Thermal state preparation via a variational quantum algorithm

Tony J.G. Apollaro, University of Malta

Overview:

- Noisy Intermediate-Scale Quantum (NISQ) Computers
- Structure of a Variational Quantum Algorithm (VQA)
- Gibbs state preparation via VQA
- Results on the quantum transverse field Ising model
- Conclusions and Perspectives

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THE NISQ ERA

John Preskill (2018) defines NISQ as:

- Noisy: imperfect control over qubits
- Intermediate-scale: 50-100 qubits
- Quantum: self-explanatory
- Computers: Unitary operations on qubits

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Factorisation of large integers

Experimental study of Shor's factoring algorithm using the IBM Q Experience

Mirko Amico, Zain H. Saleem, and Muir Kumph
Phys. Rev. A **100**, 012305 – Published 8 July 2019

✔ 15 ✔ 21 ✖ 35

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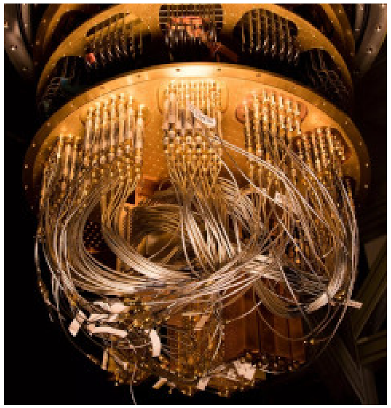
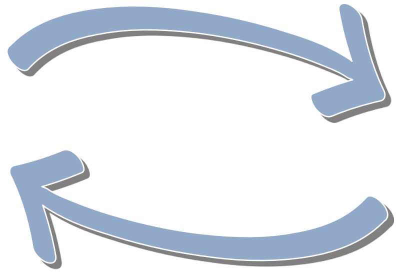
Take home message
<u>Use a quantum computer as little as possible</u>

Variational Quantum Algorithm (VQA)

Quantum Computer



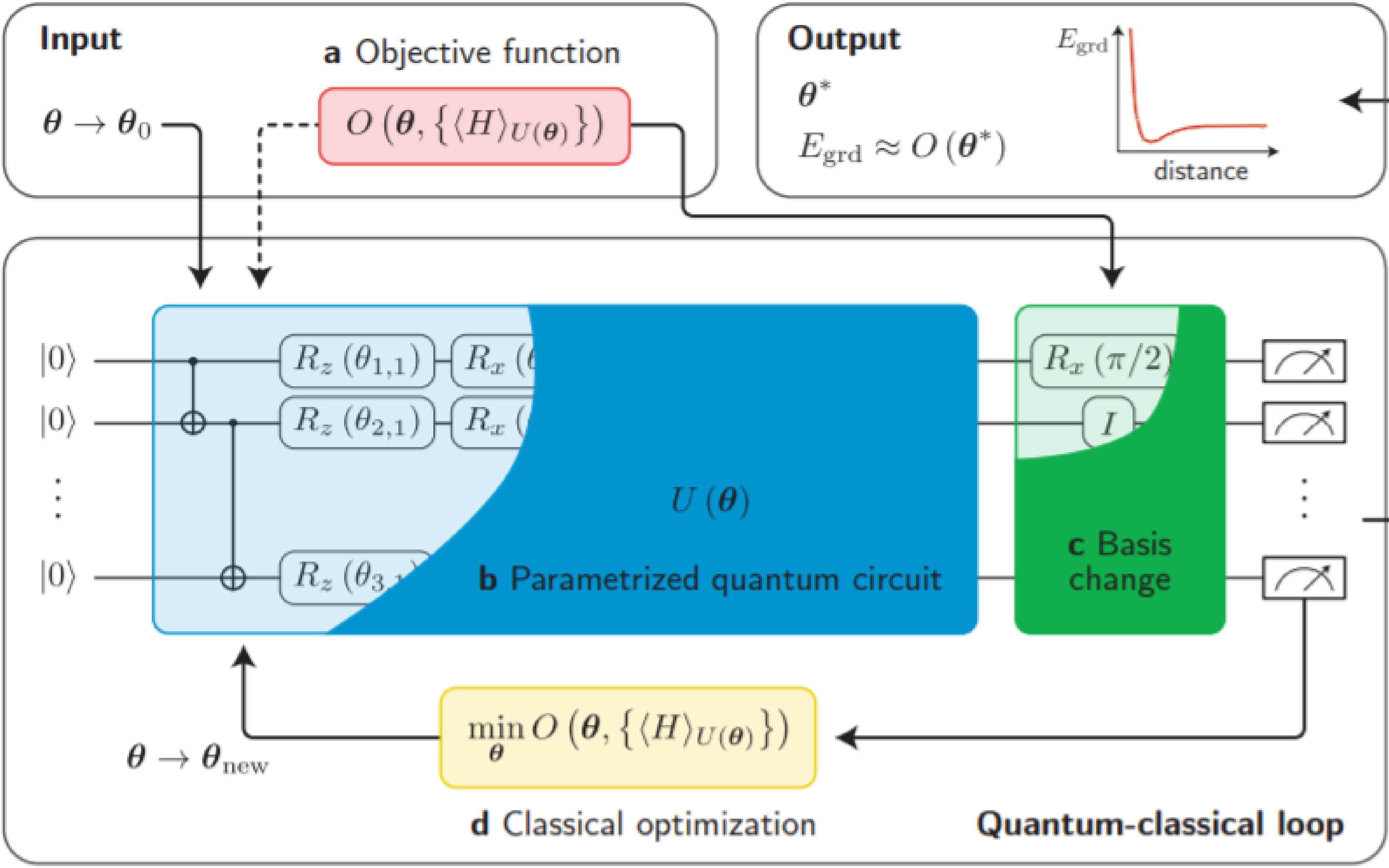


Classical optimizer

Output: cost function

Update parameters
Call the QC

Variational Quantum Algorithm (VQA)



Bharti et al., *Noisy intermediate-scale quantum algorithms,* Rev. Mod. Phys. 94, 015004 (2022)

Structure of a VQA- A. Cost function

A1: An objective function can be defined as $\min_{\theta} O\left(\theta, \left\{\langle \hat{H} \rangle_{U(\theta)}\right\}\right)$

A2: Given a parameterized unitary (PQC), one can expand it into

$$\langle \hat{H} \rangle_{U(\theta)} = \langle 0|^{\otimes N} U^{\dagger}(\theta) \hat{H} U(\theta) |0\rangle^{\otimes N}$$

A3: The Hamiltonian is hence decomposed into Pauli strings

$$\hat{H} = \sum_{i=1}^{N} c_i \hat{P}_i \ , \ \hat{P}_i = \prod_{j=1}^{N} \hat{\sigma}_j^{\alpha_j}$$

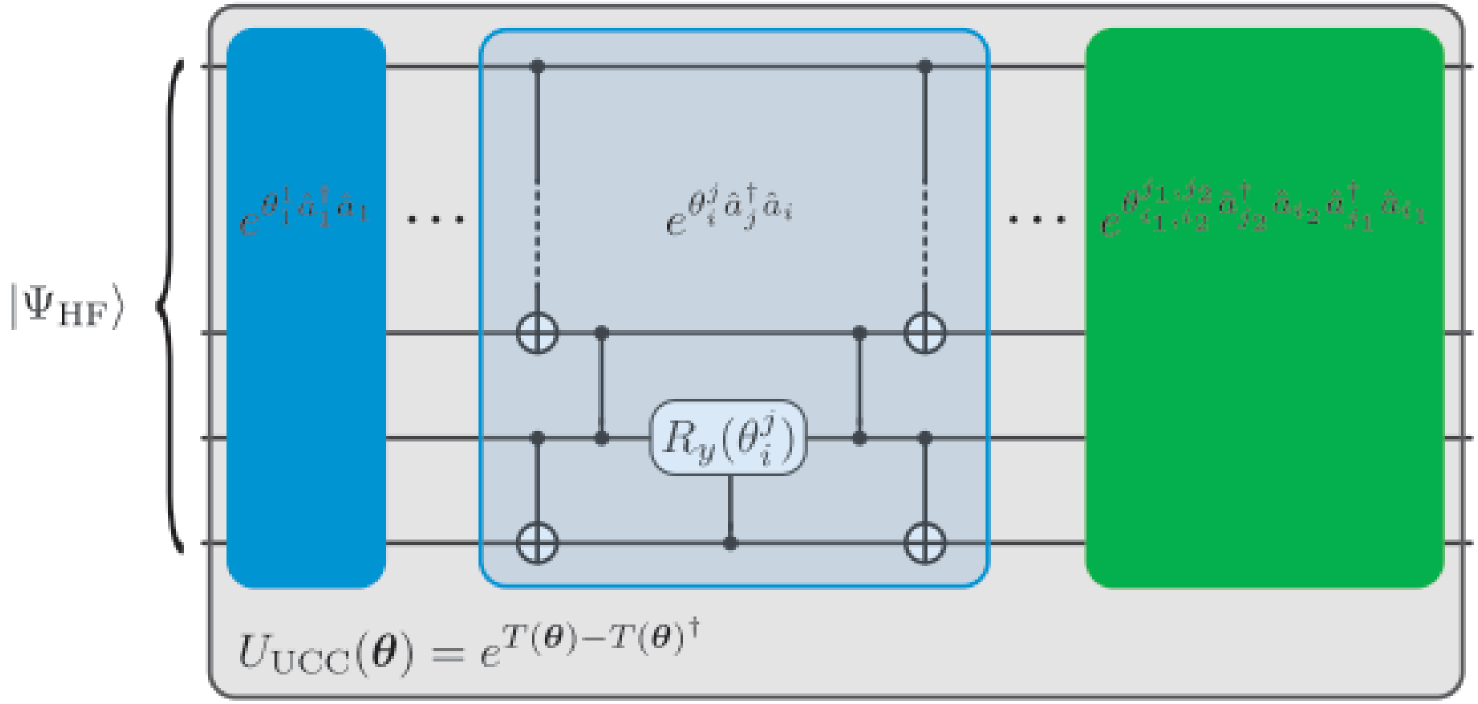
A4: The Hamiltonian expectation values is evaluated for each string

$$\langle \hat{H} \rangle_{U(\theta)} = \sum_{i=1}^{N} c_i \langle \hat{P}_i \rangle_{U(\theta)}$$

Structure of a VQA- B. PQC

Problem inspired vs Hardware efficient Ansatze

B1: Problem-inspired Ansatz

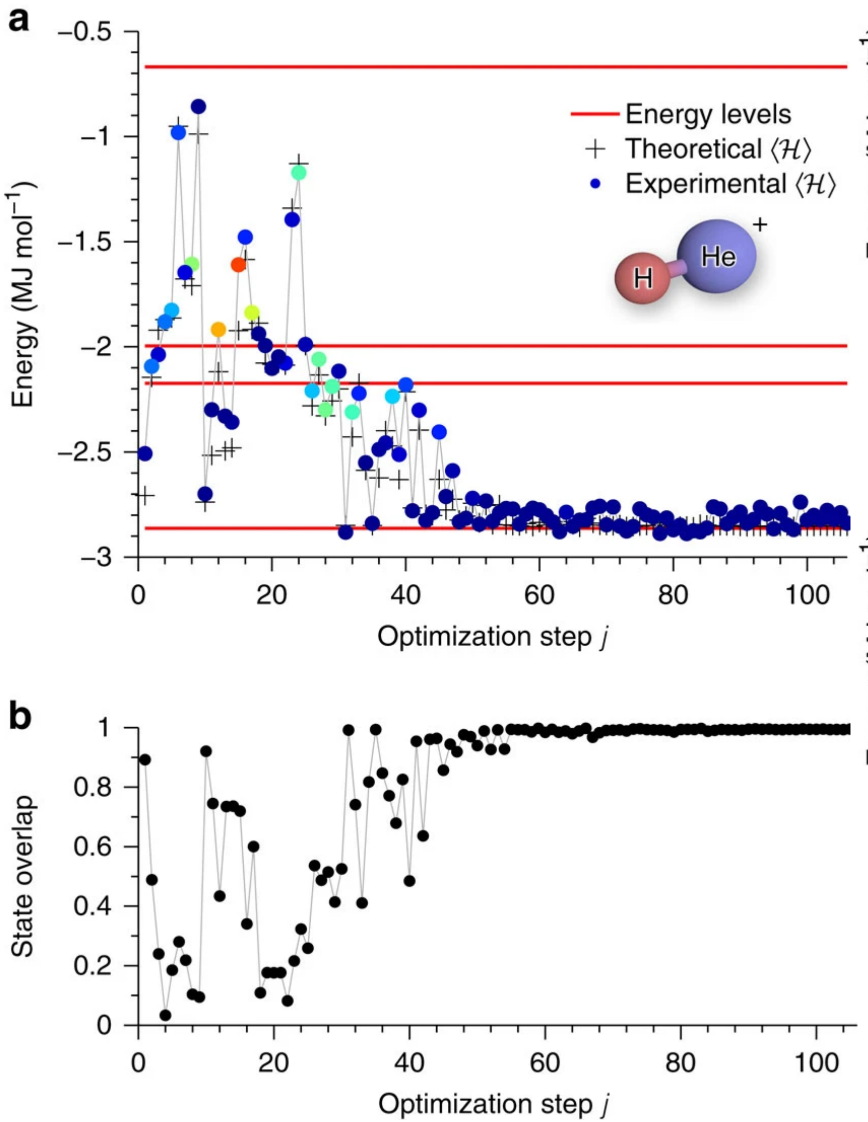


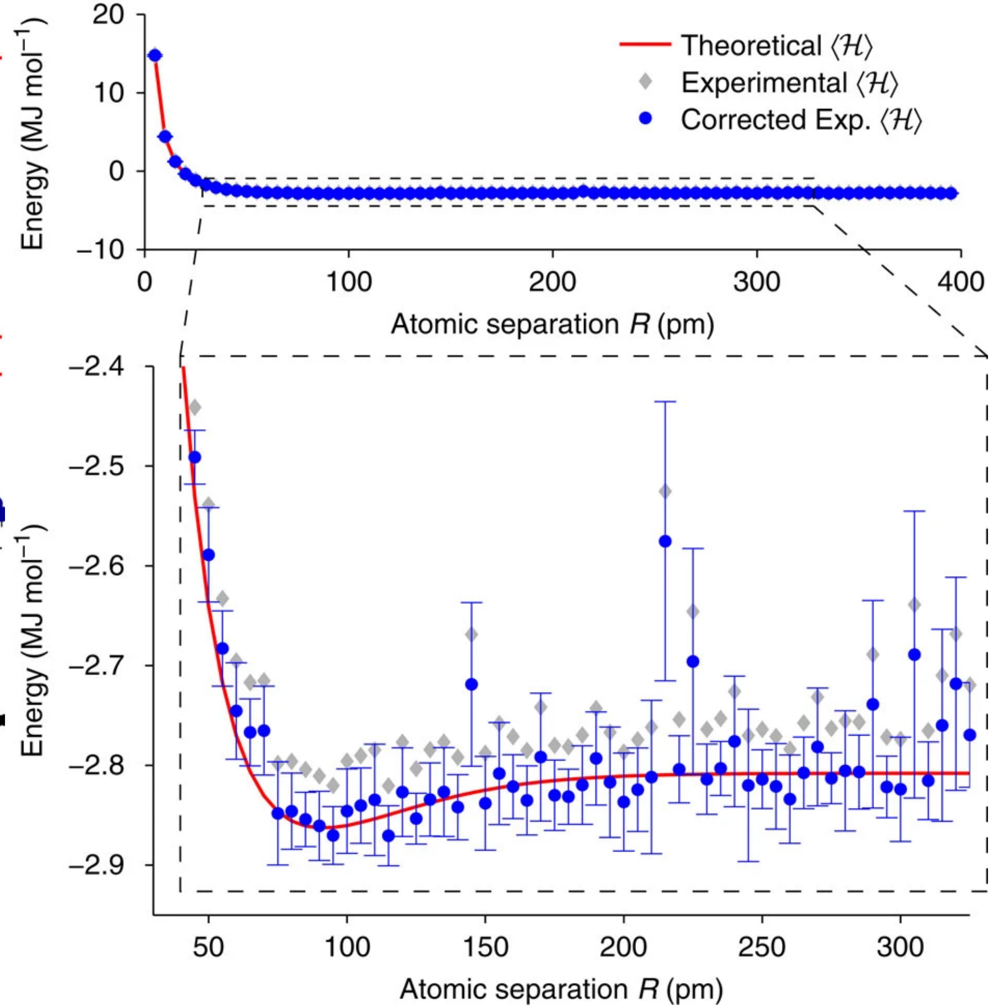
The Unitary Coupled Cluster (UCC): It adds quantum correlations to the Hartree-Fock (HF) approximation (a classically-inefficient procedure).

Other problem inspired Ansatze: QAOA, VQE, VHA, ….

Molecular quantum chemistry

Ground state of He–H+ for a specific molecular separation



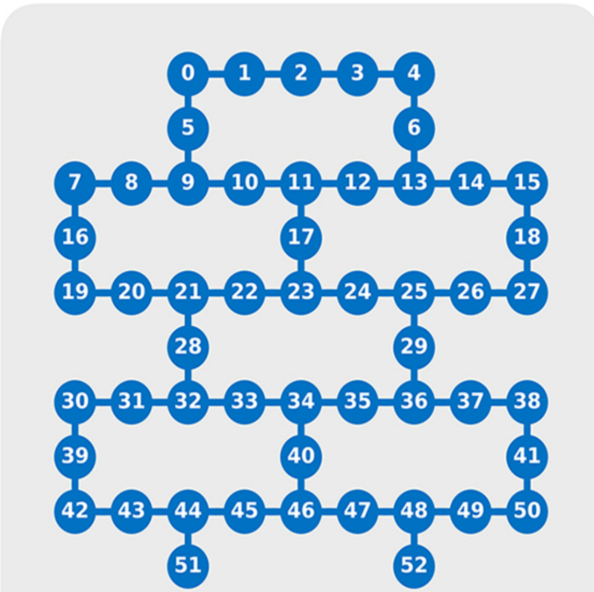


Bond dissociation curve of the He-H+ molecule.

Peruzzo et al. *A variational eigenvalue solver on a photonic quantum processor*. Nat Commun 5, 4213 (2014). https://doi.org/10.1038/ncomms5213

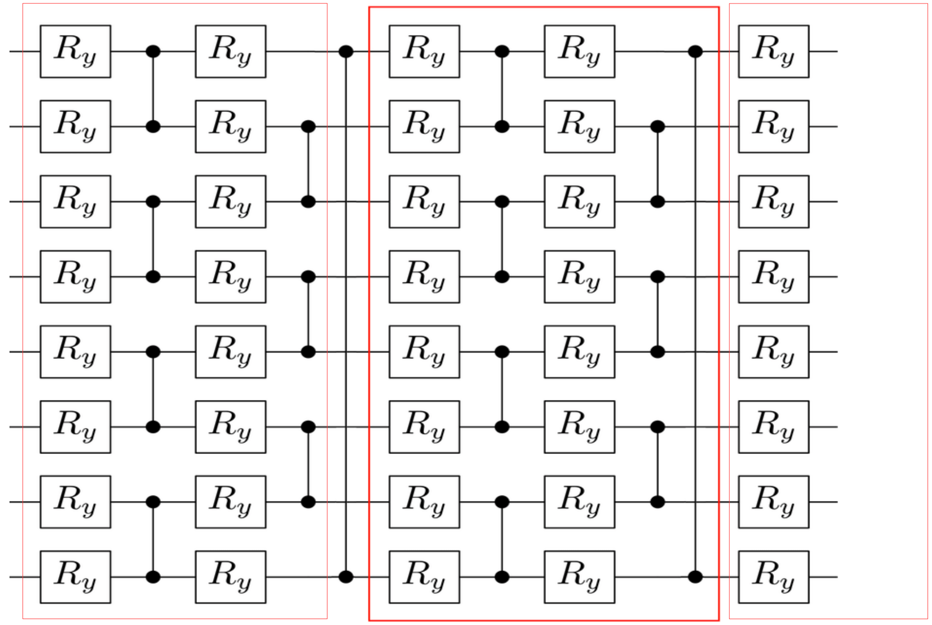
B2: Hardware-efficient Ansatz

53 Qubit Rochester Device



limited connectivity

limited set of basis gates



1st layer **2nd layer** **...**

gates errors and decoherence

Qubit	Energy relaxation time T1 (μs)	Dephasing time T2 (μs)	Frequency (GHz)	Readout error rate	Single-qubit U2 error rate	CNOT error rate
Q0	98.33551265	46.82808058	4.641200919	5.50000e-2	3.19722e-4	cx0_1: 9.422e-3
Q1	66.80352570	84.08716319	4.719992563	6.05e-2	5.76695e-4	cx1_0: 9.422e-3 cx1_2: 1.594e-2 cx1_3: 1.747e-2
Q2	77.96055113	88.27547132	4.761962111	4.04999e-2	6.51329e-4	cx2_1: 1.594e-2
Q3	93.81392649	86.04122557	4.687003753	5.04999e-2	5.11595e-4	cx3_1: 1.747e-2 cx3_4: 1.208e-2
Q4	57.44885729	40.31605568	4.923978085	4.00000e-2	6.05968e-4	cx4_3: 1.208e-2
Ave.	78.87247466	69.10959927	4.746827487	4.93e-2	5.33062e-4	1.37e-2

Limited Quantum Volume

8192

Quantinuum

(20 qubits)

Structure of a VQA

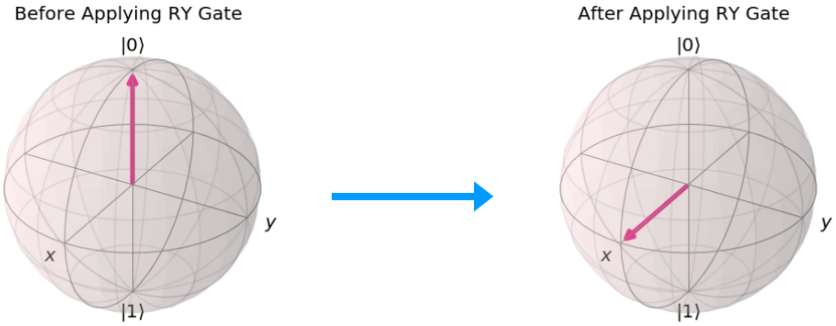
C. Measurements & D. Optimisation

On a QC measures are performed in the computational basis

$$\langle \hat{\sigma}^z \rangle = p_0 - p_1$$

Measurements on a different basis are preceded by a rotation

$$\langle \hat{\sigma}^x \rangle = \langle R_y^\dagger\left(\frac{\pi}{2}\right)\hat{\sigma}^z R_y\left(\frac{\pi}{2}\right)\rangle$$



Pauli strings measured accordingly

$$\langle \hat{P} \rangle = \langle \prod_{j=1}^{N} \hat{\sigma}_j^z \rangle_{R_j^\alpha}$$

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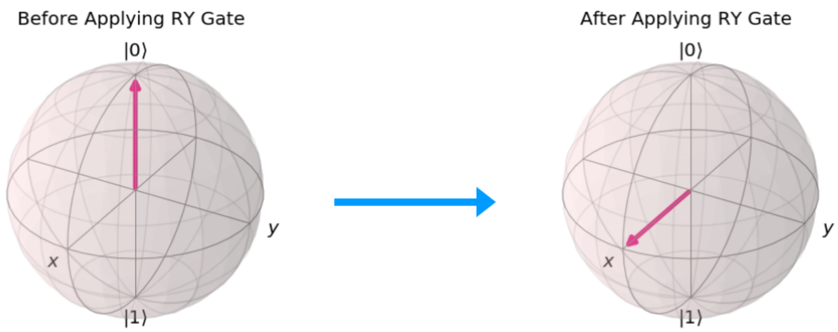

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$$\min_\theta O\left(\theta, \left\{\langle \hat{H} \rangle_{U(\theta)}\right\}\right)$$

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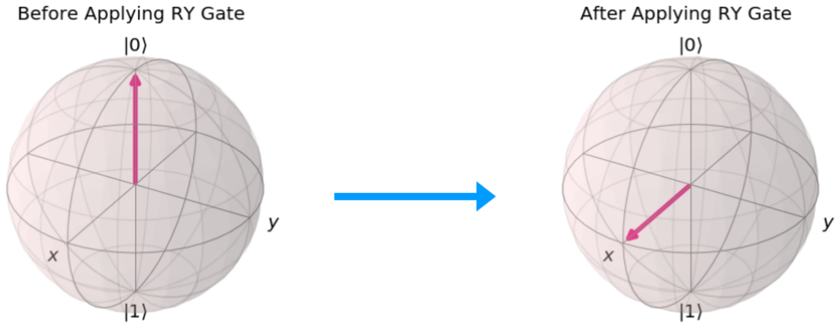

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- Gradient-free approaches (Bayesian optimisation, Nelder-Mead method, genetic algorithms,…): Global optimisers that find efficiently a global minimum, but very costly.

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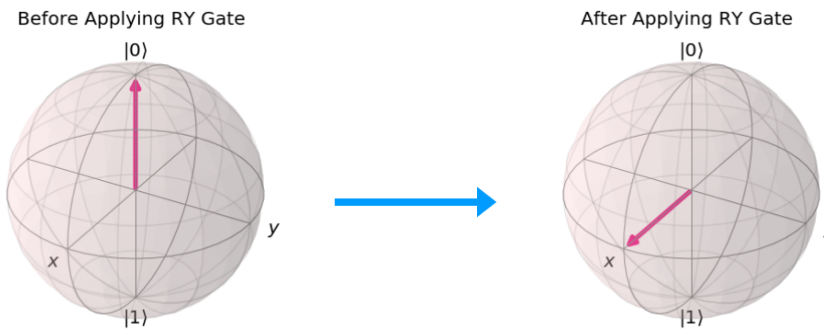

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However, on a QC:

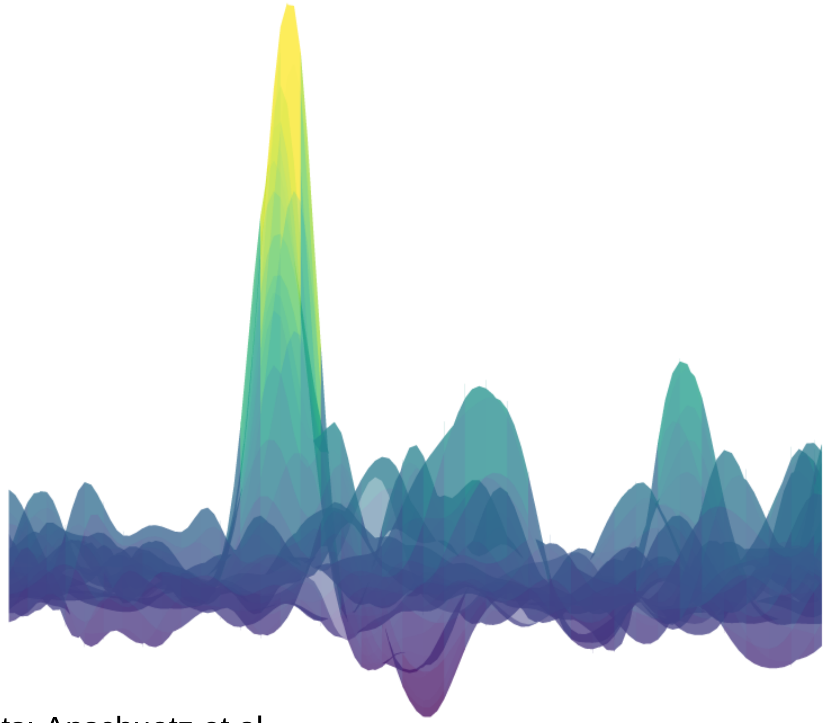
- Sampling noise and gate noise on NISQ devices disturb the landscape of the objective function
- The precision of the measured expectation value is limited by the sample shot number

Structure of a VQA

C. Measurements & D. Optimisation

$$\min_\theta O\left(\theta, \left\{\langle\hat{H}\rangle_{U(\theta)}\right\}\right)$$

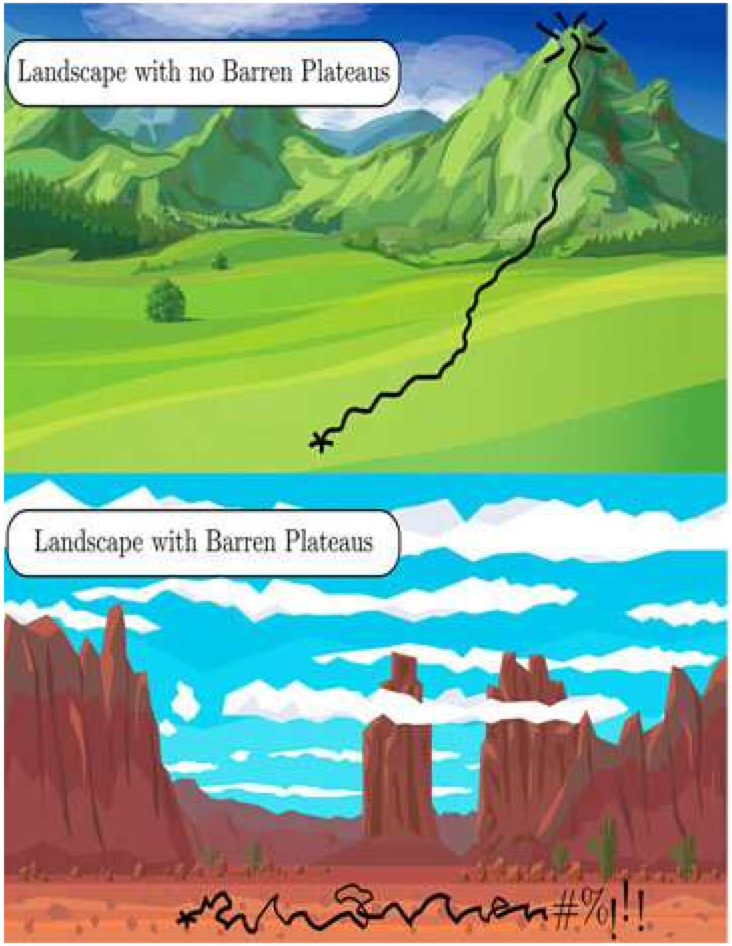
Local minima



Credits: Anschuetz et al.,
Quantum variational algorithms are swamped with traps.
Nat Commun 13, 7760 (2022).
https://doi.org/10.1038/s41467-022-35364-5

Arrasmith et al., *Effect of barren plateaus on gradient-free optimization*, Quantum 2021, 5, 558

Barren Plateaus



Credits: Los Alamos National Laboratory

Gibbs state on a QC
motivations

Definition of Gibbs states

$$\rho_\beta = \frac{e^{-\beta H}}{Z_\beta}\ , \ \beta = \frac{1}{k_B T}$$

$$Z_\beta = Tr\left\{e^{-\beta H}\right\} = \sum_{i=1}^{d} e^{-\beta E_i}$$

Usefulness of Gibbs states

quantum simulation
quantum machine learning
quantum optimization
open quantum systems
Sampling from Gibbs states used in:
combinatorial optimization problems
semidefinite programming
training quantum Boltzmann machines

Properties of Gibbs states

- Minimizes the Helmholtz free energy

$$F_\beta(\rho) = \mathrm{Tr}\left[H\rho\right] - \beta^{-1} S(\rho)$$

where the von Neumann entropy is

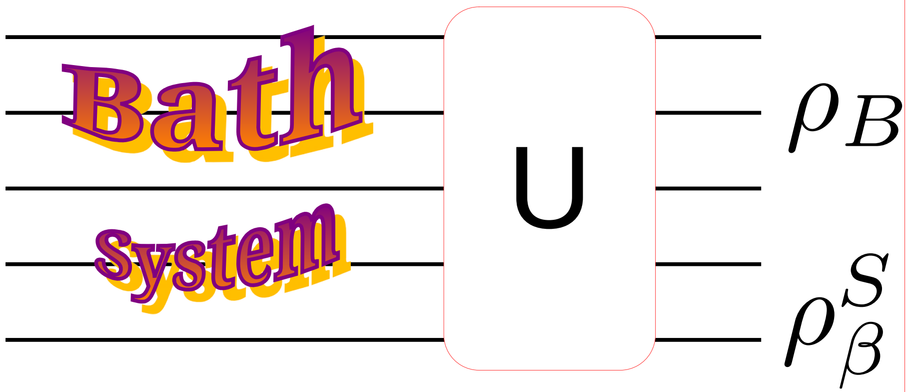
$$S(\rho) = -\mathrm{Tr}\left[\rho \ln \rho\right] = -\sum_{i=1}^{d} p_i \ln p_i$$

- It is an equilibrium state
- It is unique (for quantum spin models on finite lattices)
- It is a completely passive state

Matsui, *Purification and Uniqueness of Quantum Gibbs States*, Commun. Math. Phys. 162, 321-332 (1994)

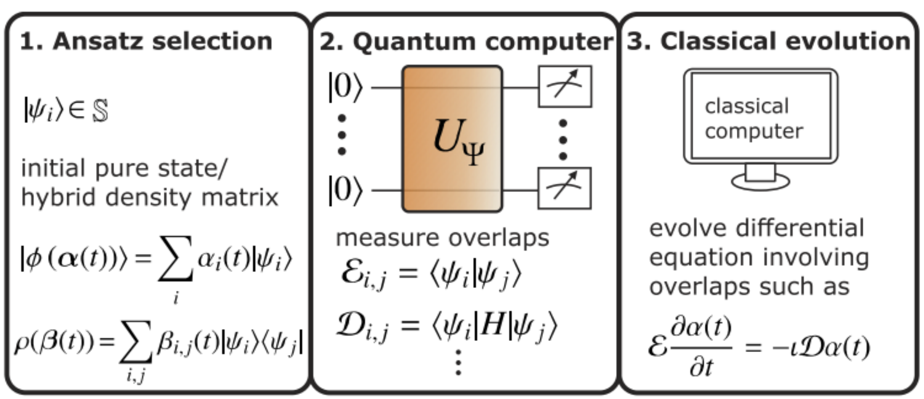
Gibbs state on a QC
a set of approaches

Mimick the process of thermalisation



Drawbacks: thermalisation time, reservoir qubits,..

Riera, A.; Gogolin, C.; Eisert, J.
Thermalization in Nature and on a Quantum Computer.
Phys. Rev. Lett. 2012, 108, 080402−080406

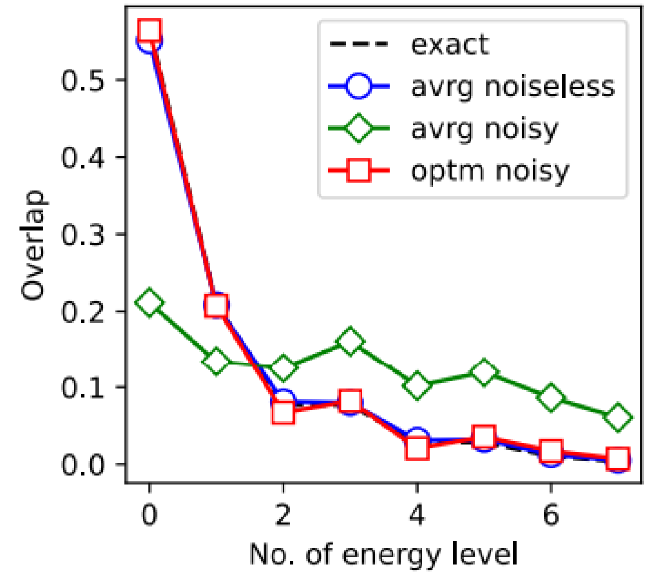


Haug and Bharti, *Generalized quantum assisted simulator* 2022
Quantum Sci. Technol. 7 045019

Implement effective imaginary-time evolution

$$\mathbb{E}_\psi e^{-\beta H/2}|\psi\rangle\langle\psi|e^{-\beta H/2} \propto \exp(-\beta H)$$

$|\psi\rangle$ is a random initial state



Heisenberg Hamiltonian with 3 system qubits and 2 ancilla qubits

Drawbacks: ITE requires non-unitary dynamics

Shtanko et al., *Algorithms for Gibbs state preparation on noiseless and noisy random quantum circuits,* arXiv:2112.14688

Motta et al., *Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution.* Nat. Phys. 16, 205–210 (2020). https://doi.org/10.1038/s41567-019-0704-4

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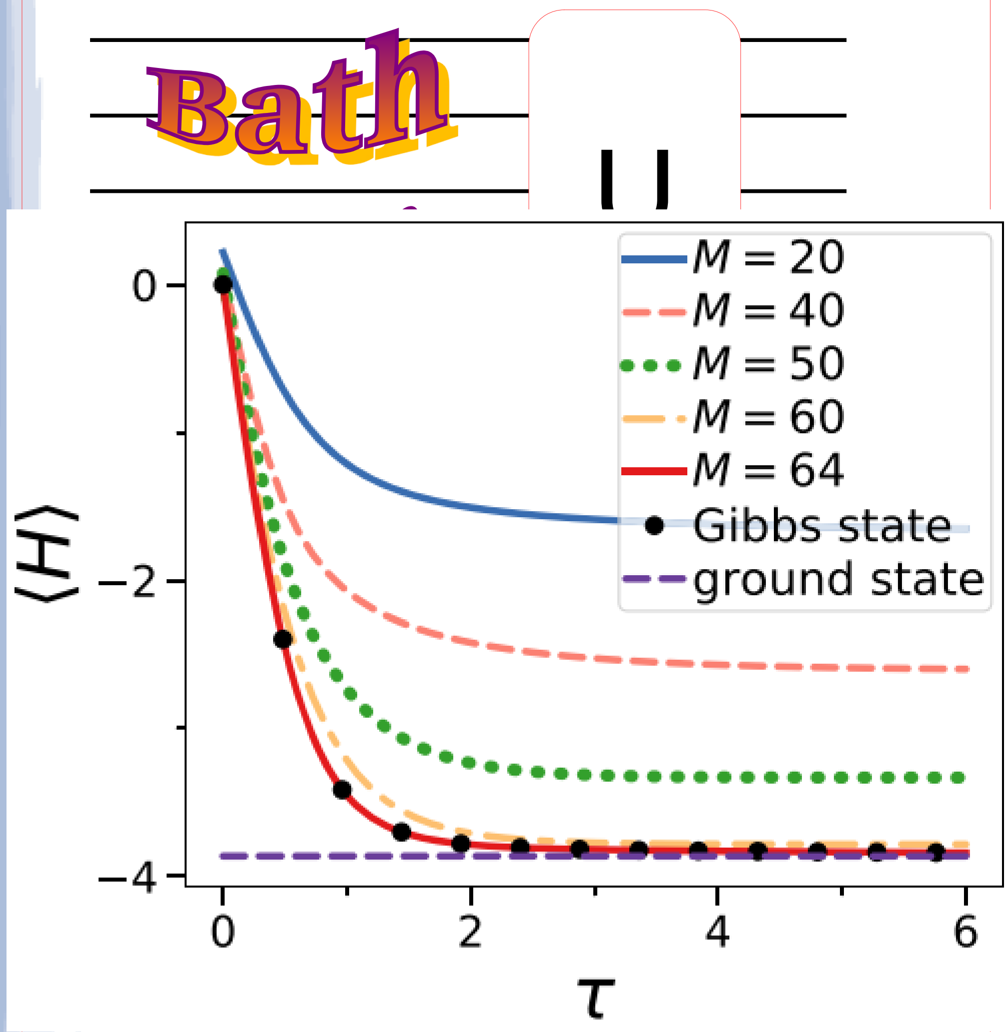

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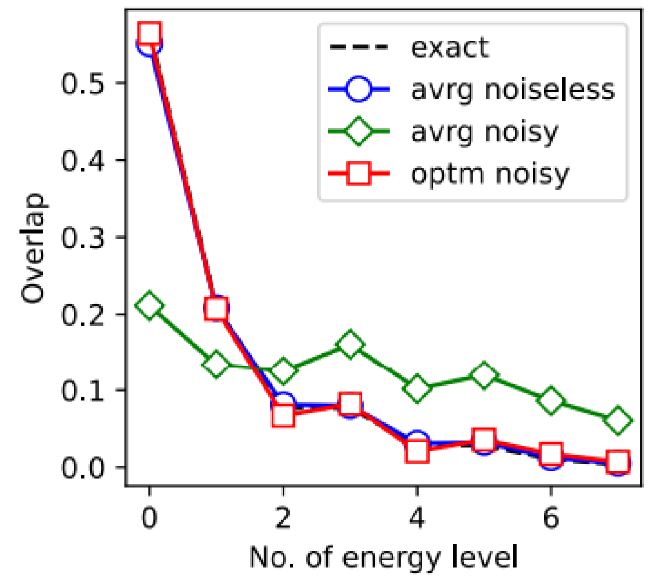

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Gibbs state on a QC
the variational approach

The free energy is
a faithful cost function

$$F_\beta(\rho) = \mathrm{Tr}\,\{H\rho\} - \beta^{-1} S(\rho)$$

$\mathrm{Tr}\{H\rho\}$ can be “easily” measured

$\mathrm{S}(\rho)$ however, is not an observable!

Approaches to estimate
the von Neumann entropy

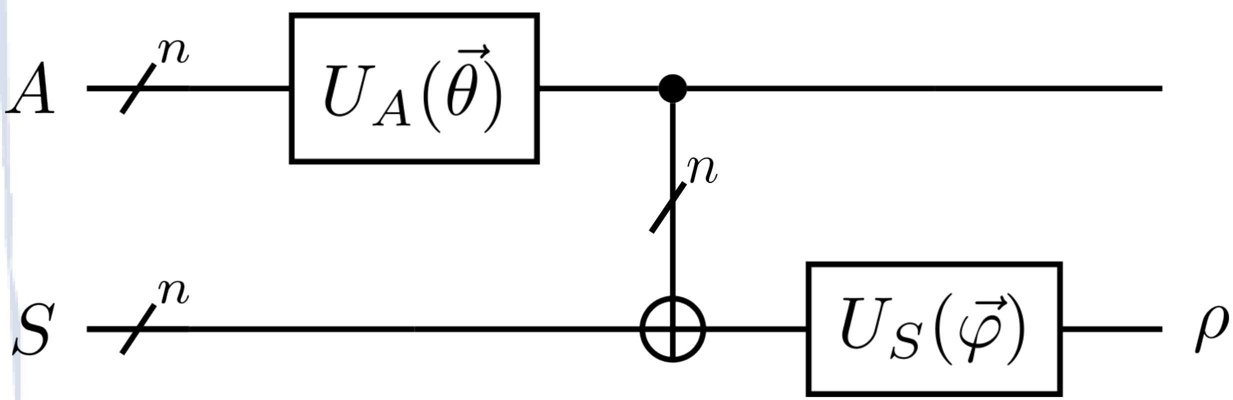
$$\tilde{S}(\rho) = \sum_{m=1}^{M} \left(b_m^{(1)} \mathrm{Tr}(\rho \cos(pt_m)) + b_m^{(2)} \mathrm{Tr}(\rho\, sin(pt_m)) \right)$$

Chowdhury, A. N., G. H. Low, and N. Wiebe (2020), arXiv:2002.00055 .

$$S_K(\rho) = \sum_{k=1}^{K} \frac{(-1)^k}{k} \mathrm{tr}[(\rho - I)^k \rho] = \sum_{j=0}^{K} C_j\, \mathrm{tr}(\rho^{j+1}).$$

Y. Wang, G. Li, and X. Wang, Phys. Rev. Applied 16,054035 (2021).

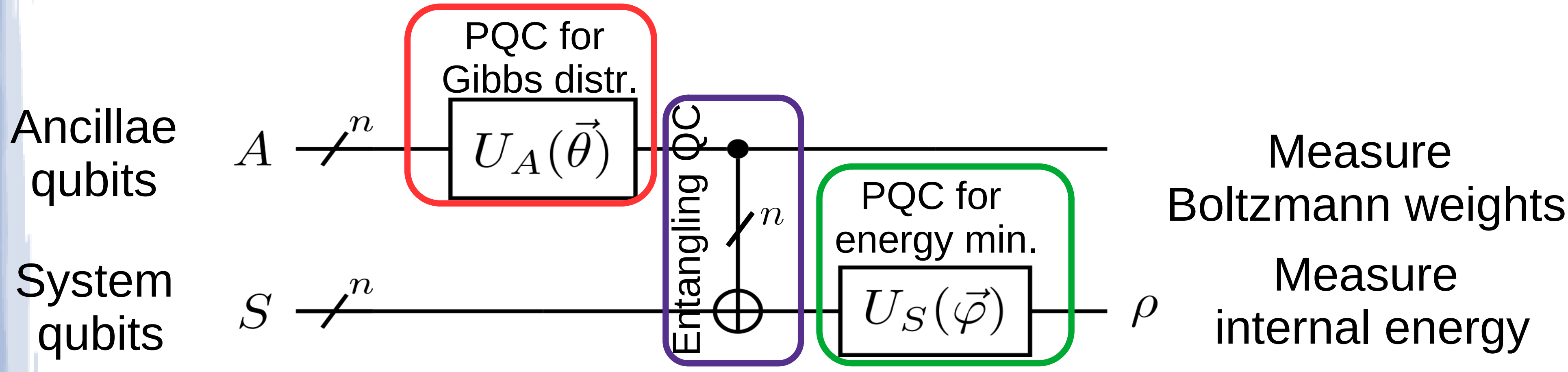
Our approach: generate a **diagonal** probability distribution function



$$\mathcal{S}(\rho) = -\sum_{i=1}^{d} p_i \ln p_i$$

$$\mathrm{Tr}\{\mathcal{H}\rho\}$$

Cost function $F_\beta(\rho) = \mathrm{Tr}\{H\rho\} - \beta^{-1}S(\rho)$



The unitary on the ancillae generates $(U_A \otimes I_S)\,|0\rangle_{AS}^{\otimes 2n} = |\psi\rangle_A \otimes |0\rangle_S^{\otimes n}$

A set of CNOT gates is applied between ancillae and system qubits $\mathrm{CNOT}_{AS} \equiv \bigotimes_{i=1}^{n} \mathrm{CNOT}_{A_i S_i}$

The reduced density matrices of A and S are identical

$$\mathrm{Tr}_S\left\{\mathrm{CNOT}_{AS}(|\psi\rangle\langle\psi|_A \otimes |0\rangle\langle 0|_S^{\otimes n})\mathrm{CNOT}_{AS}^\dagger\right\} = \mathrm{diag}\,(p_1, p_2, \ldots, p_d)$$

$$\mathrm{Tr}_A\left\{\mathrm{CNOT}_{AS}(|\psi\rangle\langle\psi|_A \otimes |0\rangle\langle 0|_S^{\otimes n})\mathrm{CNOT}_{AS}^\dagger\right\} = \mathrm{diag}\,(p_1, p_2, \ldots, p_d)$$

The unitary on the system rotates from the computational basis to a different basis

$$\rho = U_S \mathrm{diag}\left(p_1, p_2, \ldots, p_d\right) U_S^\dagger = \sum_i p_i \left|\psi_i\right\rangle\!\left\langle\psi_i\right|$$

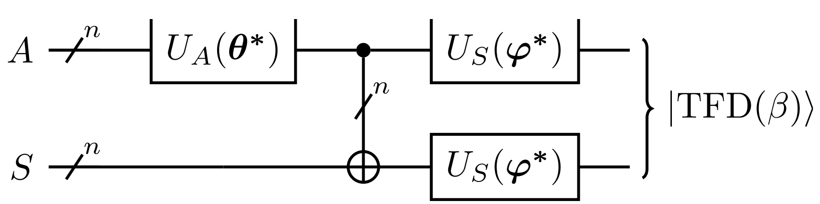
The result of the minimisation of the cost function

$$\rho_\beta = \arg\min_{\theta,\varphi} F_\beta\left(\rho\left(\theta,\varphi\right)\right) = \arg\min_{\theta,\varphi}\left(Tr\left\{H\rho_S(\theta,\varphi)\right\} - \beta^{-1} S\left(\rho_A(\theta)\right)\right)$$

$$p_i = \frac{e^{-\beta E_i}}{Z} \quad \& \quad \left|\psi_i\right\rangle = \left|E_i\right\rangle$$

The Gibbs State

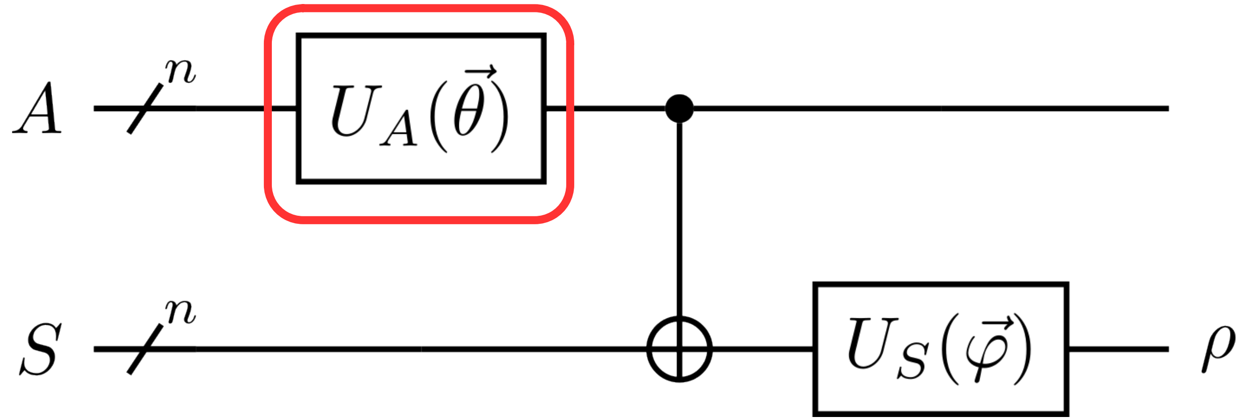
Generation of thermofield double states:
condensed matter physics, black holes and traversable wormholes

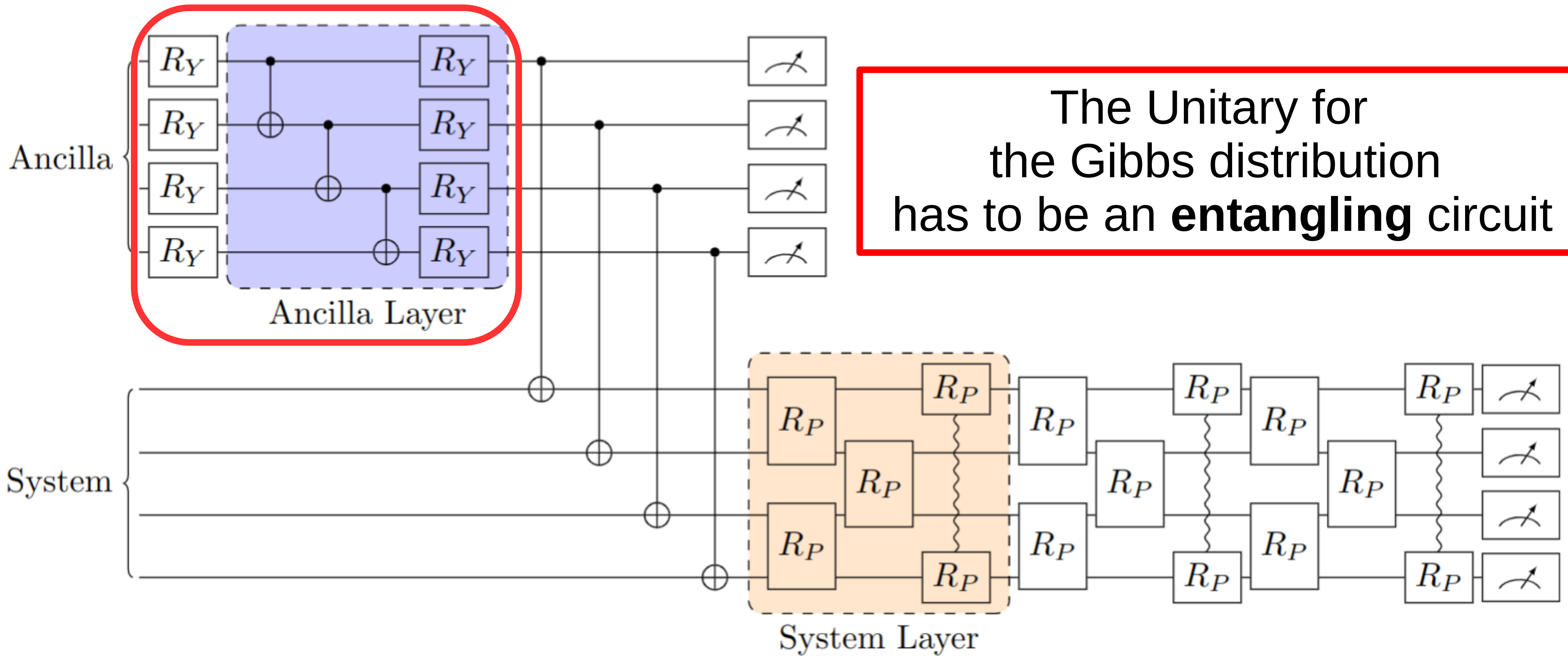


$$\left|\mathrm{TFD}(\beta)\right\rangle = \frac{1}{\sqrt{Z}} \sum_i e^{-\frac{\beta E_i}{2}} \left|i\right\rangle_A \left|i\right\rangle_S$$

Wu and Hsieh, *Variational Thermal Quantum Simulation via Thermofield Double States*, Phys. Rev. Lett. 123, 220502 (2019)
Sagastizabal et al, *Variational preparation of finite-temperature states on a quantum computer, , npj Quantum Information 7, 1 (2021),*

Generating the Gibbs distribution





The Unitary for
the Gibbs distribution
has to be an **entangling** circuit

With only local gates (non-entangling gates) only specific PDFs can be searched

$$\bigotimes_{i=0}^{n-1} R_Y(\theta_i)\,|0\rangle_i = \bigotimes_{i=0}^{n-1} (b_i\,|0\rangle_i + b_i\,|1\rangle_i) = \sum_{i=0}^{d-1} \prod_{j\in S_{i=0}} a_i \prod_{k\in S_{i=1}} b_i\,|i\rangle = \sum_{i=0}^{d-1} p_i\,|i\rangle$$

As each p_i is the Boltzmann weight of the Gibbs distribution

$$p_i = \prod_{j\in S_{i=0}} \cos\left(\frac{\theta_j}{2}\right) \prod_{k\in S_{i=1}} \sin\left(\frac{\theta_k}{2}\right) = \frac{e^{-\beta E_i}}{Z}$$

Only PDFs satisfying very restictive criteria can be searched
(the non-entangling Ansatz has little expressibility)

$$\frac{p_0}{p_1} = \frac{a_0}{b_0}$$

$$\frac{p_0}{p_2} = \frac{a_1}{b_1}$$

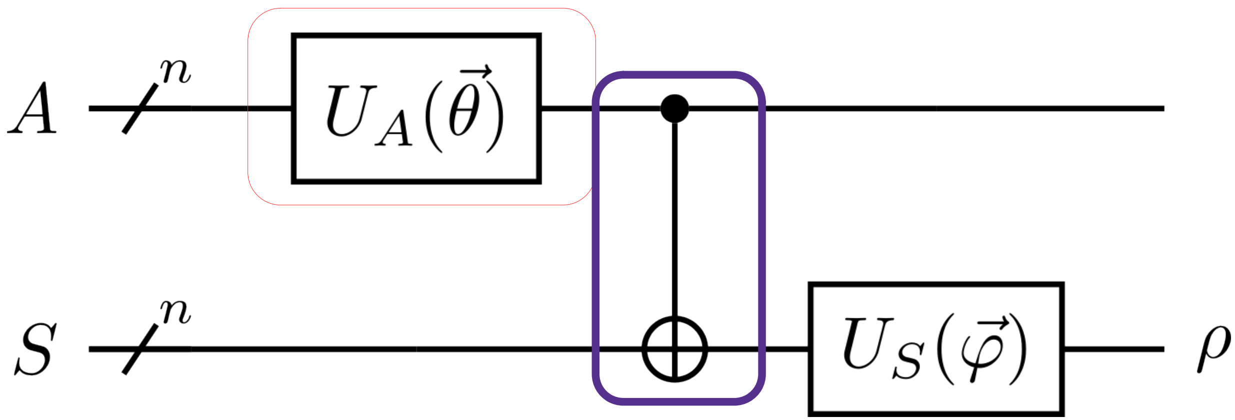
$$\frac{p_0}{p_3} = \frac{a_0 a_1}{b_0 b_1}$$

$$p_0 p_3 = p_1 p_2$$

$$e^{-\beta E_0} e^{-\beta E_3} = e^{-\beta E_1} e^{-\beta E_2}.$$

$$E_0 + E_3 = E_1 + E_2$$

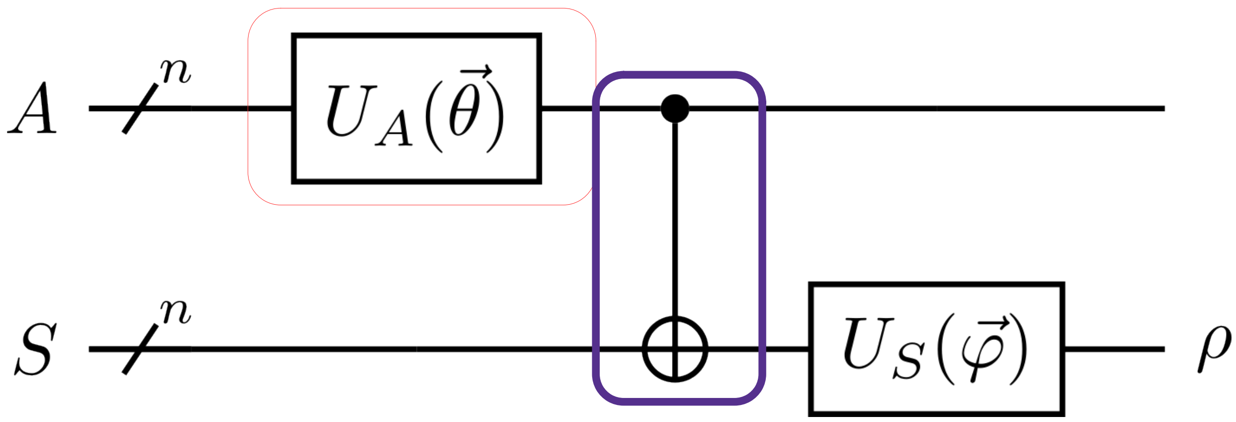
Mapping the PDF to the system



$$U_A = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1d} \\ u_{21} & u_{22} & \cdots & u_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ u_{d1} & u_{d2} & \cdots & u_{dd} \end{pmatrix}$$

$$|\psi_{AS}\rangle = \sum_{i=1}^{d} u_{i1} |\mathbf{i}\rangle_A |\mathbf{0}\rangle_S$$

Mapping the PDF to the system



$$U_A = \begin{pmatrix} u_{11} & u_{12} & \cdots & u_{1d} \\ u_{21} & u_{22} & \cdots & u_{2d} \\ \vdots & \vdots & \ddots & \vdots \\ u_{d1} & u_{d2} & \cdots & u_{dd} \end{pmatrix}$$

$$|\psi_{AS}\rangle = \sum_{i=1}^{d} u_{i1} |\mathbf{i}\rangle_A |\mathbf{0}\rangle_S$$

$$|\psi_{AS}\rangle = \sum_{i=1}^{d} u_{i1} |\mathbf{i}\rangle_A |\mathbf{i}\rangle_S \implies \rho_S = Tr_A[\rho_{AS}] = \sum_i |u_{i1}|^2 |\mathbf{i}\rangle\langle\mathbf{i}|$$

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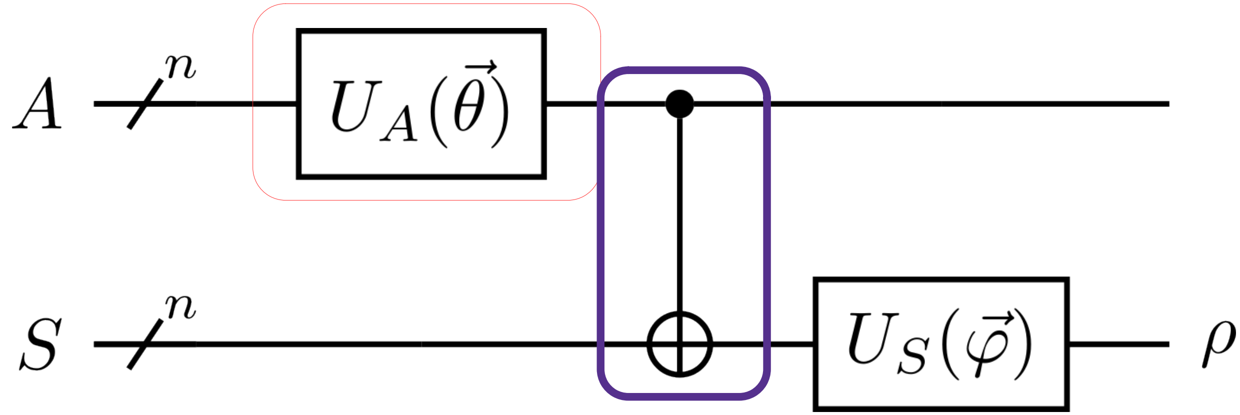

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Only the 1st column of U_A matters

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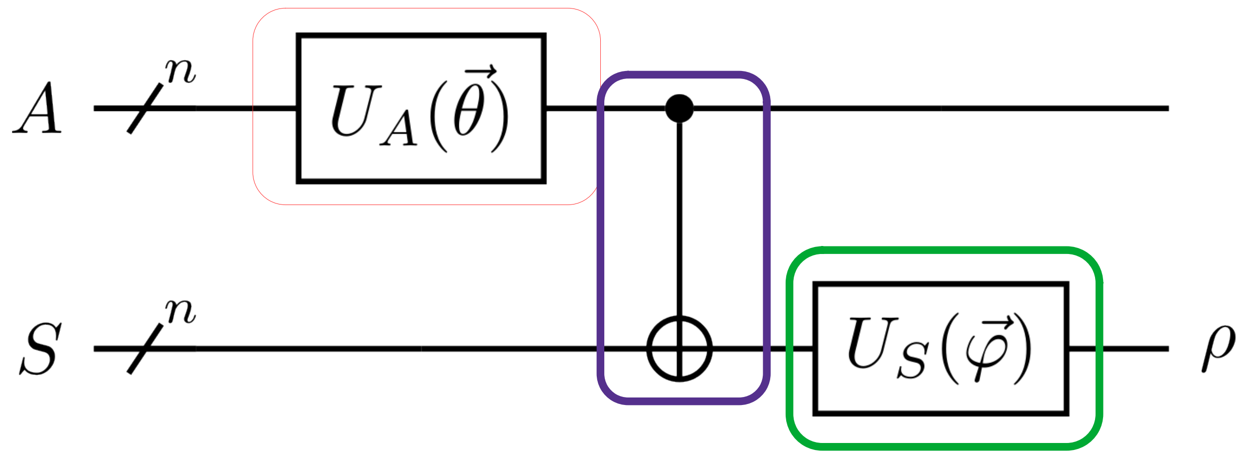
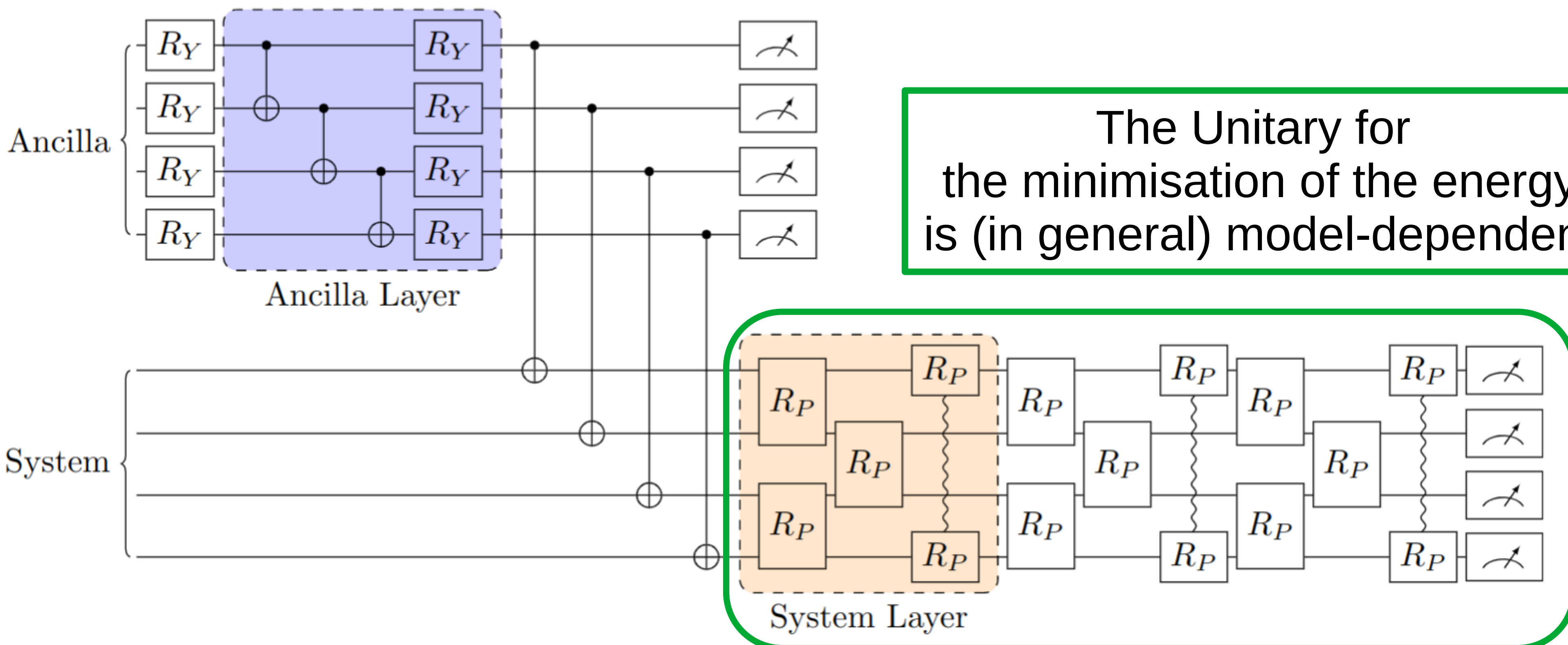
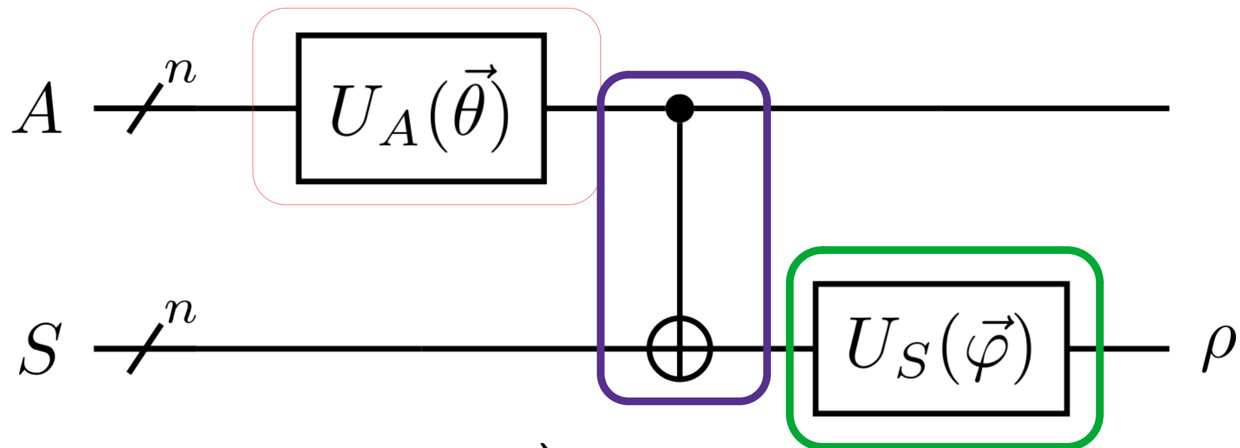
Minimising the energy





The Unitary for
the minimisation of the energy
is (in general) model-dependent

Minimising the energy



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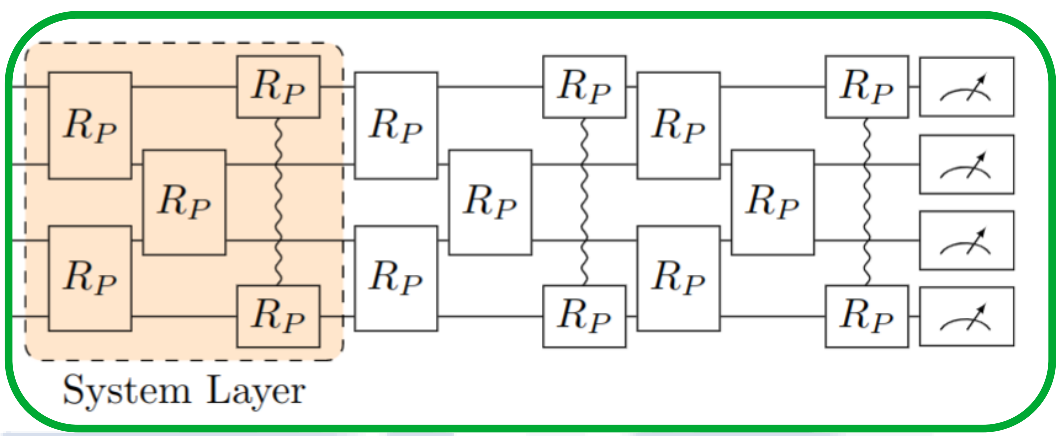
The Unitary for the minimisation of the energy is (in general) model-dependent

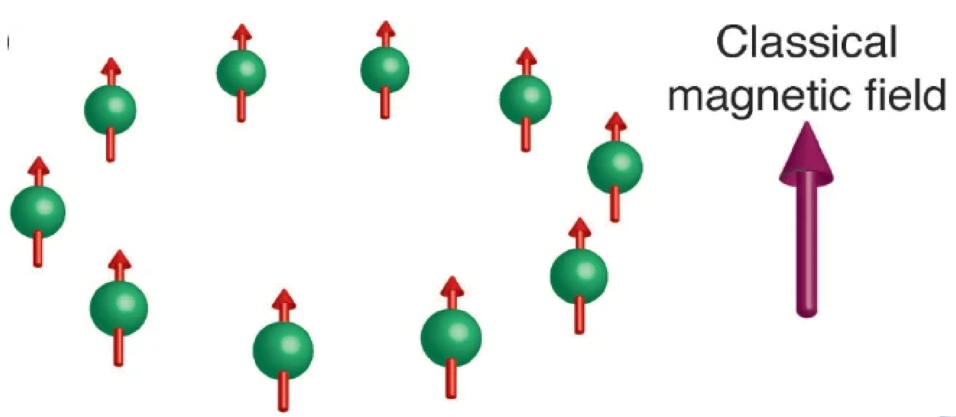
U_S rotates from the computational basis to the energy basis

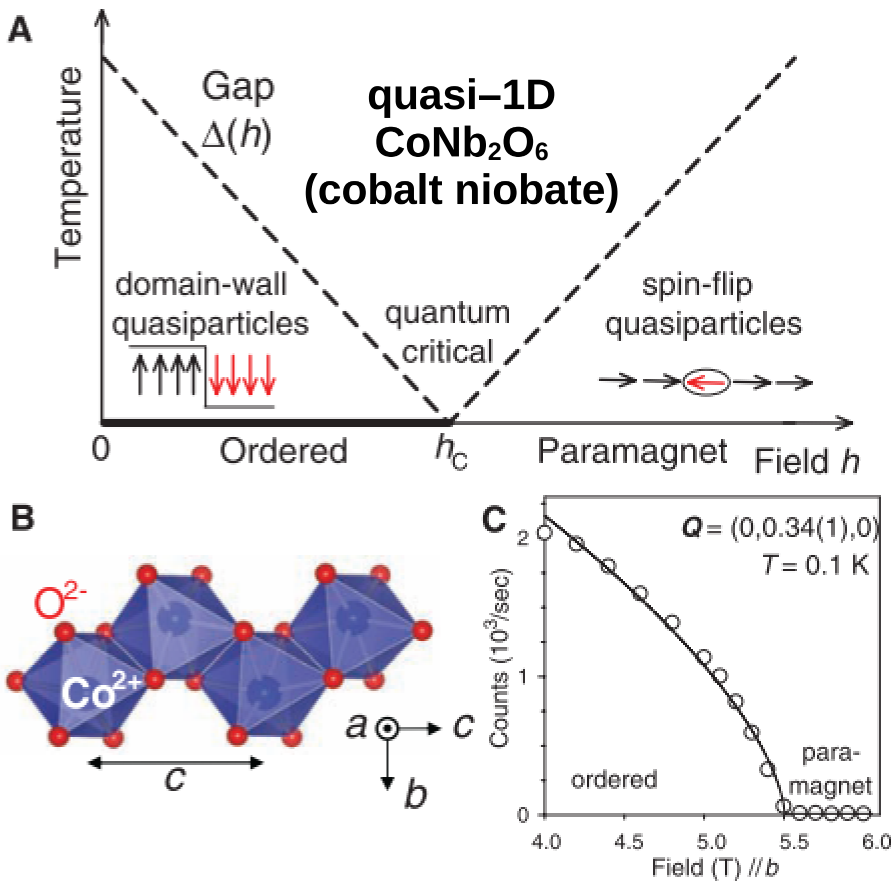
$$U_S\,|i\rangle = |E_i\rangle$$



The quantum Ising Hamiltonian

$$\hat{H} = -J \sum_n \hat{\sigma}_n^x \hat{\sigma}_{n+1}^x - h \hat{\sigma}_n^z$$





R. Coldea et al., *Quantum Criticality in an Ising Chain: Experimental Evidence for Emergent E_8 Symmetry,* Science 327, 177 (2010);

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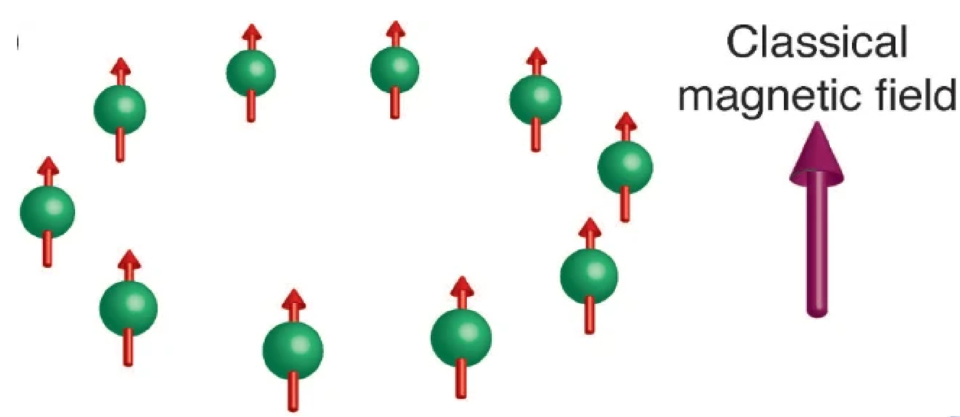
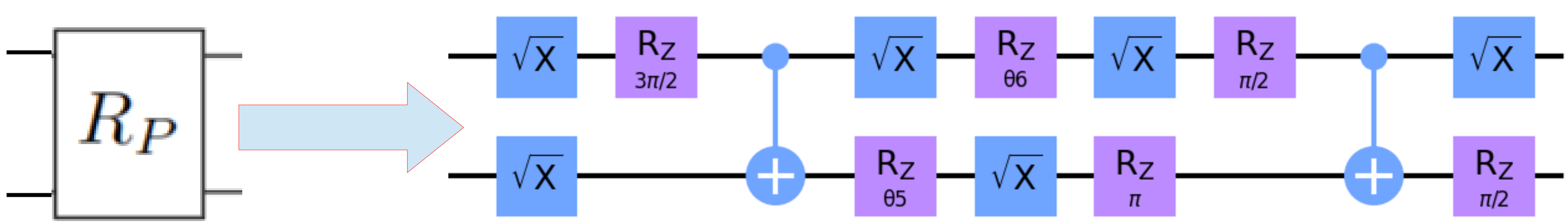


Z_2 symmetry → Parity-Preserving Ansatz

$$R_P(\varphi_i, \varphi_j) = R_{YX}(\varphi_j) \cdot R_{XY}(\varphi_i) = \begin{pmatrix} \cos\left(\frac{\varphi_i+\varphi_j}{2}\right) & 0 & 0 & \sin\left(\frac{\varphi_i+\varphi_j}{2}\right) \\ 0 & \cos\left(\frac{\varphi_i-\varphi_j}{2}\right) & -\sin\left(\frac{\varphi_i-\varphi_j}{2}\right) & 0 \\ 0 & \sin\left(\frac{\varphi_i-\varphi_j}{2}\right) & \cos\left(\frac{\varphi_i-\varphi_j}{2}\right) & 0 \\ -\sin\left(\frac{\varphi_i+\varphi_j}{2}\right) & 0 & 0 & \cos\left(\frac{\varphi_i+\varphi_j}{2}\right) \end{pmatrix}$$



2 CNOT
+
6 √x
gates

Results (state vector)

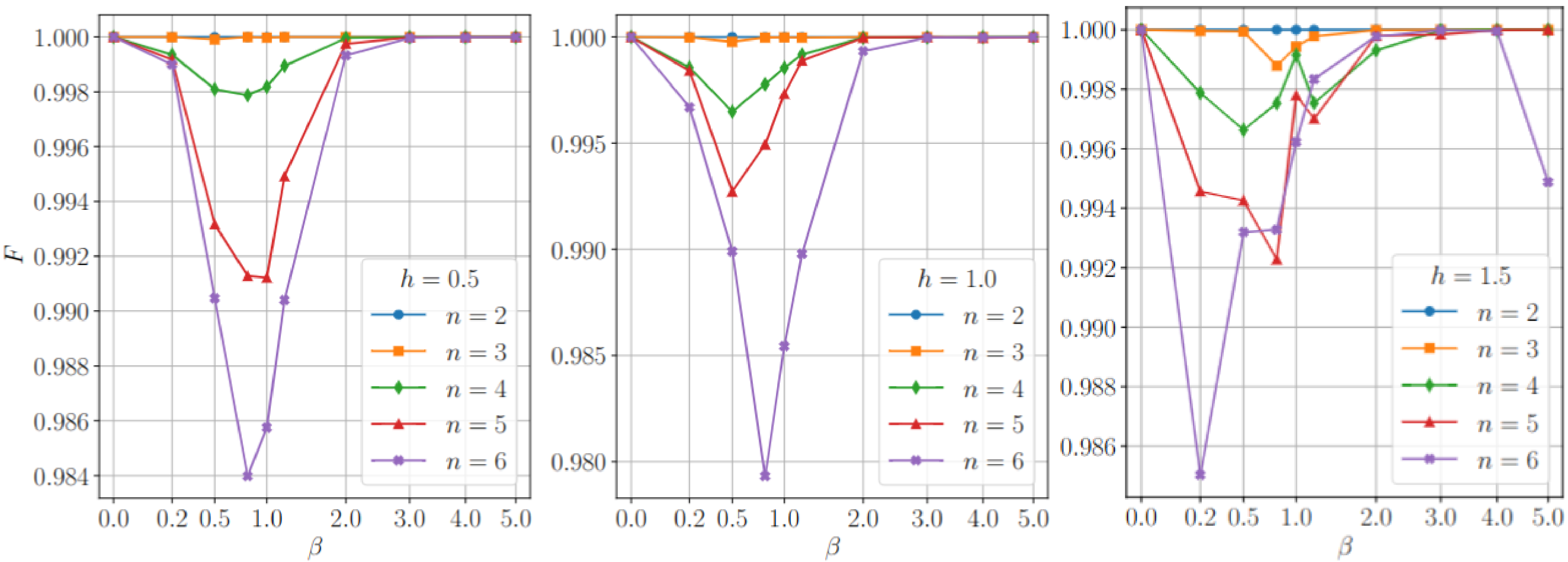
Measures for determining the quality of the prepared Gibbs state

$$F(\rho_1, \rho_2) = \sqrt{\sqrt{\rho_2}\rho_1\sqrt{\rho_2}}$$

$$D(\rho_1, \rho_2) = \frac{1}{2}||\rho_1 - \rho_2||_1$$

$$\left(||A||_1 := Tr\left\{\sqrt{A^\dagger A}\right\}\right)$$

$$1 - F(\rho_1, \rho_2) \leq D((\rho_1, \rho_2) \leq \sqrt{1 - F^2(\rho_1, \rho_2)}$$



Results (noisy-simulations & QC)

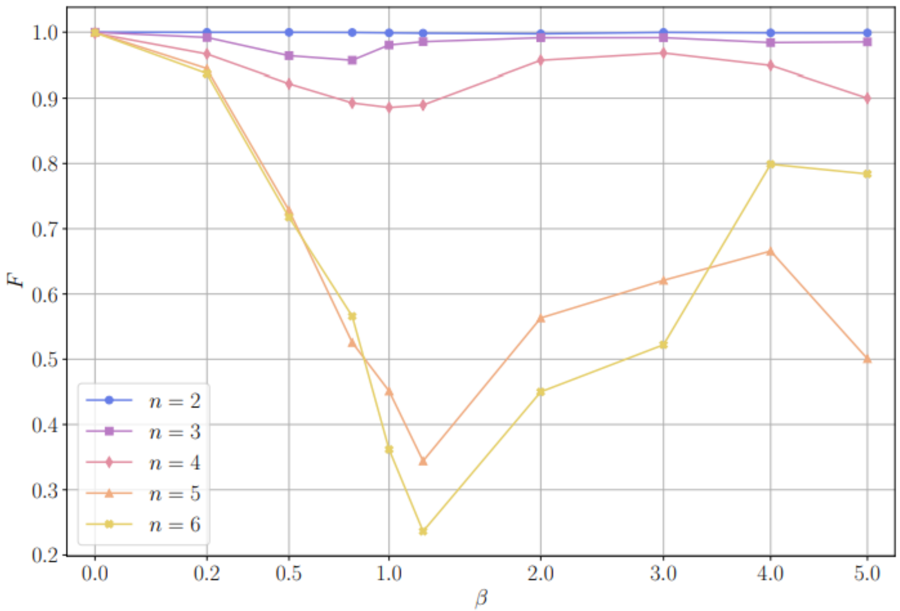


Figure 5: Fidelity F, of the obtained state via noisy simulations (using SPSA) of `ibmq_guadalupe` with the exact Gibbs state, vs inverse temperature β, for two to six qubits of the Ising model with $h = 0.5$. A total of ten runs are made for each point, with the optimal state taken to be the one that maximizes the fidelity.

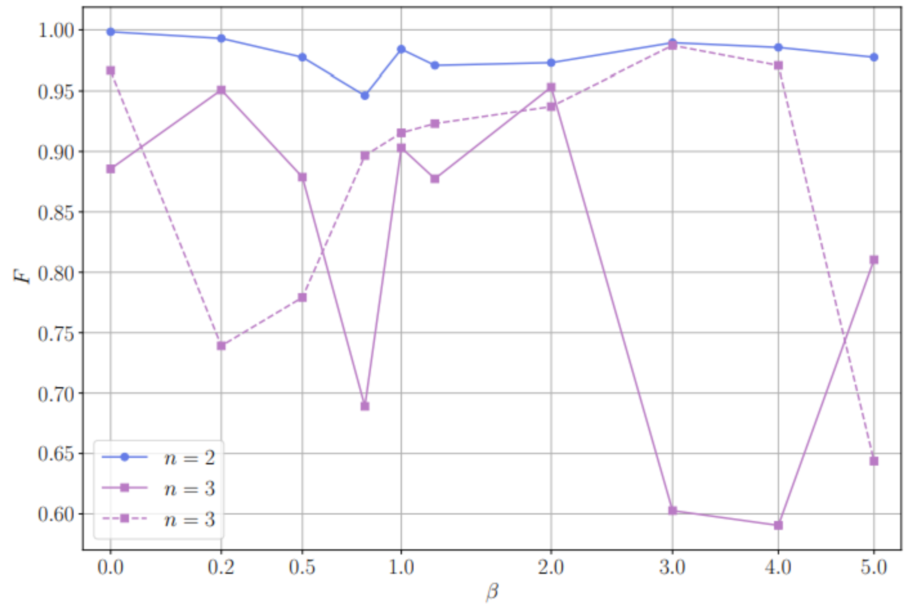
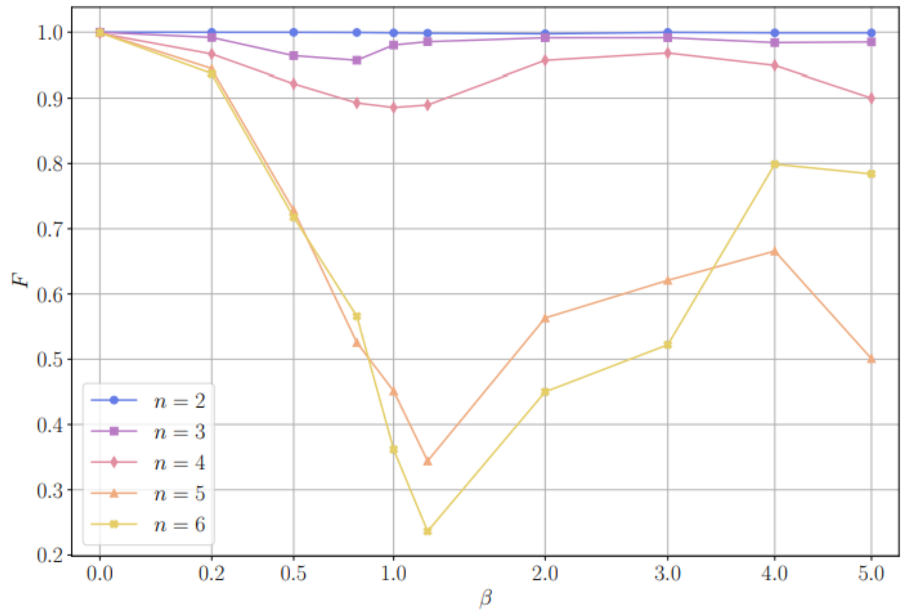


Figure 6: Fidelity F, of the obtained state (using SPSA) running directly on `ibm_nairobi` with the exact Gibbs state, vs inverse temperature β, for two and three qubits of the Ising model with $h = 0.5$. The dashed line represents the run with no R_P gate between non-adjacent qubits in the system layers. One run is carried out for $n = 2$, and $n = 3$ for the dashed line, and two runs for $n = 3$ for the solid line.

Results (noisy-simulations & QC)



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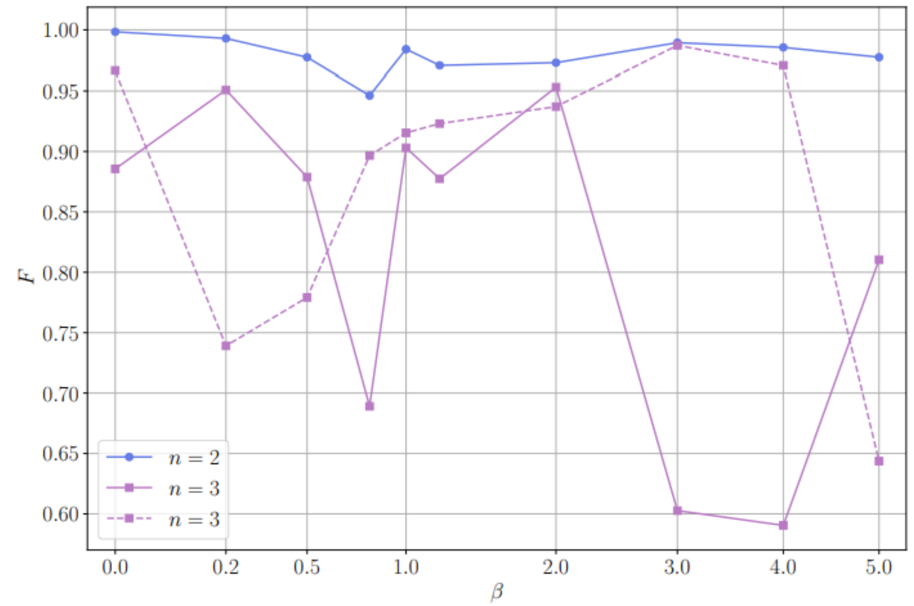

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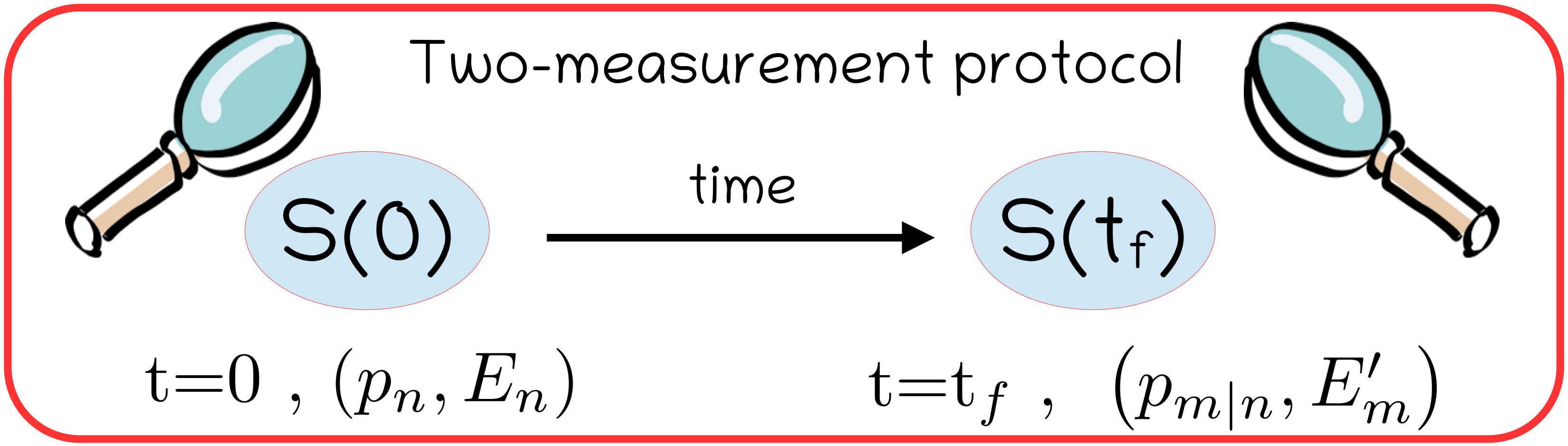
Take home messages:

- The VQA works very well...on a classical computer;
- "Use the QC as little as possible" → the algorithm works (well) within the given available quantum volume;
- Intermediate temperatures (β≃1) are more difficult to realise.

Applications in quantum thermodynamics: PDF of Work

$$p(w) = \sum_{nm} p_{m|n}(t_f)\, p_n(0)\, \delta\left(w - \left(E'_m(t_f) - E_n(0)\right)\right)$$



Peter Talkner, Eric Lutz, and Peter Hänggi, *Fluctuation theorems: Work is not an observable,* Phys. Rev. E 75, 050102R (2007)

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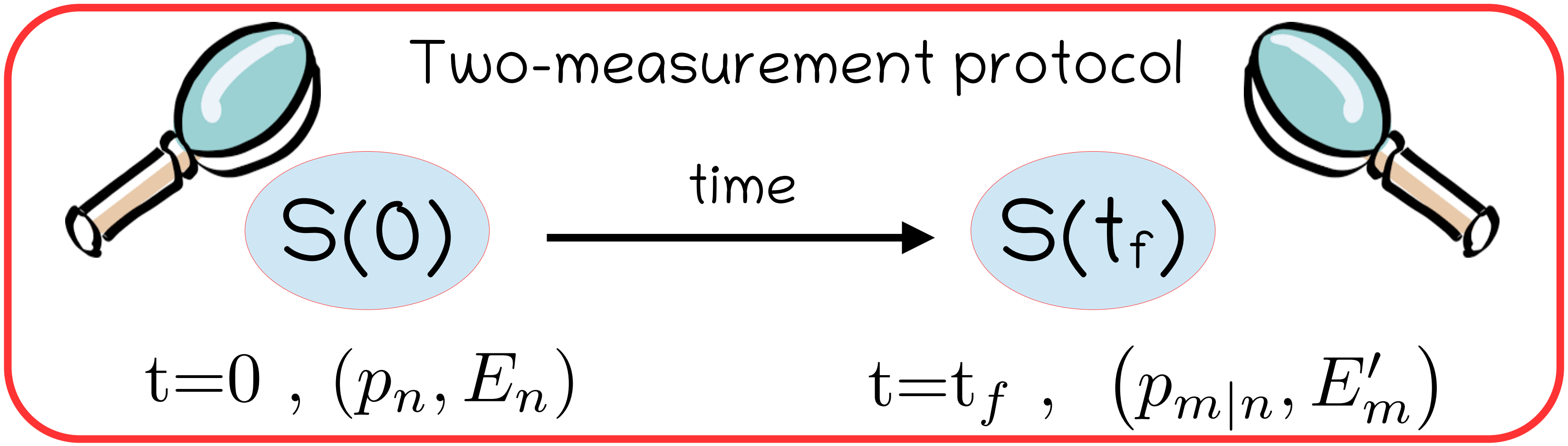

$$p_{m|n}(t_f) = \left|\langle E'_m | U(t_f) | E_n \rangle\right|^2 \xrightarrow{\text{sudden quench}} \left|\langle E'_m | E_n \rangle\right|^2$$

where U diagonalises H
and
V diagonalises H'

$$p_{m|n} = \left|\langle m' | V^\dagger U | n \rangle\right|^2$$

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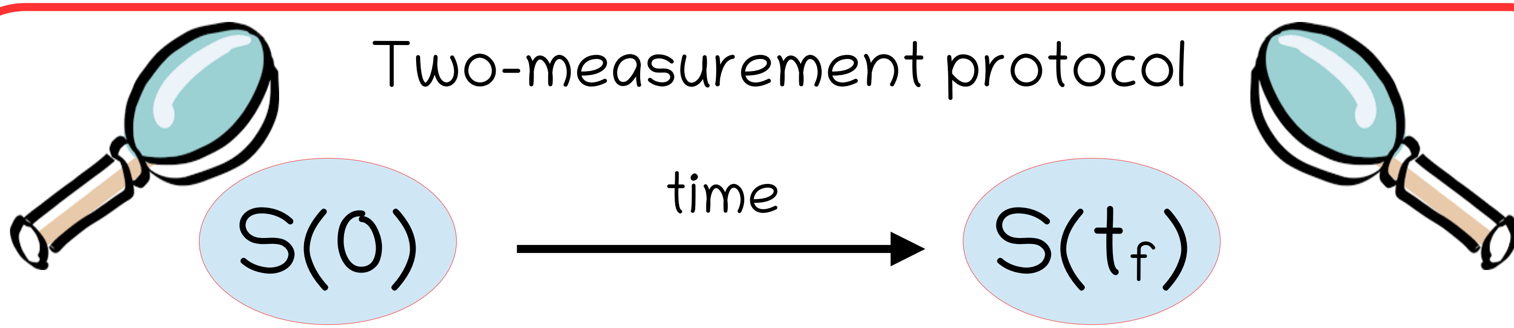
Two-measurement protocol



t=0 , (p_n, E_n) t=t$_f$, $(p_{m|n}, E'_m)$

Method for preparing Gibbs states in

Holmes et al.,
Quantum algorithms from fluctuation theorems: Thermal-state preparation,
Quantum 6, 825 (2022)

Conclusions

- Preparation of a thermal state (of an arbitrary system) on a quantum computer;
- Variational Quantum Algorithm to generate the thermal state (with an exact method to evaluate the von Neumann entropy);
- Efficient generation of the Gibbs state for the quantum Ising model at arbitrary temperatures (state-vector simulation);
- Efficient generation on a real NISQ device only for few qubits.

Outlooks

- Preparation of a thermal state of molecular systems (VQE works generally good);
- Application to the work PDF of an out-of-equilibrium protocol

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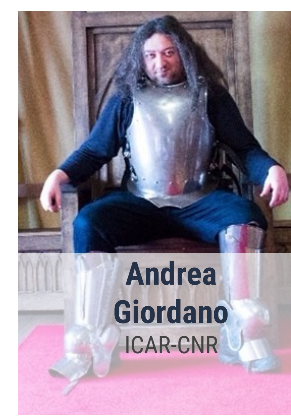
Jacopo Settino
Università della Calabria

Carlo Mastroianni
ICAR-CNR



Andrea Giordano
ICAR-CNR

Salvatore Lorenzo
University of Palermo

Variational Gibbs State Preparation on NISQ devices
https://arxiv.org/abs/2303.11276