Quantum Computation of Thermal Averages in the Presence of a Sign Problem

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for the QUBIPF collaboration*

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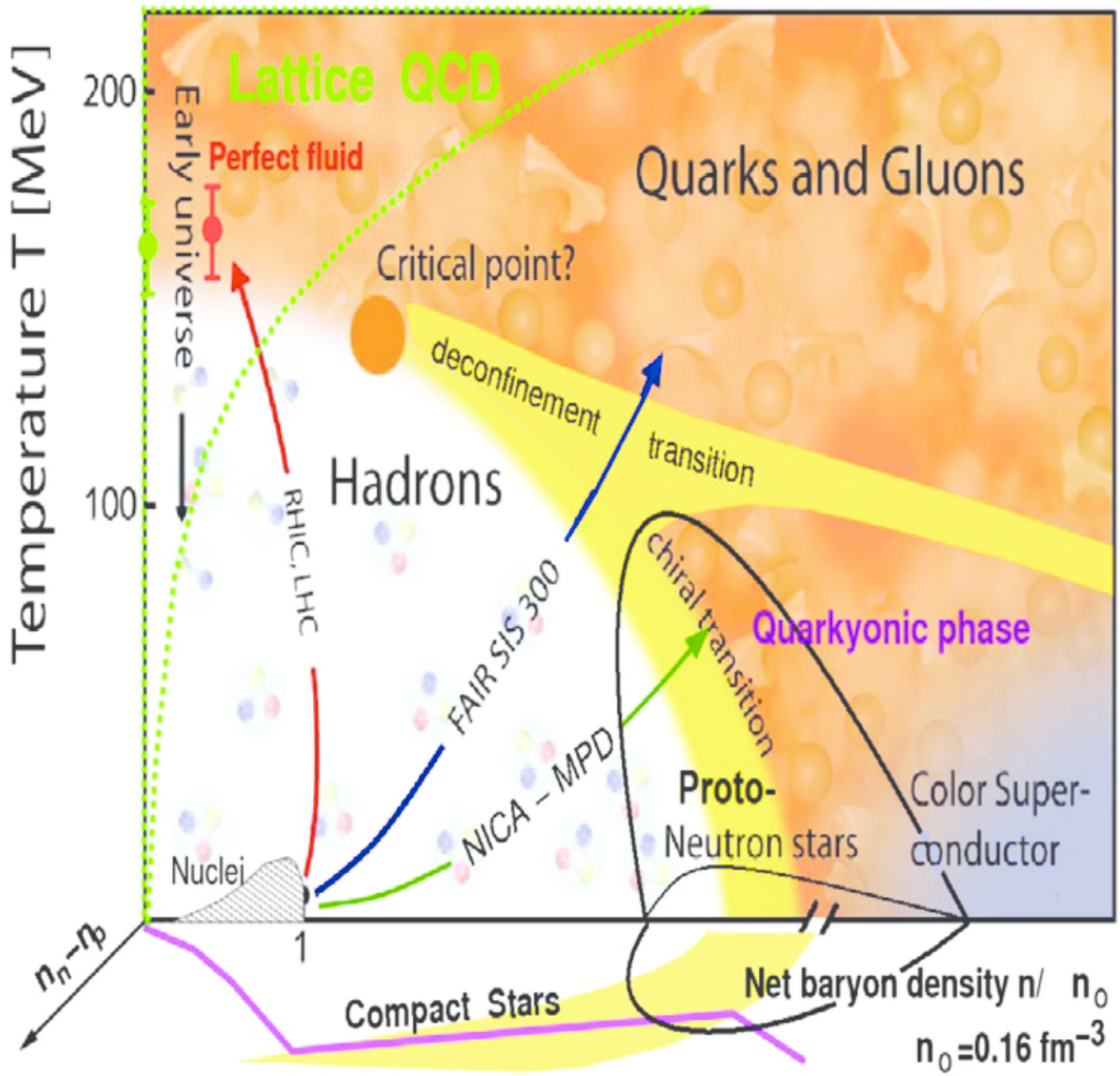
Sign Problem in QCD Classical Simulations



Sign Problem and Quantum Computing

The **sign problem** hinders classical computational methods for QCD at finite density (e.g., nuclei and neutron stars physics):

Euclidean *action* $S \notin \mathbb{R} \implies$ weight $\not> 0$ in the path-integral.

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Our goal is to generate Gibbs ensembles, **but** simultaneously trying to overcome the sign problem by QC techniques.

Computing Gibbs ensembles

Many approaches have been proposed, to mention a few:

- approaches based on variational methods; J. Whitfield *et al.* (2011)
- quantum simulated annealing; R. D. Somma *et al.* (2008)
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- others...

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We focus our analysis to the **Quantum Metropolis Sampling** (QMS) algorithm, presented in [K. Temme *et al.*, Nature **471** (2011) 87], showing its application to a system affected by sign problem and analyzing sources of systematical errors. [arXiv:2001.05328]

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Disclaimer: we studied only universal properties of the algorithm using our Simulator for Universal Quantum Algorithms (SUQA), excluding from the analysis machine-specific quantum errors.

Quantum Metropolis Sampling: general idea

[K. Temme *et al.*, Nature **471**, (2011) 87, arXiv:0911.3635 [quant-ph]].

Philosophy: sample a Gibbs ensamble of energy eigenstates, i.e., weighted as $\rho(\beta) \propto \mathrm{e}^{-\beta H}$, via a quantum-driven **Markov Chain** which satisfies a properly modified version of Detailed Balance.

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Resources:
The global state of the QMS algorithm is encoded in four registers:

- state of the system (n qubits); (digitalization)
- energy before MC step (r qubits); (incommensurability)
- energy after MC step (r qubits); (as above)
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$\Longrightarrow$ basis elements: $|acc, E^{new}, E^{old}, \psi\rangle$

QMS: sketch of the algorithm

Initialization: prepare $|0, 0, 0, \psi_k\rangle$, with $|\psi_k\rangle$ any eigenstate.

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Acceptance evaluation: apply an appropriate operator $W(E_p,E_k)$ to the acceptance qubit

$$\sum_p x_{k,p}^{(C)} |0,E_p,E_k,\psi_p\rangle \xrightarrow{W}$$

$$\sum_p x_{k,p}^{(C)} \left(f(\Delta E_{p,k}) |1\rangle + \sqrt{1-f(\Delta E_{p,k})}\, |0\rangle \right) \otimes |E_p,E_k,\psi_p\rangle ,$$

where $f(\Delta E_{p,k}) \equiv \min\left(1, e^{-\beta(E_p-E_k)/2}\right)$.

QMS: sketch of the algorithm (cont.d)

accept/reject: measure on the acceptance qubit; two possibilities:

- 1 means **accept**: we proceed with measuring on the E^{new} register, so we obtain a new eigenstate on the state register.
- 0 means **reject**: we need to *revert* the system to the initial state by trying to project back until $E^{new} == E^{old}$.
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Let's see the QMS algorithm in action on a toy model with sign problem: the *Frustrated Triangle*.

Minimal Model with Sign Problem: the Frustrated Triangle

Hamiltonian for an antiferromagnetic ($J > 0$) Ising triangle

$$H = J(\sigma_x \otimes \sigma_x \otimes \mathbb{1} + \sigma_x \otimes \mathbb{1} \otimes \sigma_x + \mathbb{1} \otimes \sigma_x \otimes \sigma_x),$$

The path-integral with a finite number N of layers with 3-qubits states $|\alpha_i\rangle$ in the computational basis reads:

$$Z[\beta] = Tr\left[\mathrm{e}^{-\beta H}\right] = \sum_{\{\alpha_i\}} \prod_{i=1}^{N} \langle \alpha_{i+1}| \, \mathrm{e}^{-\frac{\beta H}{N}} \, |\alpha_i\rangle \,,$$

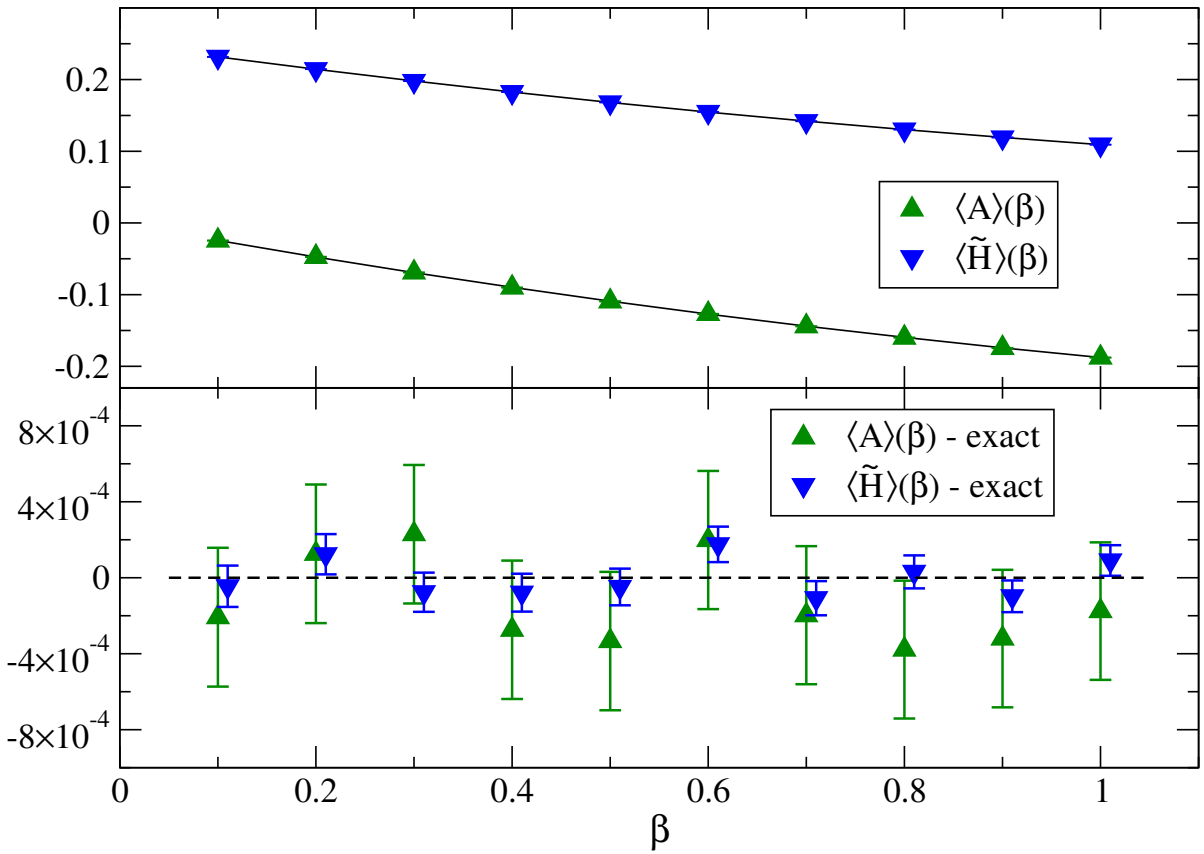
where $T \equiv \mathrm{e}^{-\frac{\beta H}{N}}$ is the **transfer matrix**.

Here the sign-problem comes from non positive off-diagonal elements in the transfer matrix (e.g. $\langle 011| \, \mathrm{e}^{-\frac{\beta H}{N}} \, |000\rangle < 0$).

Numerical Results of the QMS algorithm

Tested with non-diagonal, non-H-commuting observables, e.g.:

$$A = \sigma_x \otimes \sigma_x \otimes \left(\mathbb{1} + \sigma_y\right).$$



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These systematics are manageable, at least for small to medium scale simulations.

Summary and Perspectives

Sum up:

- the sign problem, and the role of Quantum Computing as a solution, have been discussed;
- we briefly overviewed the Quantum Metropolis Sampling (K. Temme *et al.* (2011)), showing sources of systematical errors;
- we applied the QMS algorithm to a minimal model with sign problem, the frustrated triangle, obtaining results in good agreement with the exact ones.

Work in progress:

- we are extending the analysis to increasingly complex systems, taking care of systematical errors;
- in particular, we are implementing codes for non-abelian gauge systems, for which some modification are in order, and the phase estimation needs an evolution procedure which keeps gauge-invariance. [NuQS Collaboration, PRD **11**, 114501 (2019)]

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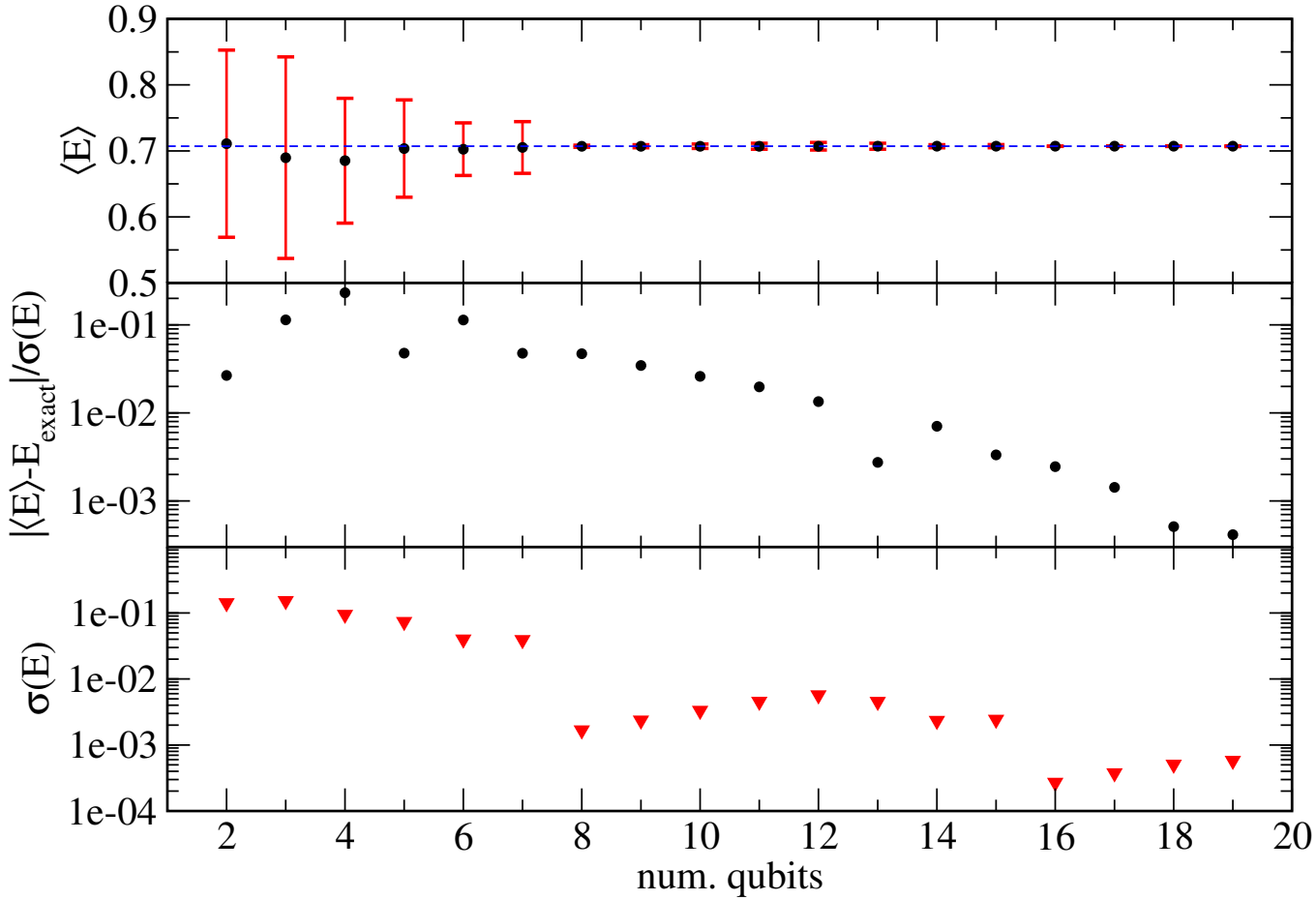
Thank you for the attention!

Additional slides

Phase estimation in general

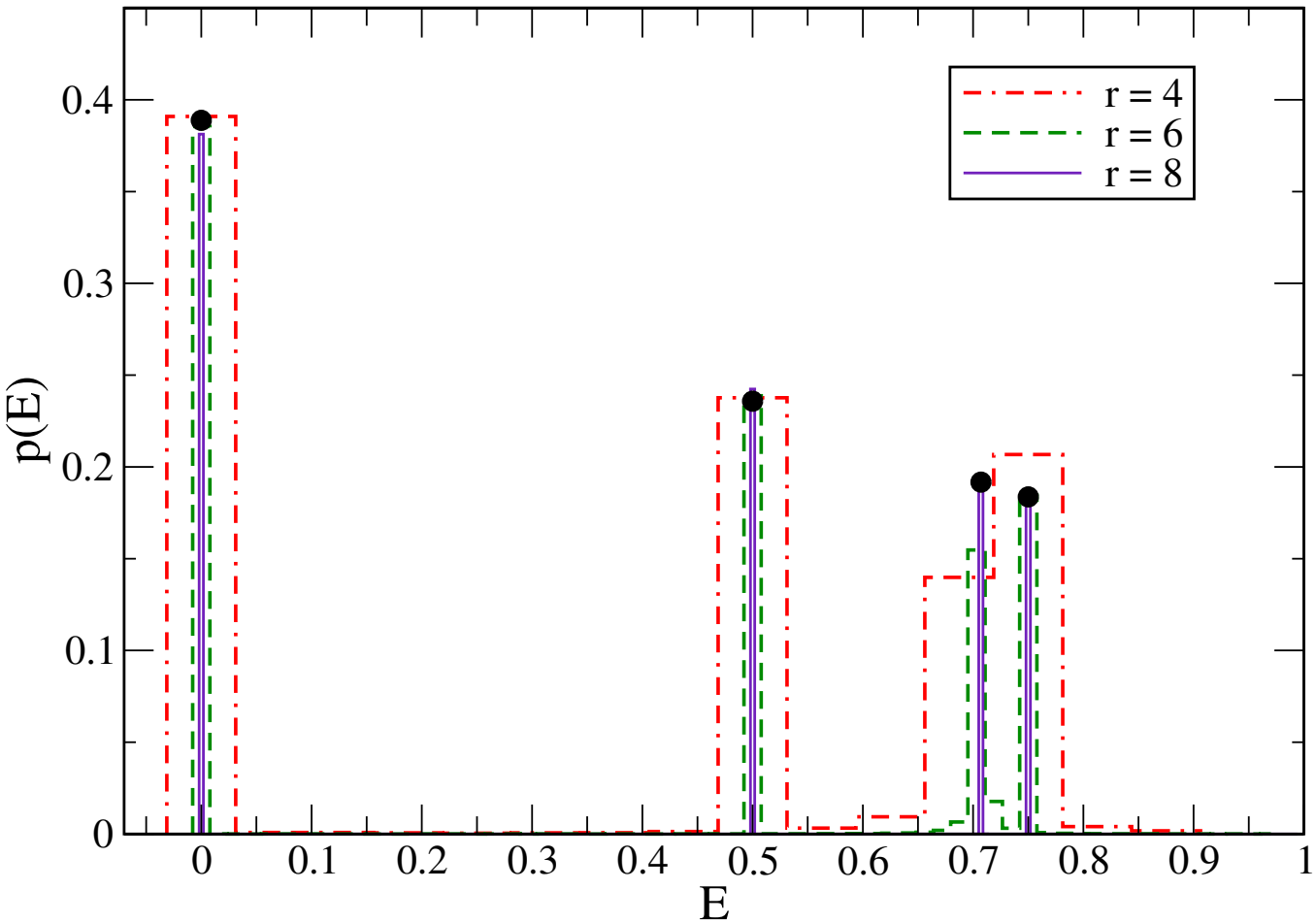
Energy estimate for an eigenstate with exact energy $\frac{1}{\sqrt{2}}$.



Error decreases as $2^{-(\text{num. qbits})}$, while the discrepancy stays of the same order of magnitude of the error.

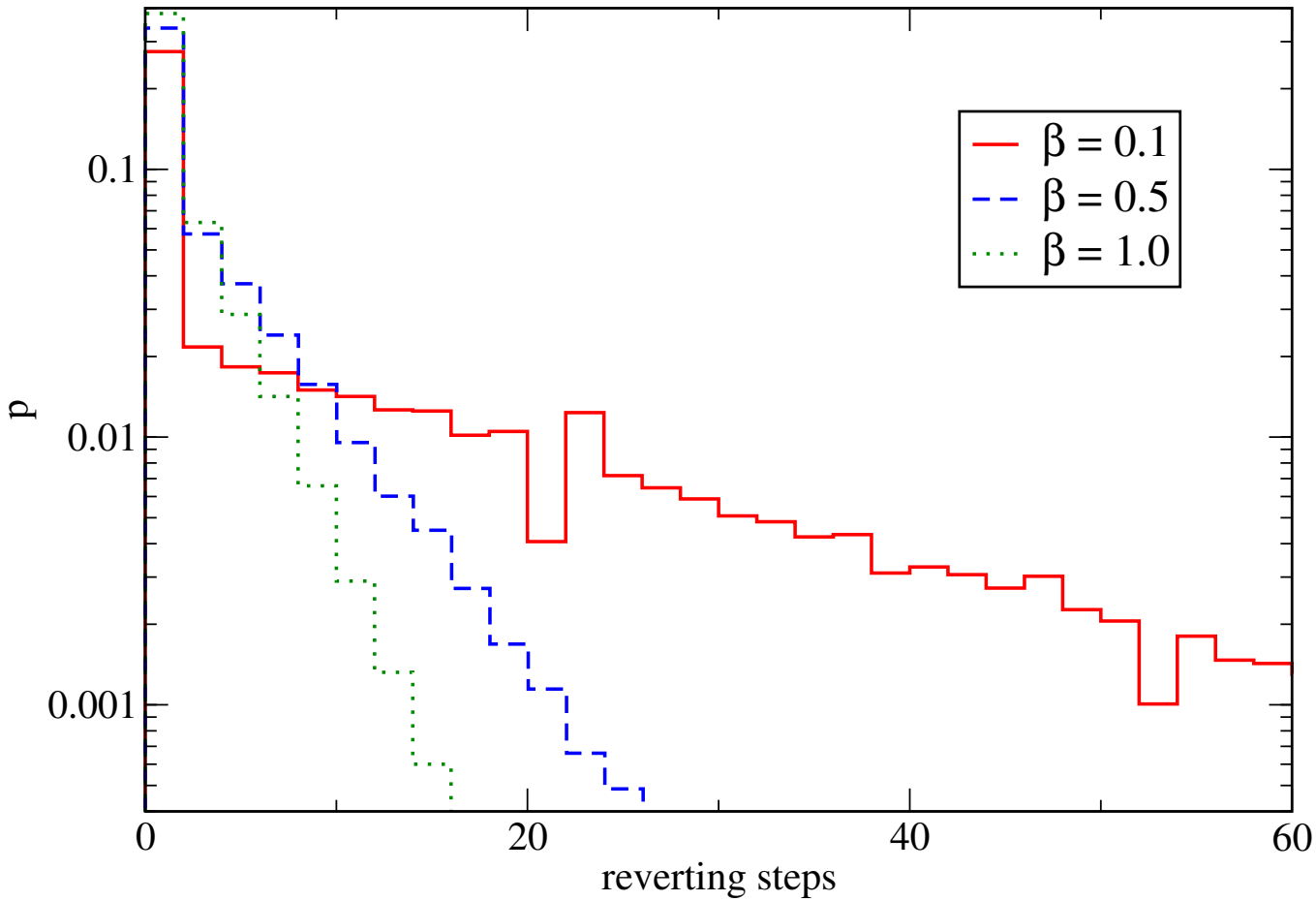
Phase estimation: QMS with incommensurable levels

Energy levels: 0, $\frac{1}{2}$, $\frac{1}{\sqrt{2}}$ and $\frac{3}{4}$.



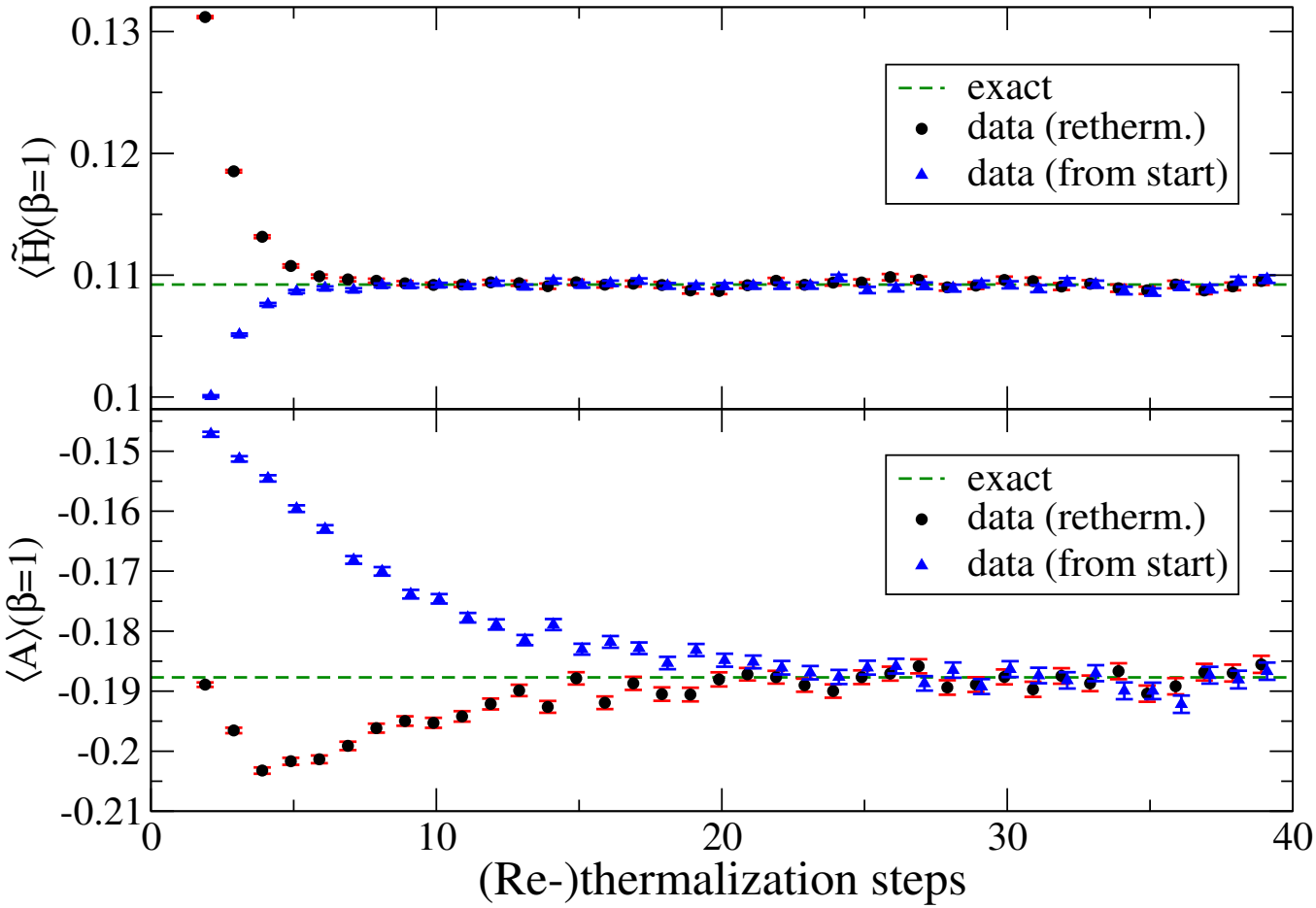
The measured energy distribution seems to converge to the exact result for increasing energy qbits.

Reversal steps in the QMS algorithm



The typical number of steps needed for reverting back the state is relatively small. Small β behave worse.

Re-thermalization process



Non H-commuting observables need more re-thermalization steps.

The Frustrated Triangle: transfer matrix

From the Hamiltonian:

$$H = J(\sigma_x \otimes \sigma_x \otimes \mathbb{1} + \sigma_x \otimes \mathbb{1} \otimes \sigma_x + \mathbb{1} \otimes \sigma_x \otimes \sigma_x),$$

straightforward calculations bring us to the following formula for the transfer matrix:

$$\mathrm{e}^{-\frac{\beta H}{N}} = \frac{1}{4}\left[\left(e^{-3\frac{\beta J}{N}} + 3e^{+\frac{\beta J}{N}}\right)\mathbb{1} + \left(e^{-3\frac{\beta J}{N}} - e^{+\frac{\beta J}{N}}\right)\frac{H}{J}\right].$$

Clearly, $\left(e^{-3\frac{\beta J}{N}} - e^{+\frac{\beta J}{N}}\right) < 0$ for $\beta J > 0$; this is the origin of the **sign problem**.