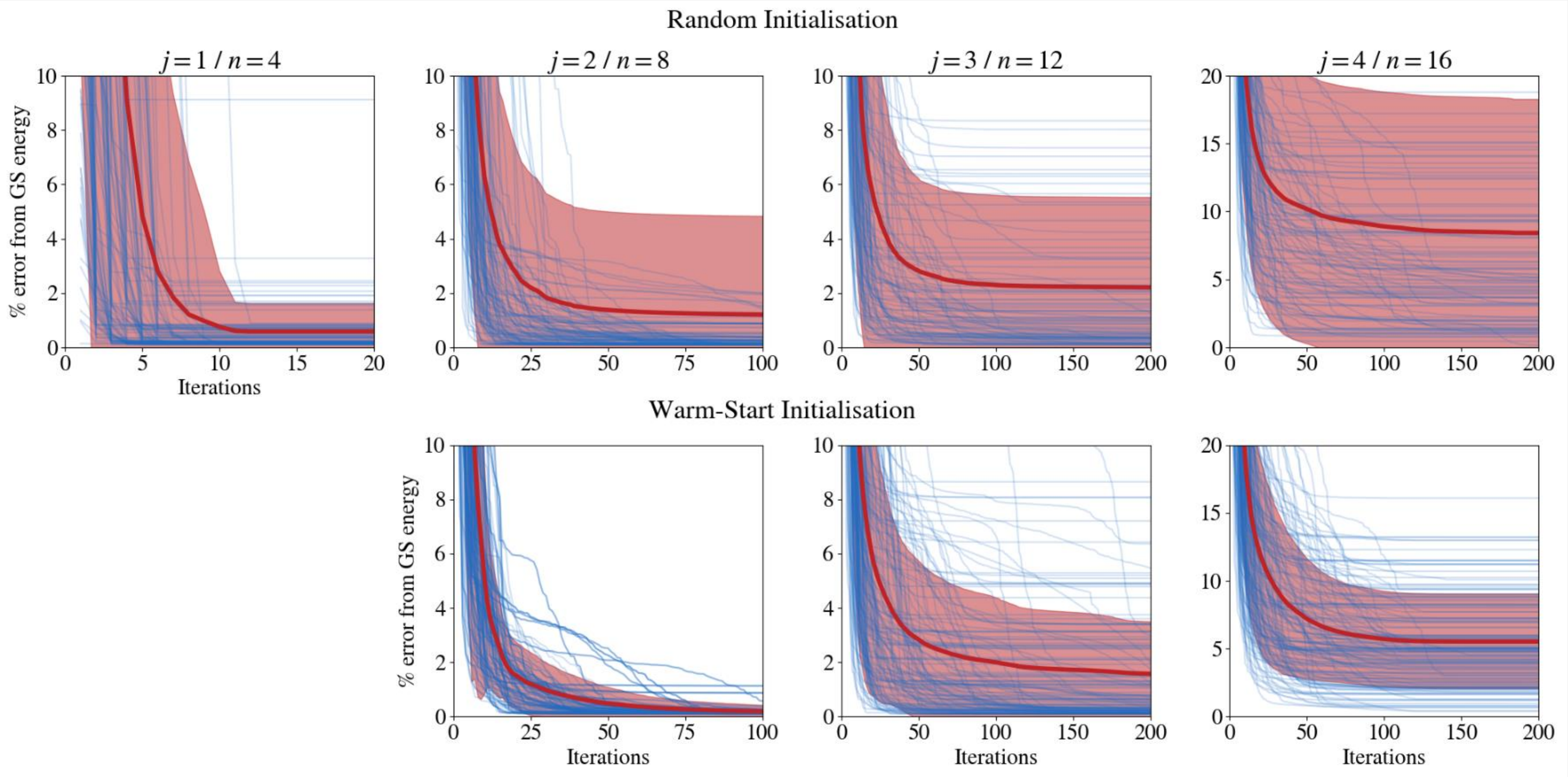
Fig. 2. Exact results for the excitation energy of the first excited state above the ground state plotted versus the interaction parameter NV/ε for $N = 4, 6, 8, 14, 30$ and 50 particles.

HVA: Hamiltonian Variational Ansatz



"*Exploiting symmetries in nuclear Hamiltonians for ground state preparation*", Joe Gibbs, Paul Stevenson, and Zoë Holmes, *submitted to Quantum Science and Technology*, arxiv:2402.10277

HVA results



"*Exploiting symmetries in nuclear Hamiltonians for ground state preparation*", Joe Gibbs, Paul Stevenson, and Zoë Holmes, *submitted to Quantum Science and Technology*, arxiv:2402.10277

Density Functional Theory (DFT)

$$\left[-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + V(\{x_i\})\right]\Phi = \mathcal{E}\Phi,$$

+

$$\begin{aligned} v_{ij}^{(2)} &= t_0\left(1 + x_0 P_\sigma\right)\delta^3\left(\vec{r}_i - \vec{r}_j\right) \\ &+ \frac{1}{2}t_1\left[\delta^3\left(\vec{r}_i - \vec{r}_j\right)k_R^2 + k_L^2\delta^3\left(\vec{r}_i - \vec{r}_j\right)\right] \\ &+ t_2\vec{k}_L\cdot\delta^3\left(\vec{r}_i - \vec{r}_j\right)\vec{k}_R \\ &+ iW_0\left(\vec{\sigma}_i + \vec{\sigma}_j\right)\cdot\vec{k}_L\times\delta^3\left(\vec{r}_i - \vec{r}_j\right)\vec{k}_R, \end{aligned}$$

=

$$\begin{aligned} E = &-\frac{\hbar^2}{2m}\sum_{i=1}^{N}\int d^3\vec{r}\left[\varphi_i^*\left(\vec{r}\right)\nabla_i^2\varphi_i\left(\vec{r}\right)\right] \\ &+ \int d^3\vec{r}\left[\frac{3}{8}t_0\rho^2\left(\vec{r}\right) + \frac{1}{16}t_3\rho^3\left(\vec{r}\right)\right]. \end{aligned}$$

Apply variational principle to get a nonlinear Schroedinger eqn:

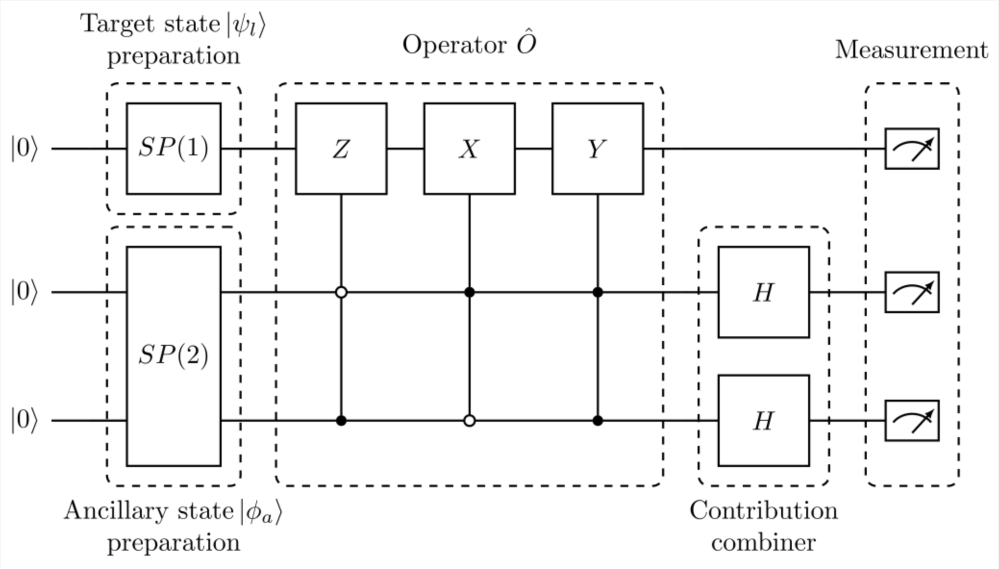
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + \frac{3}{4}t_0\rho\left(\vec{r}\right) + \frac{3}{16}t_3\rho^2\left(\vec{r}\right)\right]\varphi_j\left(\vec{r}\right) = \varepsilon_j\varphi_j\left(\vec{r}\right).$$

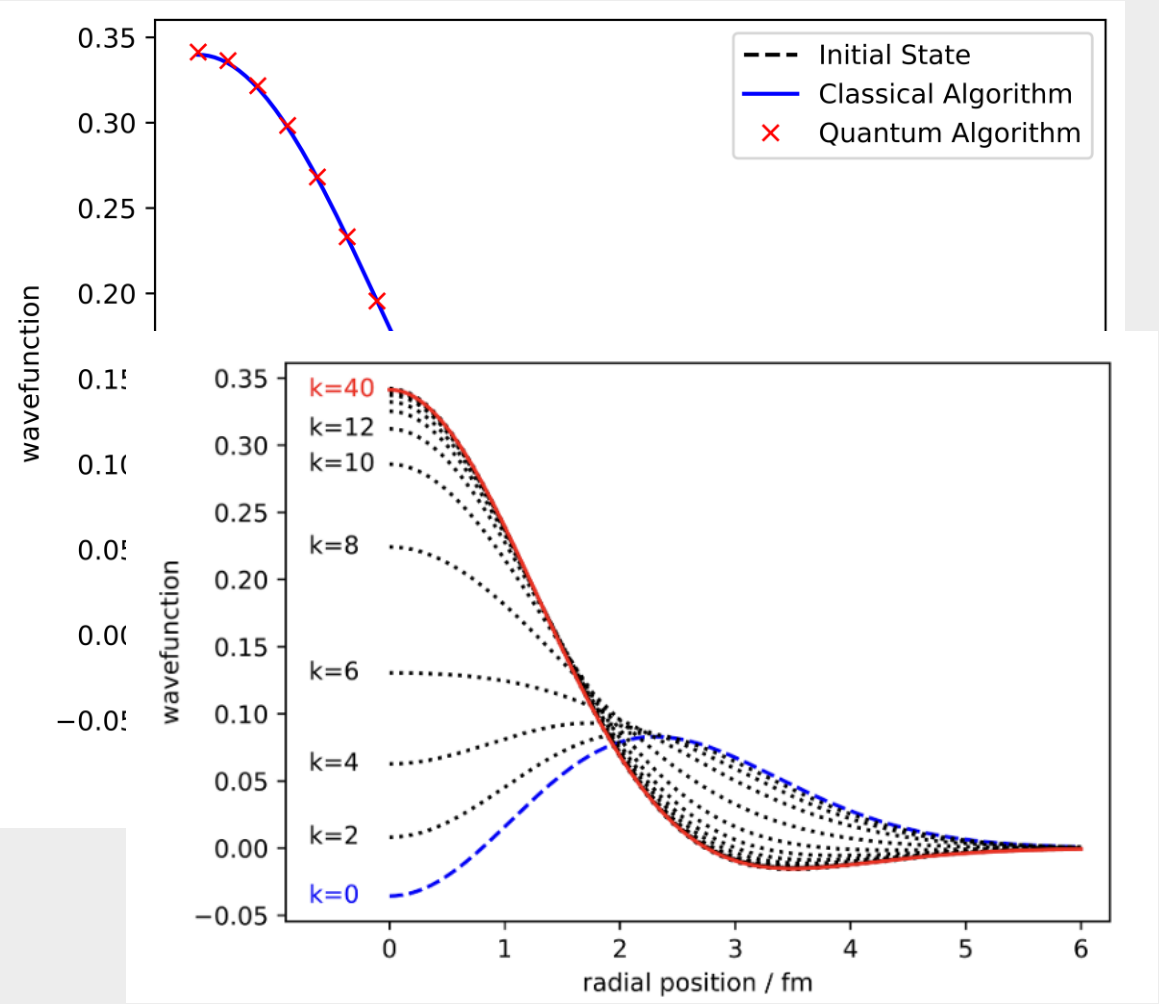
Imaginary time-evolution from initial state: Kills off high energy components -> ground state can be found

$$\left|\psi\left(r,\tau\right)\right\rangle = \mathcal{N}\exp\left(-\frac{\hat{H}_{hf}^{l}}{\hbar}\tau\right)\left|\psi\left(r,0\right)\right\rangle,$$

Non-Unitary operator – needs special treatment on quantum computer

Density Functional Theory on QC





"*A Quantum Simulation Approach to Implementing Nuclear Density Functional Theory via Imaginary Time Evolution*", Yang Hong Li, Jim Al-Khalili, and Paul Stevenson, *accepted for publication in Phys. Rev. C*, arxiv: 2308.15425

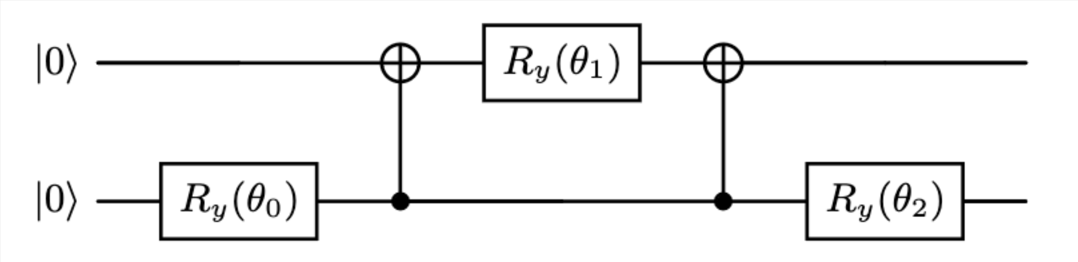
"*Solving coupled Non-linear Schrödinger Equations via Quantum Imaginary Time Evolution*", Yang Hong Li, Jim Al-Khalili and Paul Stevenson, arxiv:2402.01623

Variance Minimisation

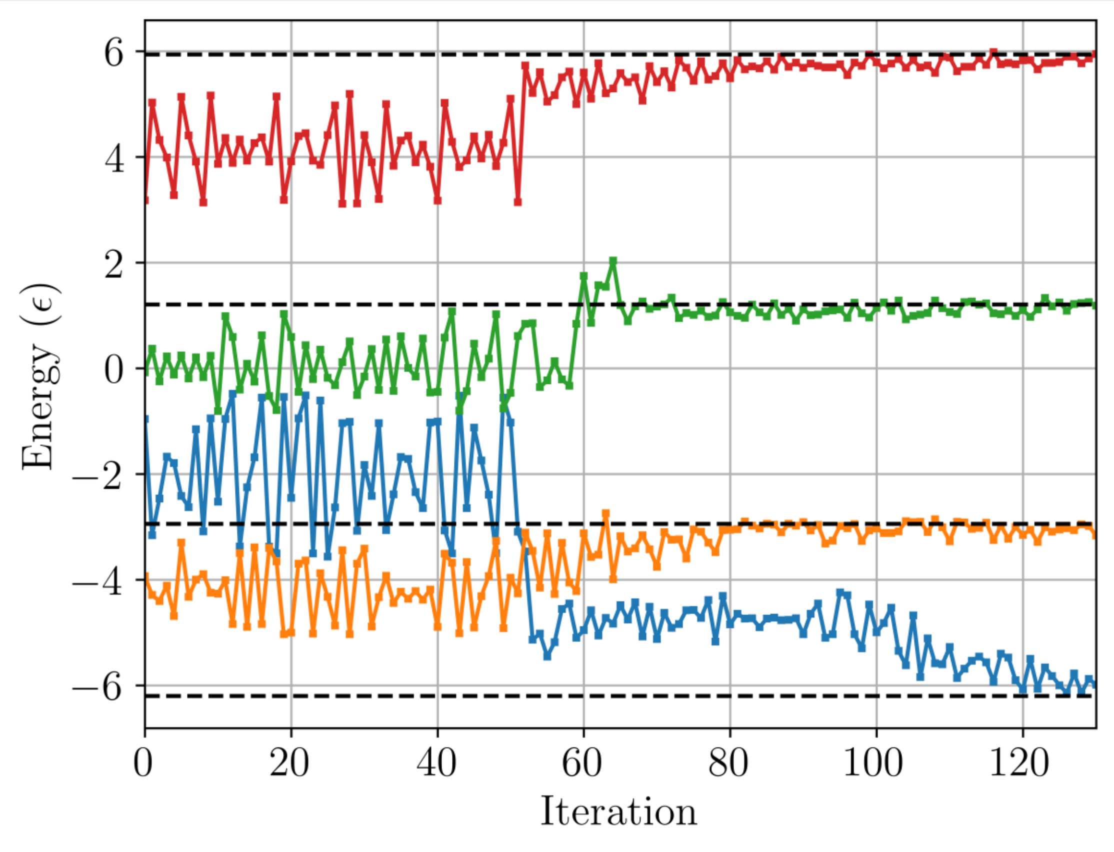
Variational methods usually used to find ground state (because that's how they work).

But, can minimize variance rather than energy to find any eigenstate

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



IBM_Nairobi real QC results



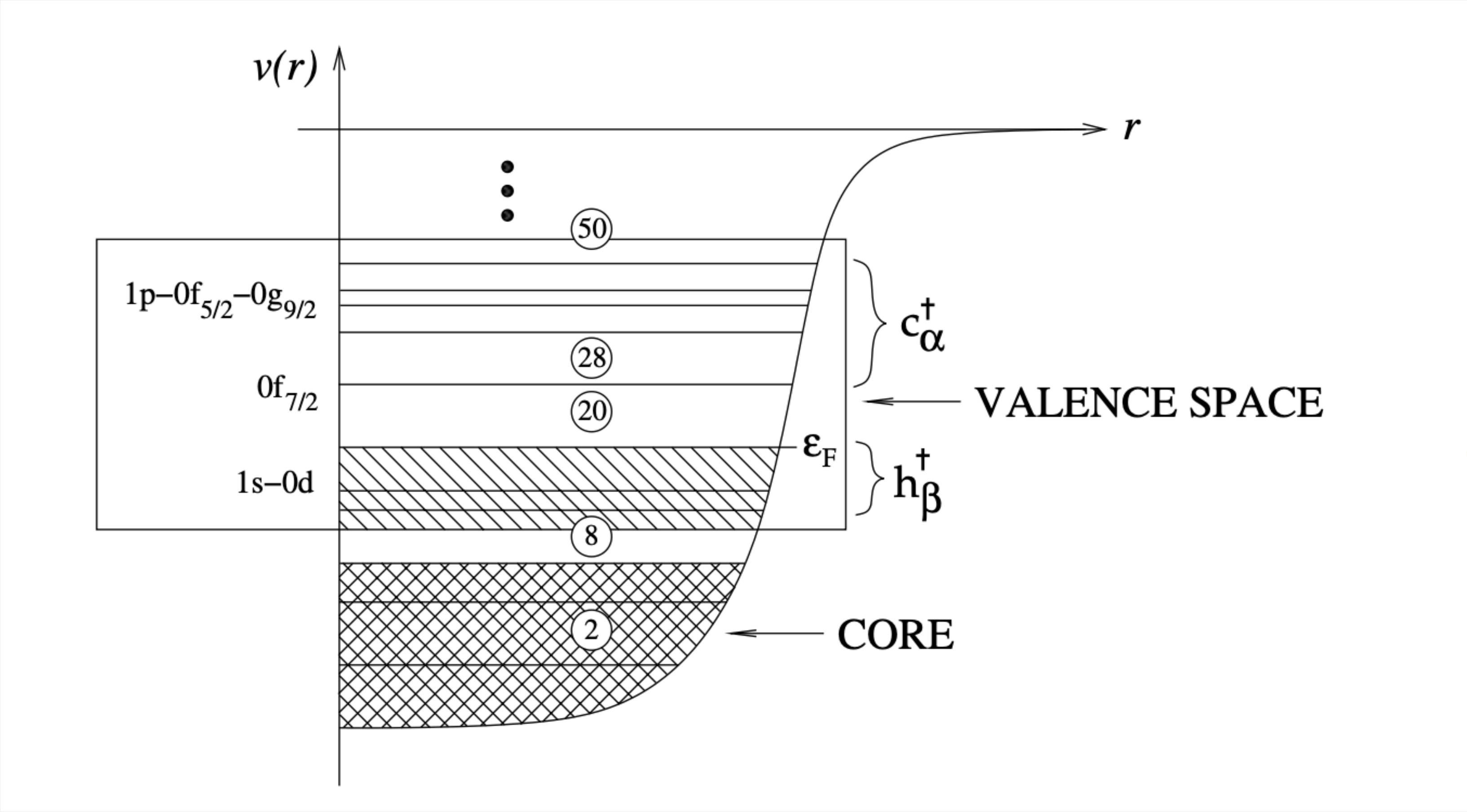
"*Quantum Computing Calculations for Nuclear Structure and Nuclear Data*", Isaac Hobday, Paul. D. Stevenson, and James Benstead, Proc. SPIE 12133, Quantum Technologies 2022, 121330J (2022) arxiv: 2205.05576

"*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

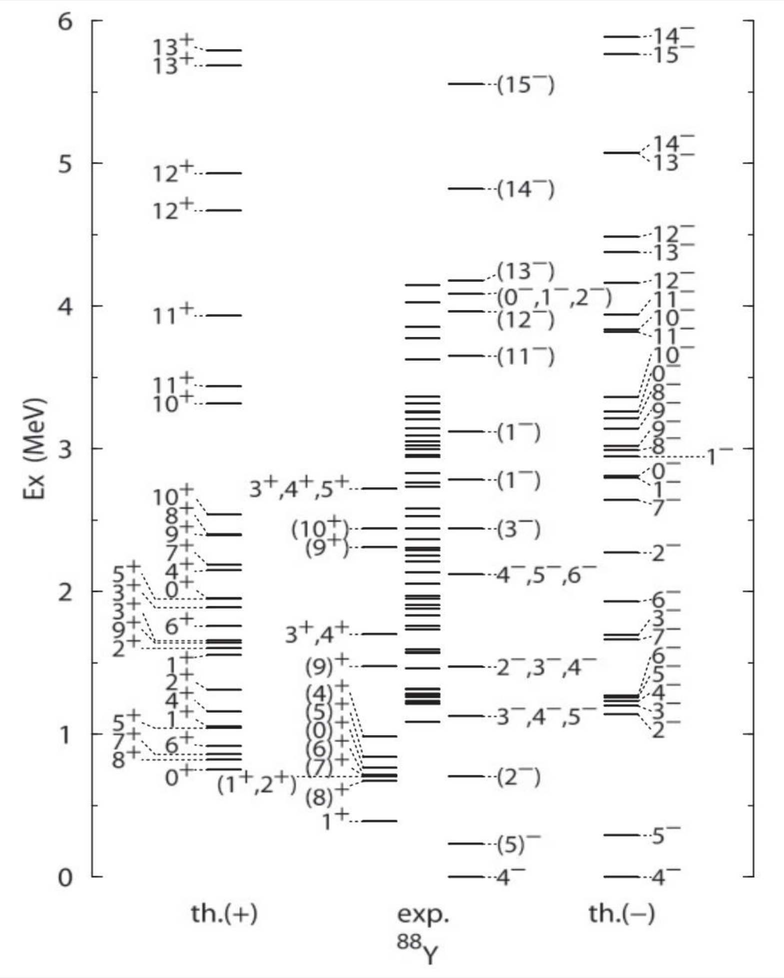
"*Variance Minimisation of the Lipkin-Meshkov-Glick Model on a Quantum Computer*", I. Hobday, P. Stevenson, and J. Benstead, submitted to Phys Rev C, arxiv:2403.08625

I. Hobday in 11:00 → 12:30 Wednesday II Session H

Shell Model



Suhonon, *From Nucleons to Nucleus, Springer Verlag*



Honma et al PRC80, 064323 (2009)

Shell Model: Ni-58

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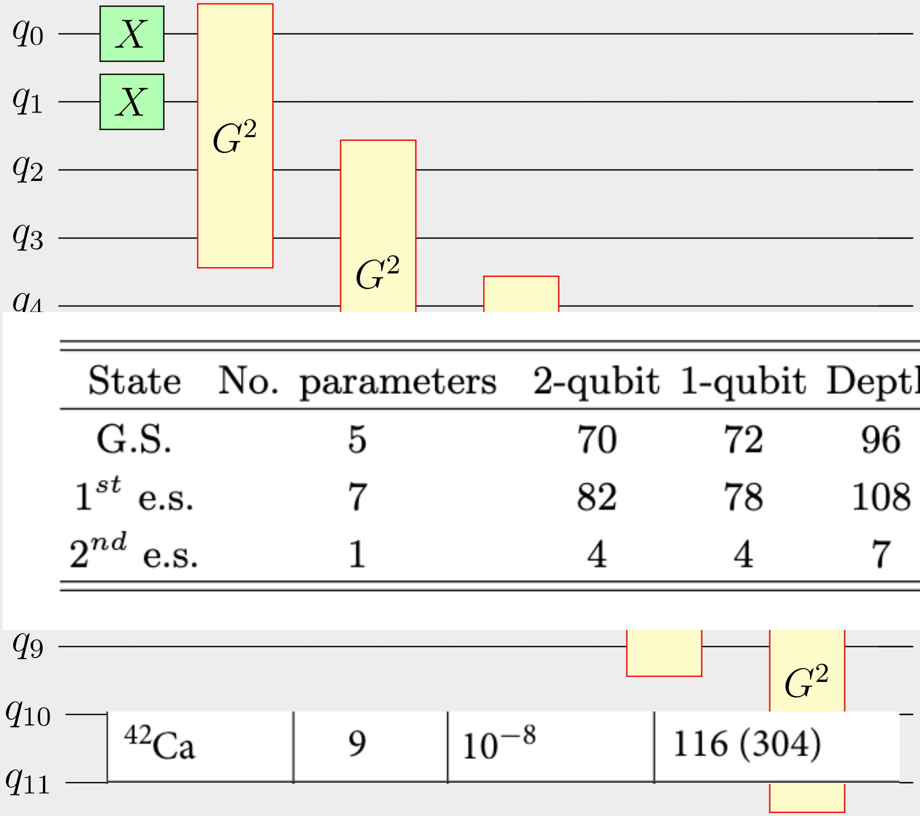
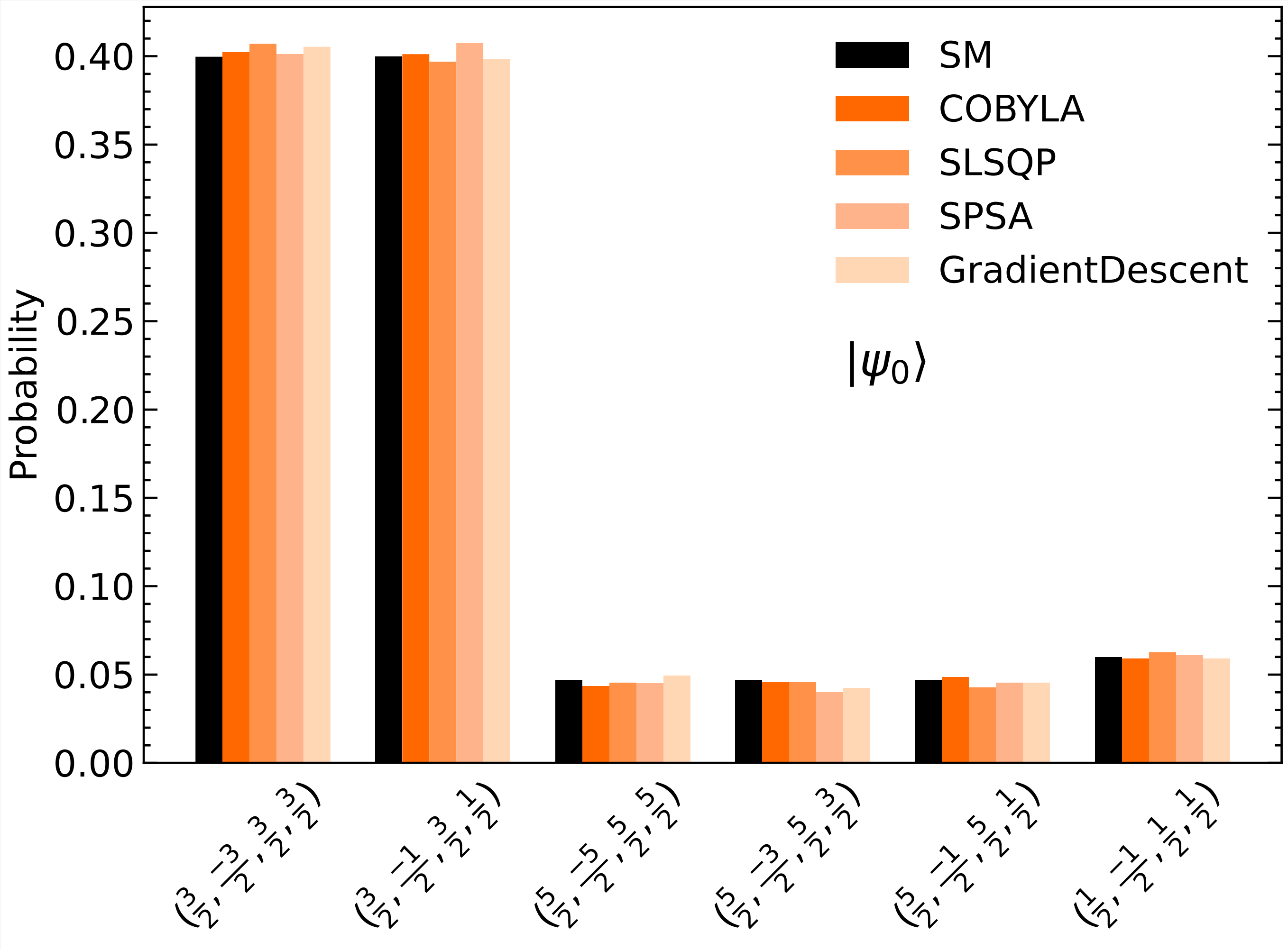


State	No. parameters	2-qubit	1-qubit	Depth
G.S.	5	70	72	96
1^{st} e.s.	7	82	78	108
2^{nd} e.s.	1	4	4	7

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

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



"*Shell-model study of 58Ni using quantum computing algorithm*", Bharti Bhoy and Paul Stevenson, *submitted to New Journal of Physics*, arxiv:2402.15577

B. Bhoy in Parallel Sessions: Wednesday I Session H 0900-1030:

Acknowledgements

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STFC under Quantum Technologies for Fundamental Physics programme
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STFC, AWE, SEPnet for PhD funding

Isaac Hobday, Joe Gibbs, Lance Li, Bharti Bhoy, James Benstead, Matteo Vorabbi, Jim Al-Khalili, Zoe Gibbs

Theoretical Nuclear Physics Industrial Studentship

University of Surrey > School of Mathematics and Physics

Dr N Timofeyuk, Dr Matteo Vorabbi   Monday, April 29, 2024

Funded PhD Project (UK Students Only)

← PhD opportunity for nuclear reaction studies working with AWE / LLNL

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