INVESTIGATING THE BOSE-HUBBARD MODEL WITH IBM QUANTUM EXPERIENCE

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BY:
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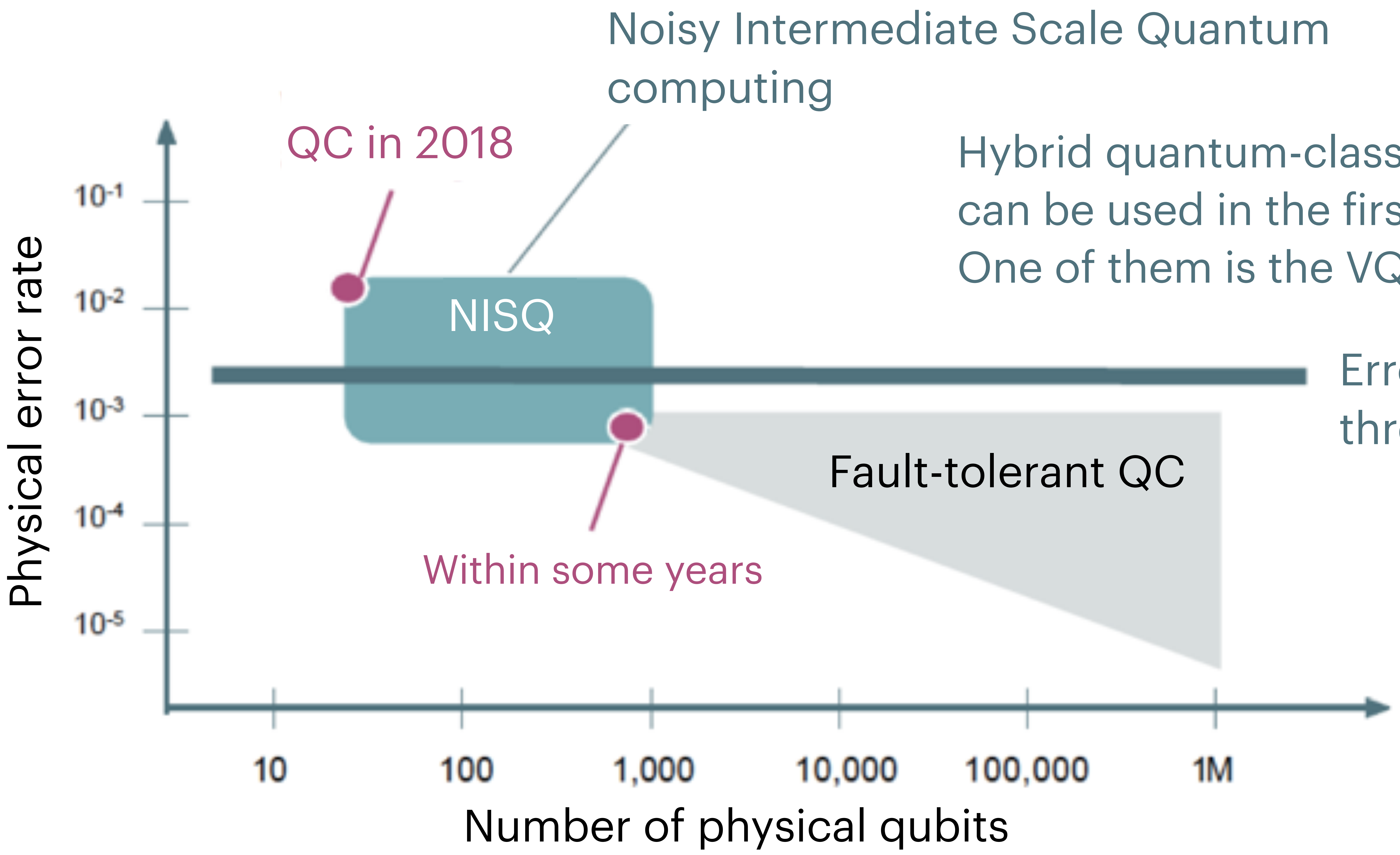
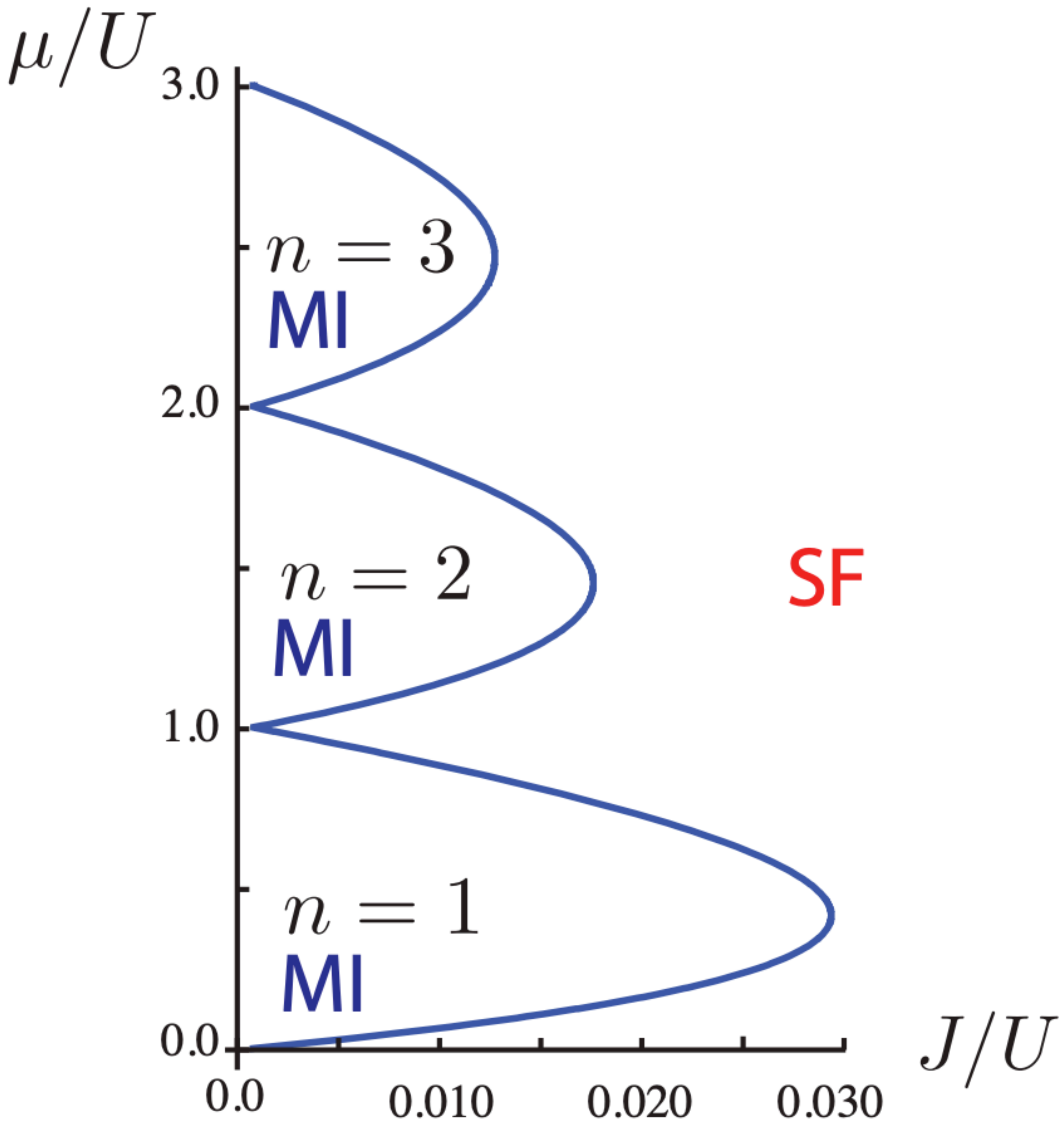
OUTLINE



Hybrid quantum-classical algorithms can be used in the first applications. One of them is the VQE.

Error correction threshold



BOSE-HUBBARD MODEL

$$\hat{H} = -J \sum_{\langle i,j \rangle} b_i^\dagger b_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$

Describes interacting spinless bosons in a lattice.

- J: hopping between sites.
- U: boson interaction.
- μ: number of particles in the system.

Quantum phase transition from a Mott insulator (MI) to a superfluid (SF). For N total particles, possible only if N is commensurate with the number of sites.

T=0, only ground state considered.

TWO-SITE MODEL

$$\hat{H} = -J(b_R^\dagger b_L + b_L^\dagger b_R) + \frac{U}{2}[\hat{n}_R(\hat{n}_R - 1) + \hat{n}_L(\hat{n}_L - 1)]$$

For N particles, there are N+1 possible occupation states of the system:

$$|i, N-i\rangle = |i\rangle_L \otimes |N-i\rangle_R$$

The hamiltonian can be easily diagonalized for low N.

Amplitudes c_i of the eigenvector's occupations are written in terms of U, for simplicity J=1.

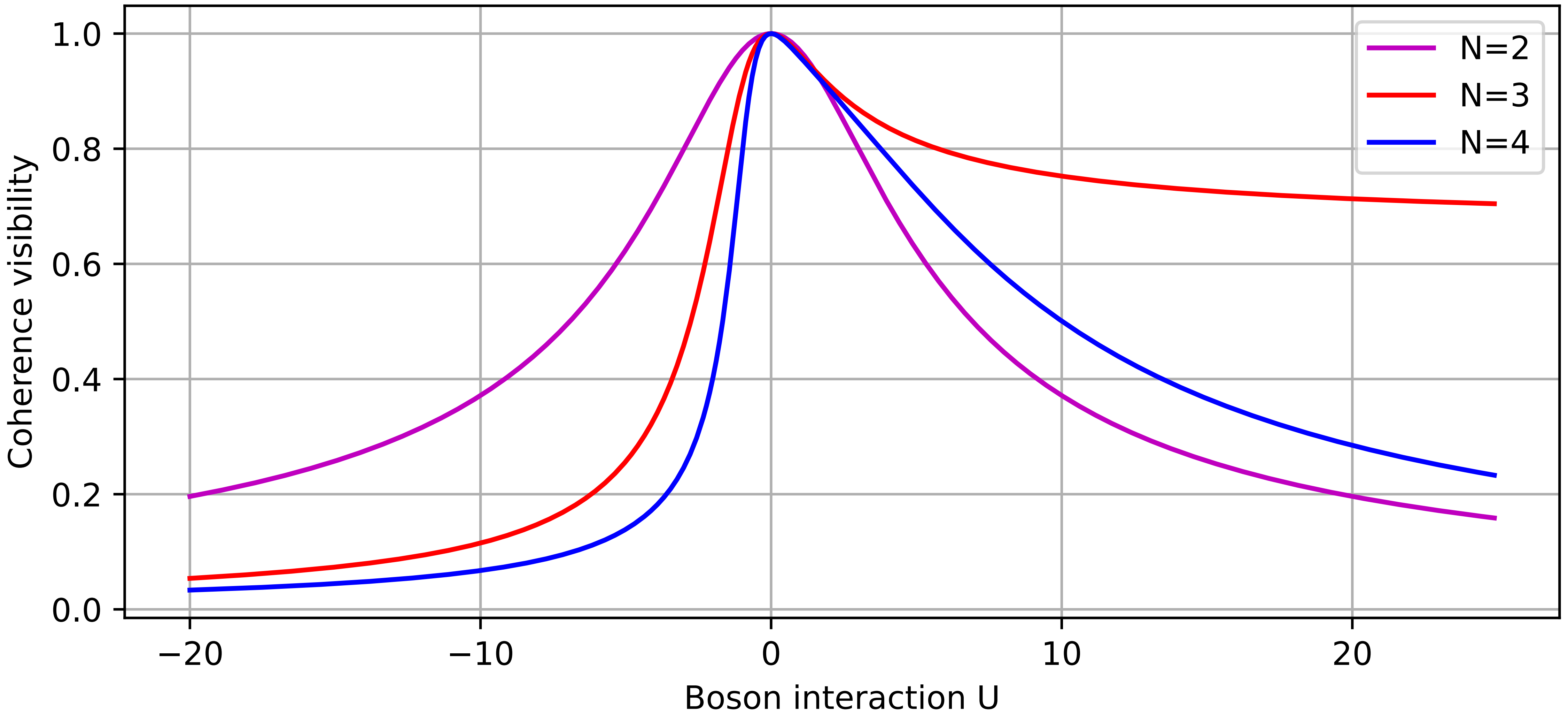
Symmetry of the system: the sites must have the same average occupation.

Metrics regarding the correlations in the system can be computed from the amplitudes.

CORRELATION METRICS

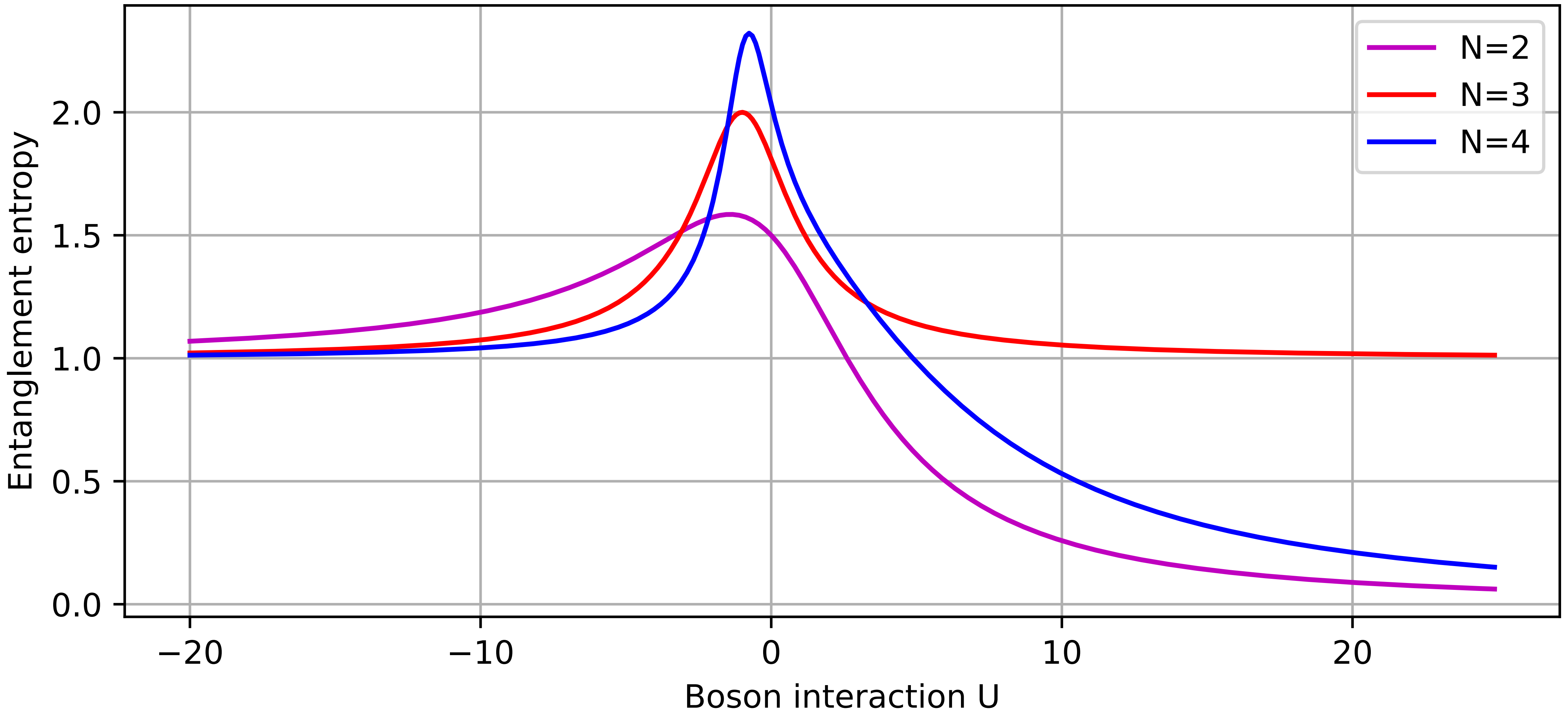
COHERENCE VISIBILITY

$$\alpha = \frac{2}{N} \sum_{i=0}^{N} c_i^* c_{i+1} \sqrt{(i+1)(N-i)}$$

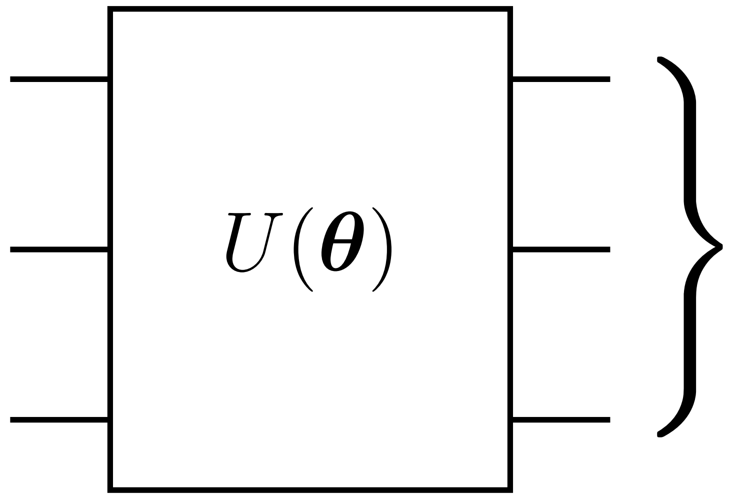


ENTANGLEMENT ENTROPY

$$S = -\sum_{i=0}^{N} |c_i|^2 \log_2 |c_i|^2$$



THE VQE



$|\psi(\boldsymbol{\theta})\rangle$

The state is prepared by the variational form.

The energy expectation value is measured.

$$\langle\psi(\boldsymbol{\theta})|\,\mathcal{H}\,|\psi(\boldsymbol{\theta})\rangle = E(\boldsymbol{\theta})$$

The parameters are updated by a classical optimizer.

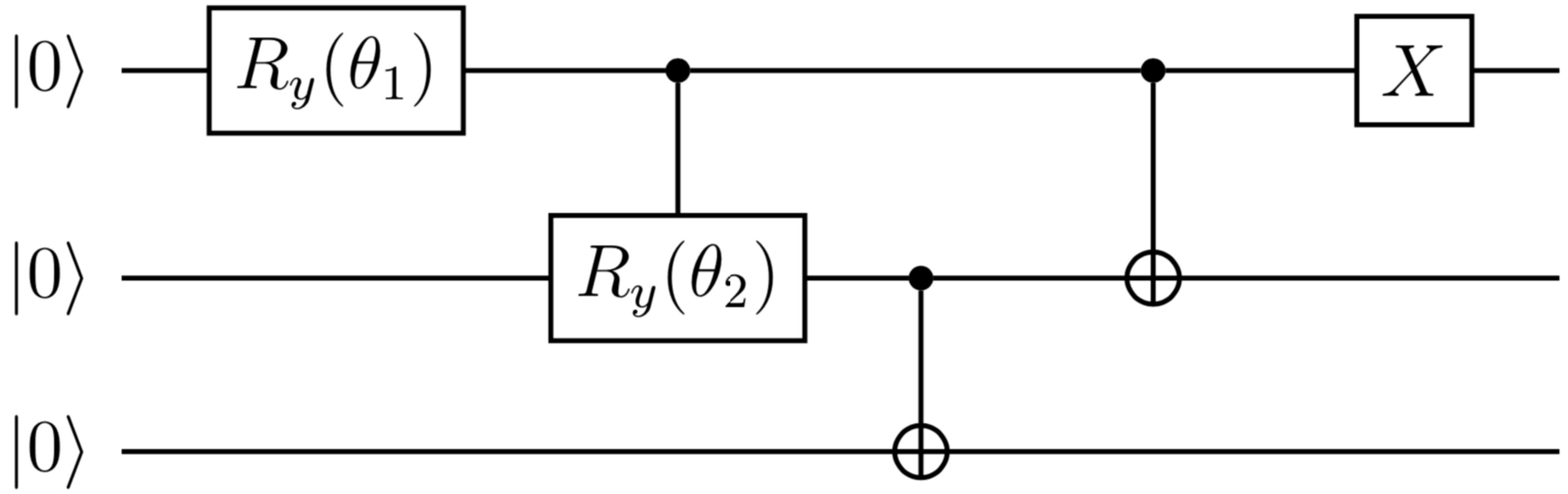
$$\boldsymbol{\theta} \to \boldsymbol{\theta}'$$

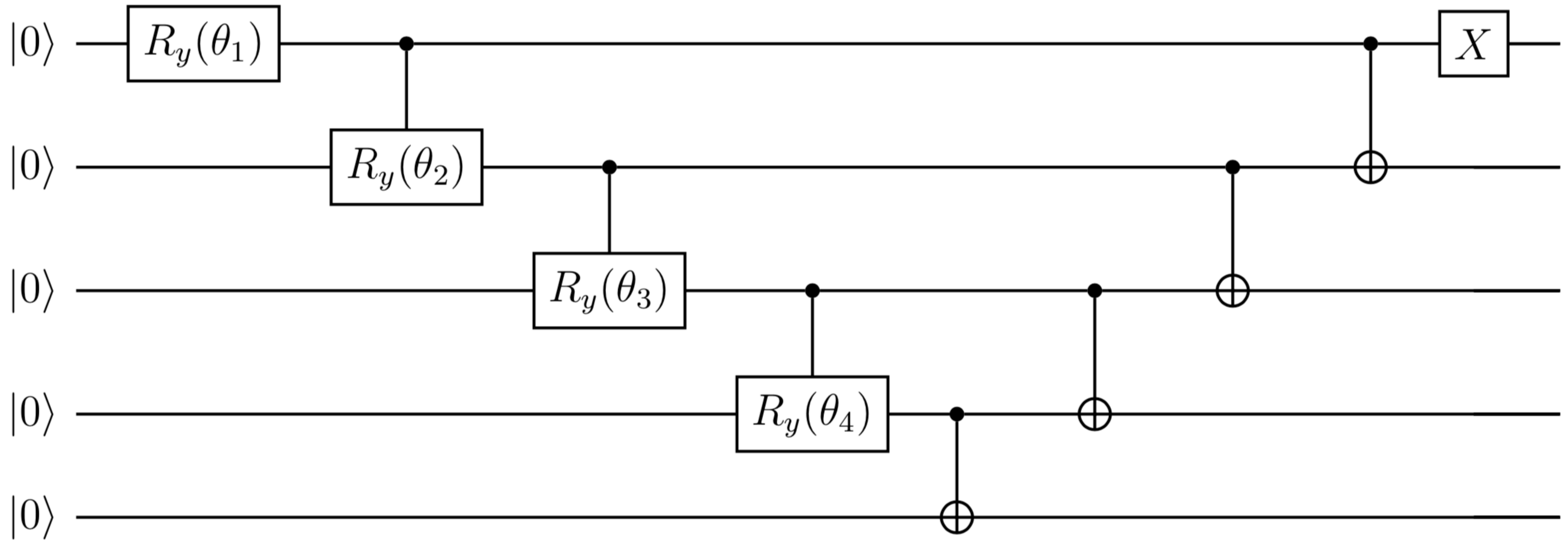
UNARY MAPPING

Straightforward extension to any N.

N+1 qubits used, many states have no physical meaning.

$$
\begin{array}{ccc}
|1000...0\rangle & \leftrightarrow & |0, N\rangle \\
|0100...0\rangle & \leftrightarrow & |1, N-1\rangle \\
|0010...0\rangle & \leftrightarrow & |2, N-2\rangle \\
\vdots & & \vdots \\
|0000...1\rangle & \leftrightarrow & |N, 0\rangle
\end{array}
$$





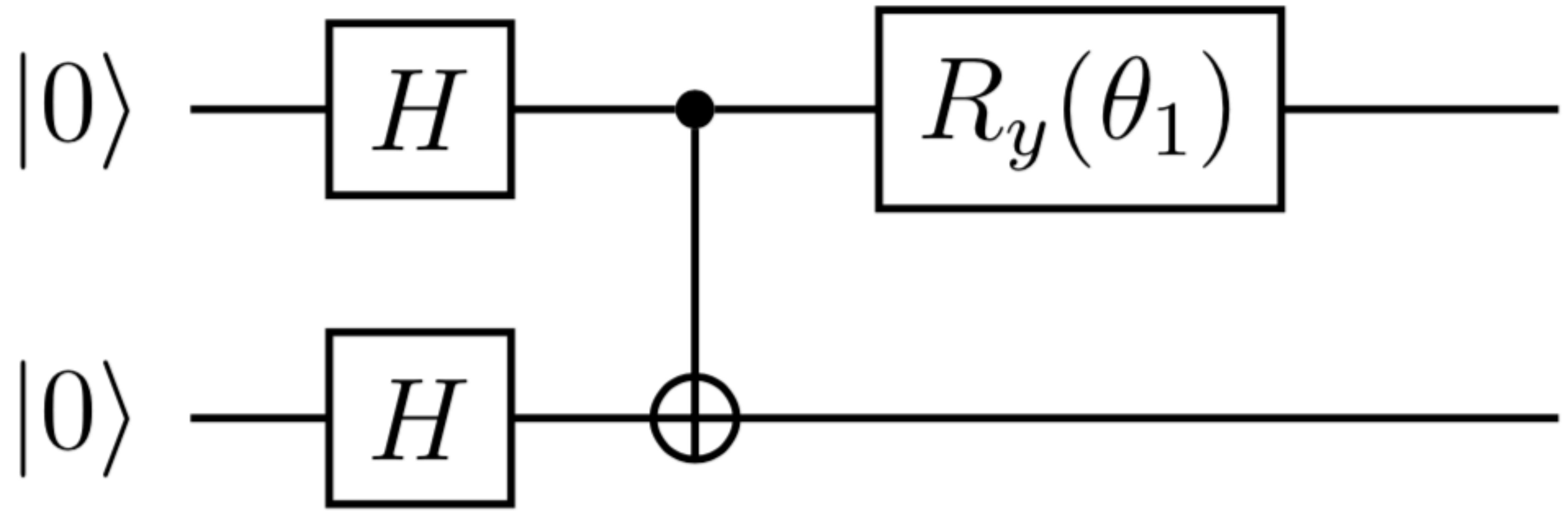
GRAY CODE MAPPING

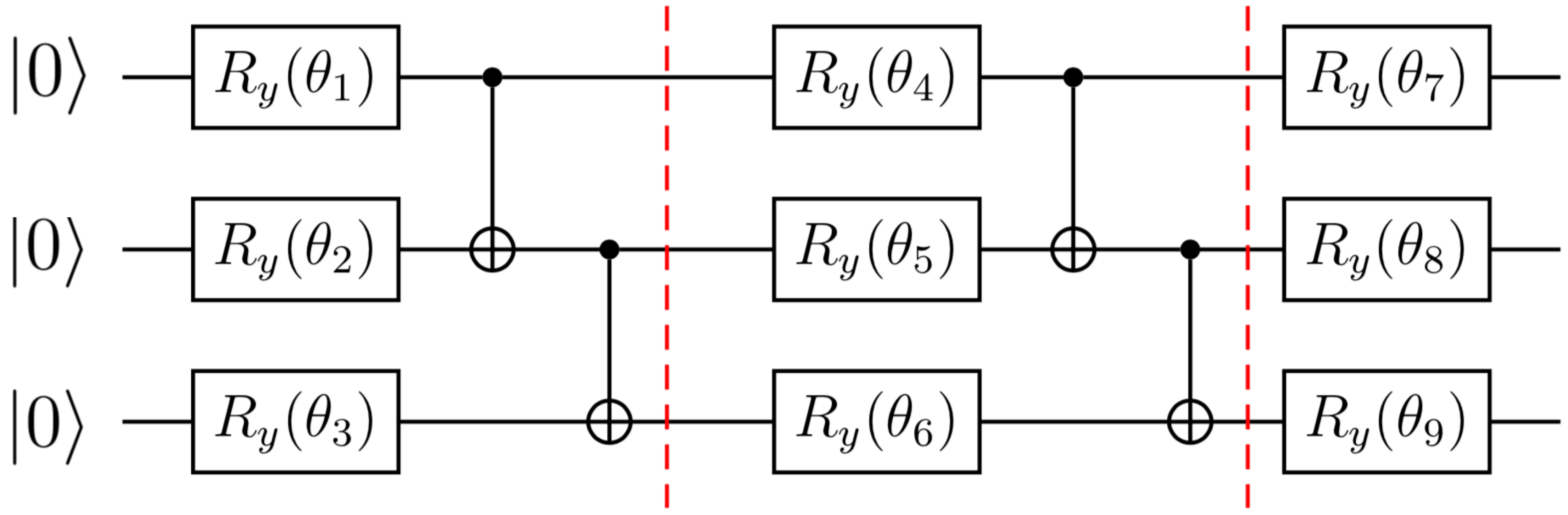
All qubit states are used if N+1 is a power of two.

Hardware efficient ansatze can be employed.

Becomes more complex for higher N.

$$\begin{array}{ccc} |00\rangle & \leftrightarrow & |0,3\rangle \\ |01\rangle & \leftrightarrow & |1,2\rangle \\ |11\rangle & \leftrightarrow & |2,1\rangle \\ |10\rangle & \leftrightarrow & |3,0\rangle \end{array}$$





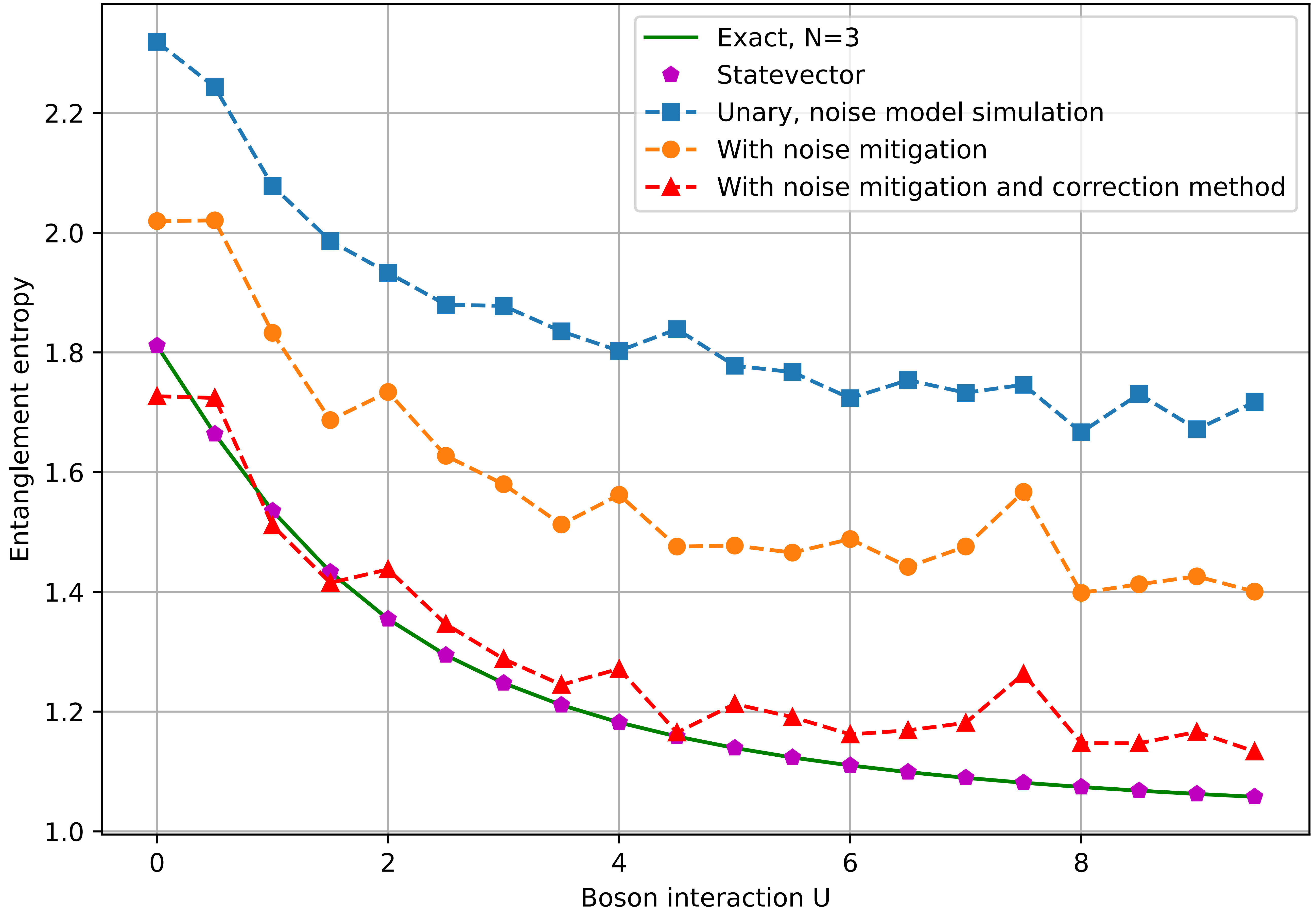
UNARY SIMULATIONS

Ideal (statevector) simulations recover exact values.

Noise introduces significant systematic errors.

Biggest source of errors is the presence of counts in non-physical states.

A simple post-processing correction method is just to consider the counts in physical states.

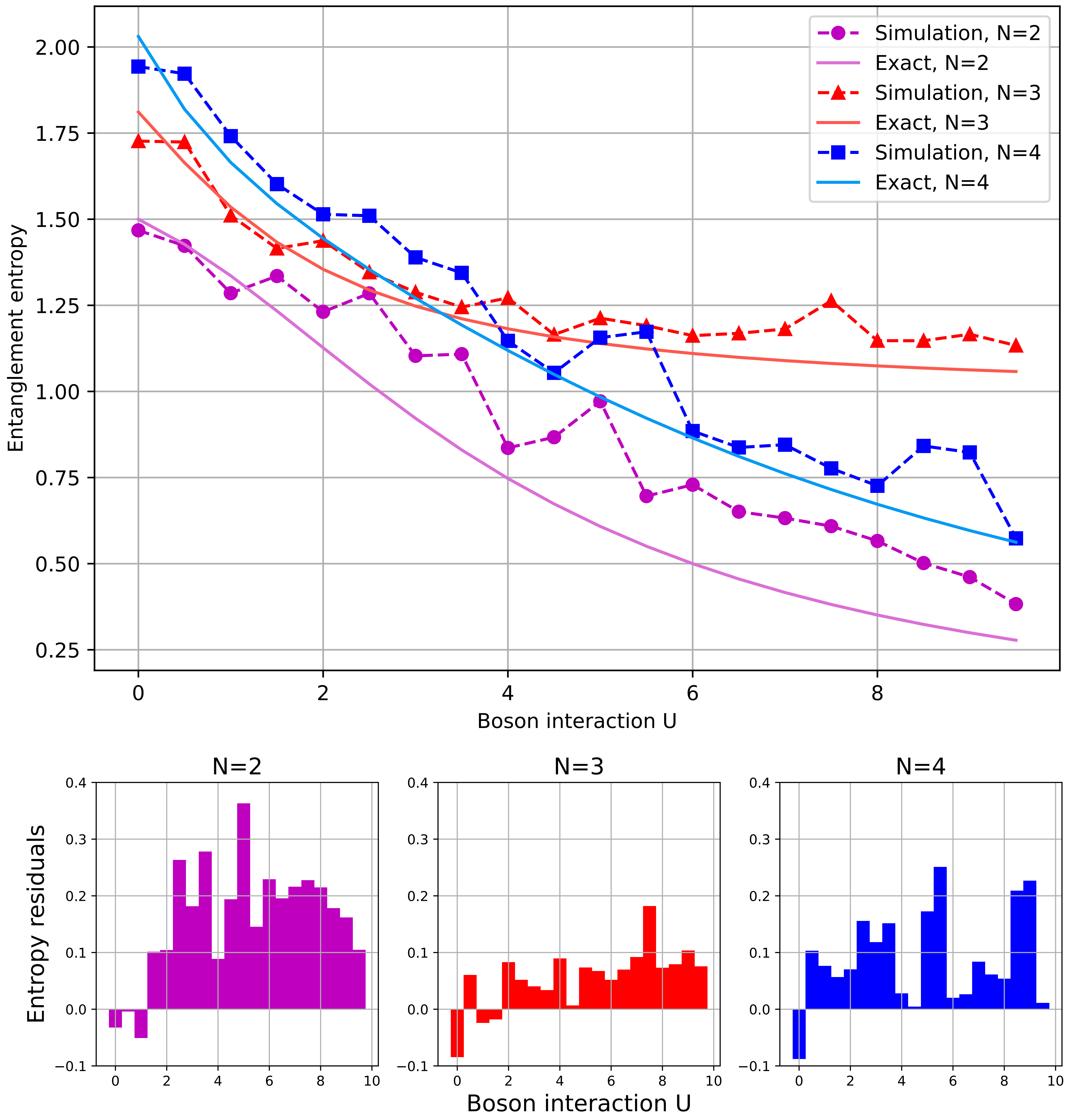


UNARY SIMULATIONS

Exact values are always overestimated.

Still, the curves are qualitatively outlined.

Most importantly, it is still possible to discern the difference between even and odd N instances.

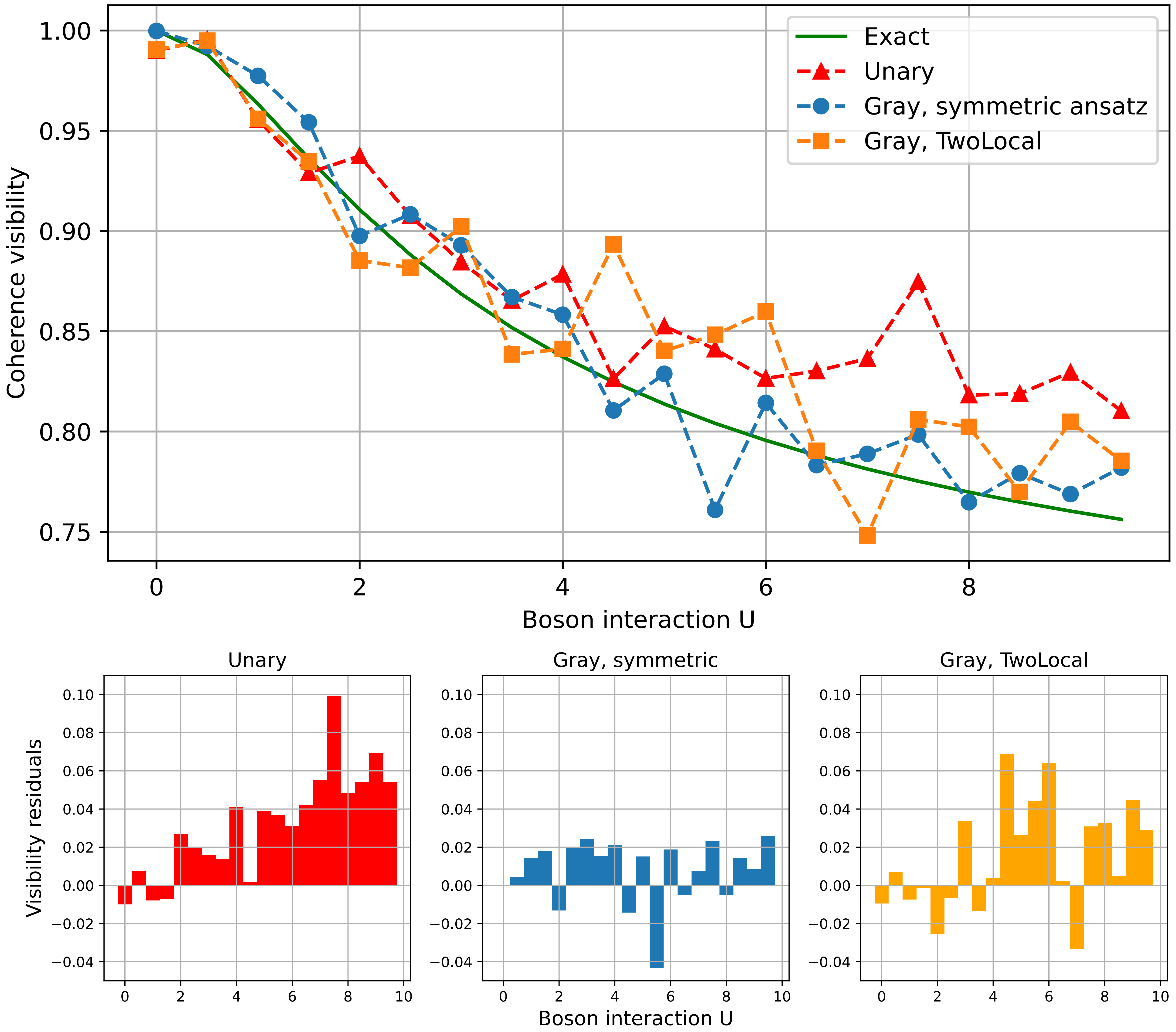


N=3, GRAY SIMULATIONS

No unphysical states.

Better performance both in terms of accuracy and computation time.

For some points, the ground state energy computed by the VQE is compatible with the exact solution.



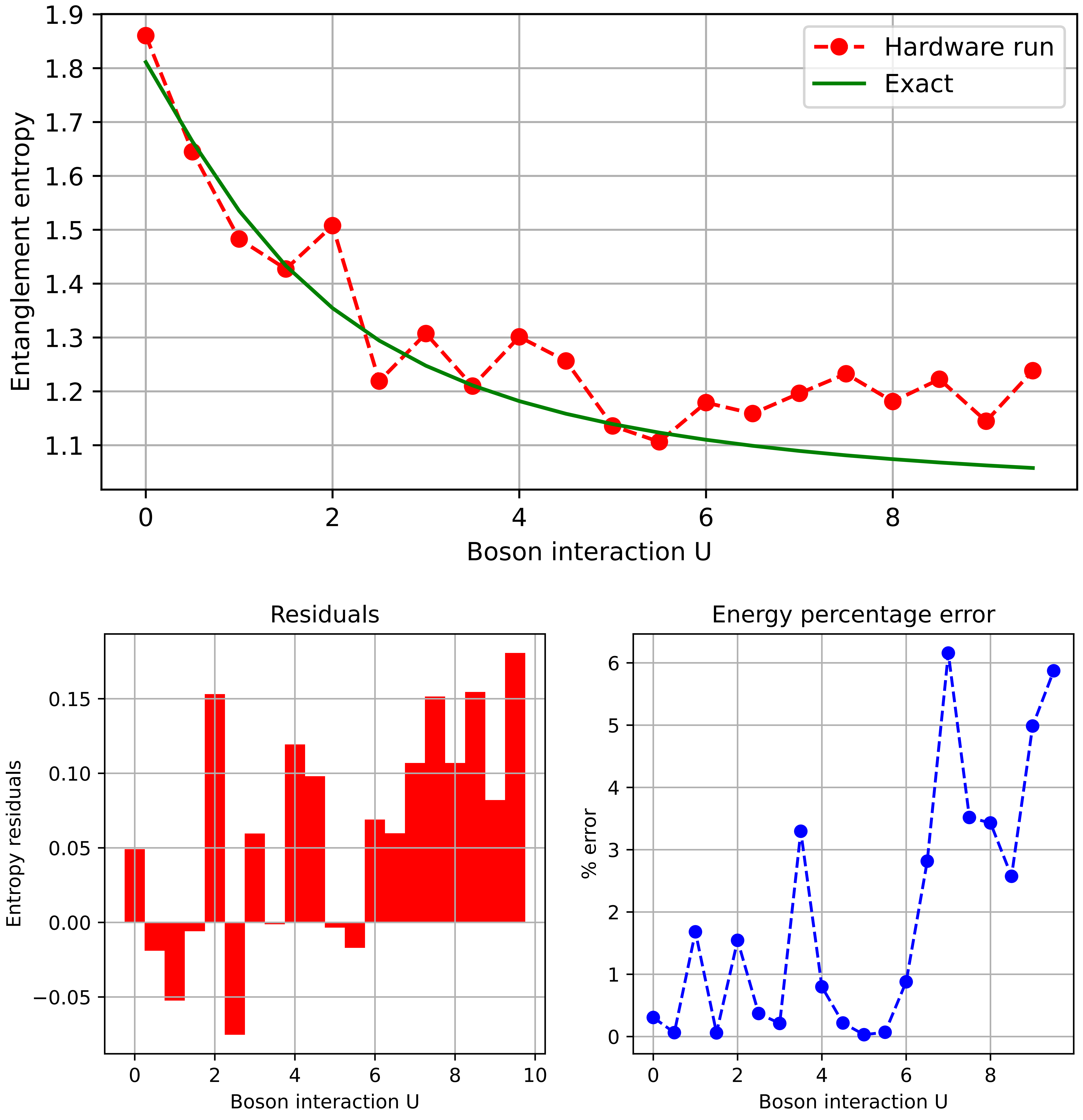
HARDWARE RUN

Gray code with symmetric ansatz was used, N=3.

Selected results from two runs, no values from simulations used to improve convergence.

Worse performance than simulation.

Still qualitative correspondence for low values of U.



RESULTS

Significant systematic errors from NISQ limitations, results not statistically compatible.

Qualitative correspondence achieved, differentiating between cases with odd or even total number of bosons.

Compact mapping far superior than unary when applicable.

Possible extension to a larger system should employ Gray coding and hardware efficient ansatz.