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

Giuseppe Clemente giuseppe.clemente@pi.infn.it

for the QUBIPF collaboration*

UNIVERSITÀ DI PISA

SM&FT Bari, 11-13 December 2019

*Quantum Bari-Pisa-Ferrara collaboration (QUBIPF):

C. Bonati, M. Cardinali, G. Clemente, L. Cosmai, M. D'Elia, A. Gabbana, D. Rossini, S. F. Schifano, R. Tripiccione and D. Vadacchino

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.

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.

Quantum Computing (QC) is often popularized as a solution, since the Hamiltonian formulation do not show sign problems.

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.

Quantum Computing (QC) is often popularized as a solution, since the Hamiltonian formulation do not show sign problems.

However, most of the work in literature focuses on real-time quantum evolution, not directly useful for computing thermal averages or studying the phase diagram.

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.

Quantum Computing (QC) is often popularized as a solution, since the Hamiltonian formulation do not show sign problems.

However, most of the work in literature focuses on real-time quantum evolution, not directly useful for computing thermal averages or studying the phase diagram.

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)
- quantum metropolis methods; B. Terhal, D. Di Vincenzo (2000)
- others...

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)
- quantum metropolis methods; B. Terhal, D. Di Vincenzo (2000)
- others...

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. (work in preparation)

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)
- quantum metropolis methods; B. Terhal, D. Di Vincenzo (2000)
- others...

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. (work in preparation)

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.

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.

Assumption: an energy eigenstate must be build to start the chain.

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.

Assumption: an energy eigenstate must be build to start the chain.

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)
- acceptance (1 qubit).

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.

Assumption: an energy eigenstate must be build to start the chain.

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)
- acceptance (1 qubit).

$\Longrightarrow$ 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.

QMS: sketch of the algorithm

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

Phase estimation (PE) on E^{old}: $|0,0,0,\psi_k\rangle \xrightarrow{\Phi^{(old)}} |0,0,E_k,\psi_k\rangle$

M. Troyer and U. J. Wiese (2005) (Trotterization)

QMS: sketch of the algorithm

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

Phase estimation (PE) on E^{old}: $|0,0,0,\psi_k\rangle \xrightarrow{\Phi^{(old)}} |0,0,E_k,\psi_k\rangle$

M. Troyer and U. J. Wiese (2005) (Trotterization)

Quantum Metropolis trial: draw classically and apply an unitary operator C to the state qubits followed by a PE on E^{new}

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

QMS: sketch of the algorithm

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

Phase estimation (PE) on E^{old}: $|0,0,0,\psi_k\rangle \xrightarrow{\Phi^{(old)}} |0,0,E_k,\psi_k\rangle$

M. Troyer and U. J. Wiese (2005) (Trotterization)

Quantum Metropolis trial: draw classically and apply an unitary operator C to the state qubits followed by a PE on E^{new}

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

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 $E^{new} == E^{old}$.
  (threshold on reversal steps)

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 $E^{new} == E^{old}$. (threshold on reversal steps)

Energy measures are taken at each MC step, without cost. Measuring non-H-commuting observables breaks the chain: a certain number of rethermalization steps are required.

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 $E^{new} == E^{old}$. (threshold on reversal steps)

Energy measures are taken at each MC step, without cost. Measuring non-H-commuting observables breaks the chain: a certain number of rethermalization steps are required.

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:

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

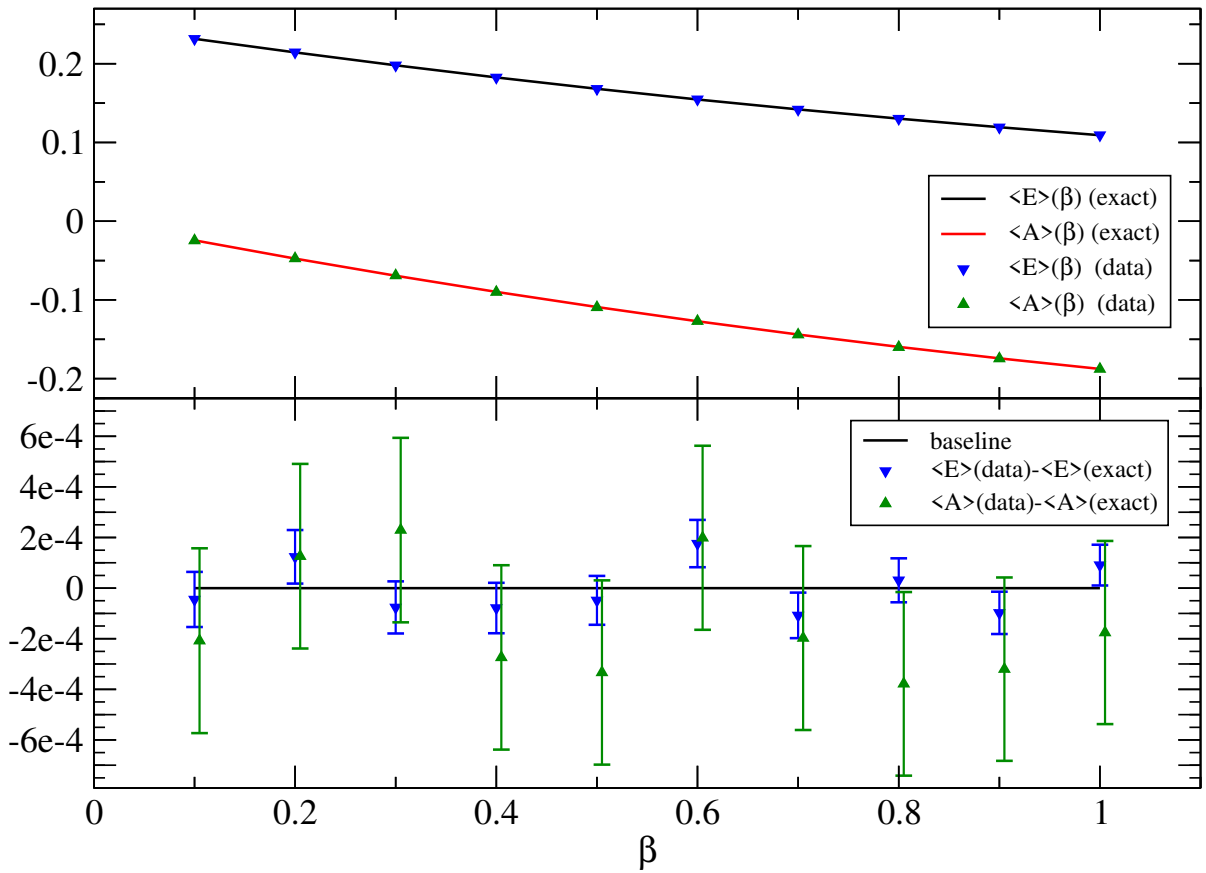
where $T \equiv \mathrm{e}^{-\frac{\beta H}{N}}$ is the **transfer matrix**.

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.:

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



We find excellent agreement: $\chi^2(E) = 10.7$ (p-value: 0.38) and $\chi^2(A) = 4.9$ (p-value: 0.90), with 10 d.o.f.

Sources of systematical errors

- Digitalization: representing physics of continuum d.o.f. with a finite number of qubits n;

  D. C. Hackett *et al.* (2019)

Sources of systematical errors

- Digitalization: representing physics of continuum d.o.f. with a finite number of qubits n;

  D. C. Hackett *et al.* (2019)

- Energy representation: distance between energy levels could be incommensurable $\Longrightarrow$ phase-estimation cannot be exact with a finite number of qubits r in the energy register;

Sources of systematical errors

- Digitalization: representing physics of continuum d.o.f. with a finite number of qubits n;

  D. C. Hackett *et al.* (2019)

- Energy representation: distance between energy levels could be incommensurable $\Longrightarrow$ phase-estimation cannot be exact with a finite number of qubits r in the energy register;
- Finite Trotter step-size in the phase-estimation procedure.

Sources of systematical errors

- Digitalization: representing physics of continuum d.o.f. with a finite number of qubits n;

  D. C. Hackett *et al.* (2019)

- Energy representation: distance between energy levels could be incommensurable $\Longrightarrow$ phase-estimation cannot be exact with a finite number of qubits r in the energy register;
- Finite Trotter step-size in the phase-estimation procedure.
- Threshold in the number of reversal attempts in case of reject;

Sources of systematical errors

- Digitalization: representing physics of continuum d.o.f. with a finite number of qubits n;

  D. C. Hackett *et al.* (2019)

- Energy representation: distance between energy levels could be incommensurable $\Longrightarrow$ phase-estimation cannot be exact with a finite number of qubits r in the energy register;
- Finite Trotter step-size in the phase-estimation procedure.
- Threshold in the number of reversal attempts in case of reject;
- Rethermalization steps after a measure;

Sources of systematical errors

- Digitalization: representing physics of continuum d.o.f. with a finite number of qubits n;

  D. C. Hackett *et al.* (2019)
- Energy representation: distance between energy levels could be incommensurable $\Longrightarrow$ phase-estimation cannot be exact with a finite number of qubits r in the energy register;
- Finite Trotter step-size in the phase-estimation procedure.
- Threshold in the number of reversal attempts in case of reject;
- Rethermalization steps after a measure;

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)]

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:

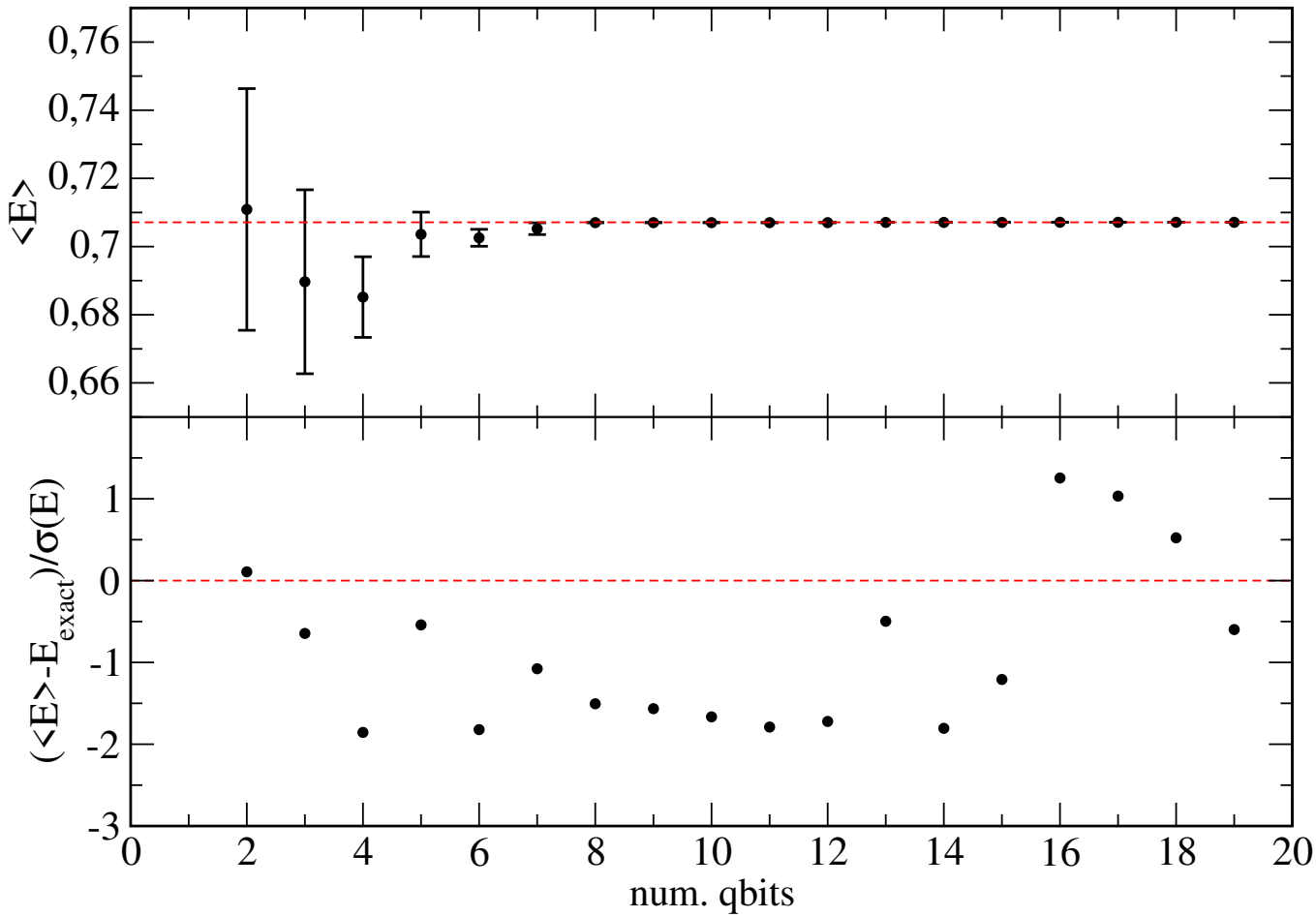
- we are extending the analysis to increasingly complex systems, taking care of systematical errors;
- in particular, we are implementing codes for non-abelian gauge systems, for which some modification are in order, and the phase estimation needs an evolution procedure which keeps gauge-invariance.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

Thank you for the attention!

Additional slides

Phase estimation in general

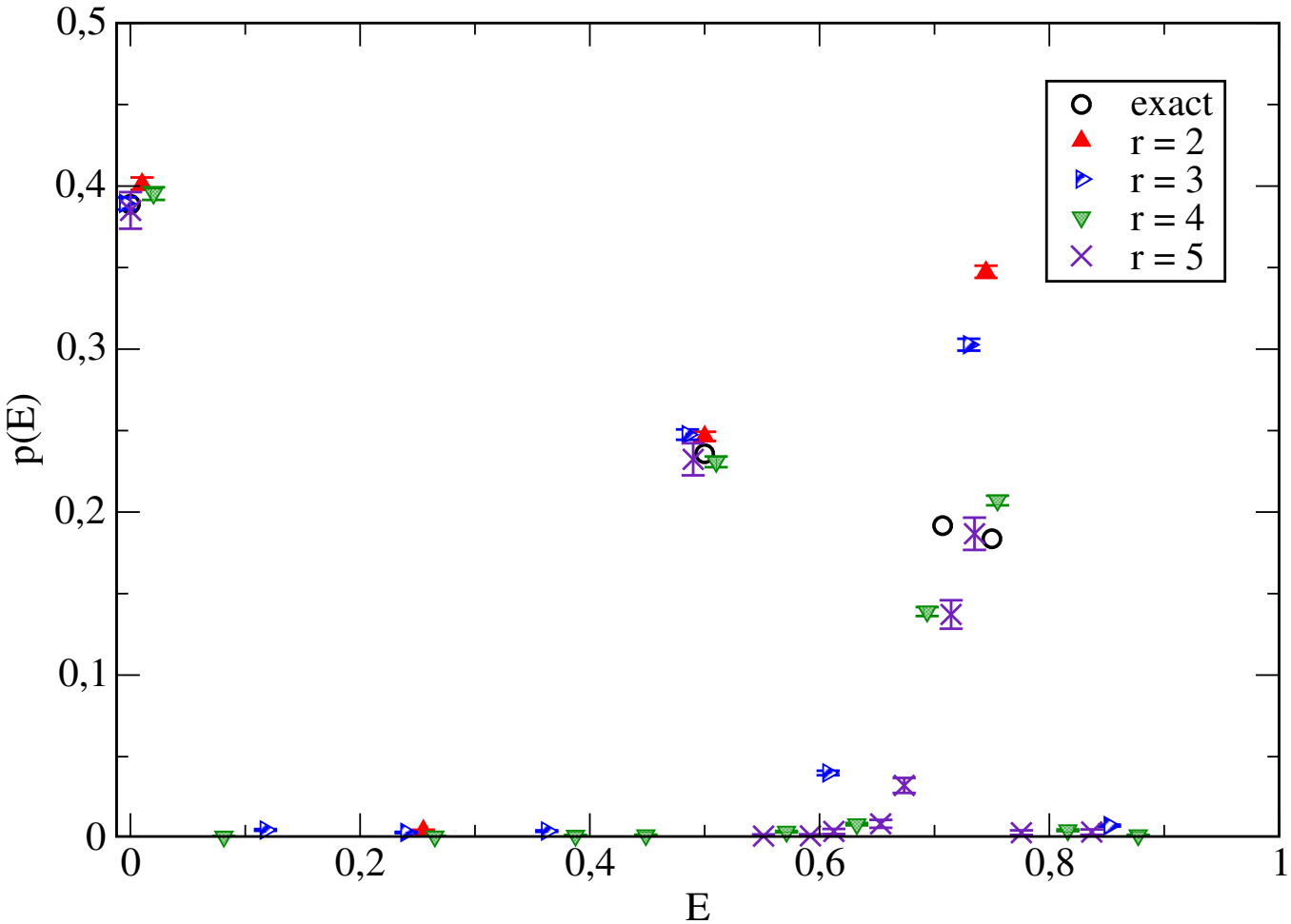
Energy estimate for an eigenstate with exact energy $\frac{1}{\sqrt{2}}$.



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

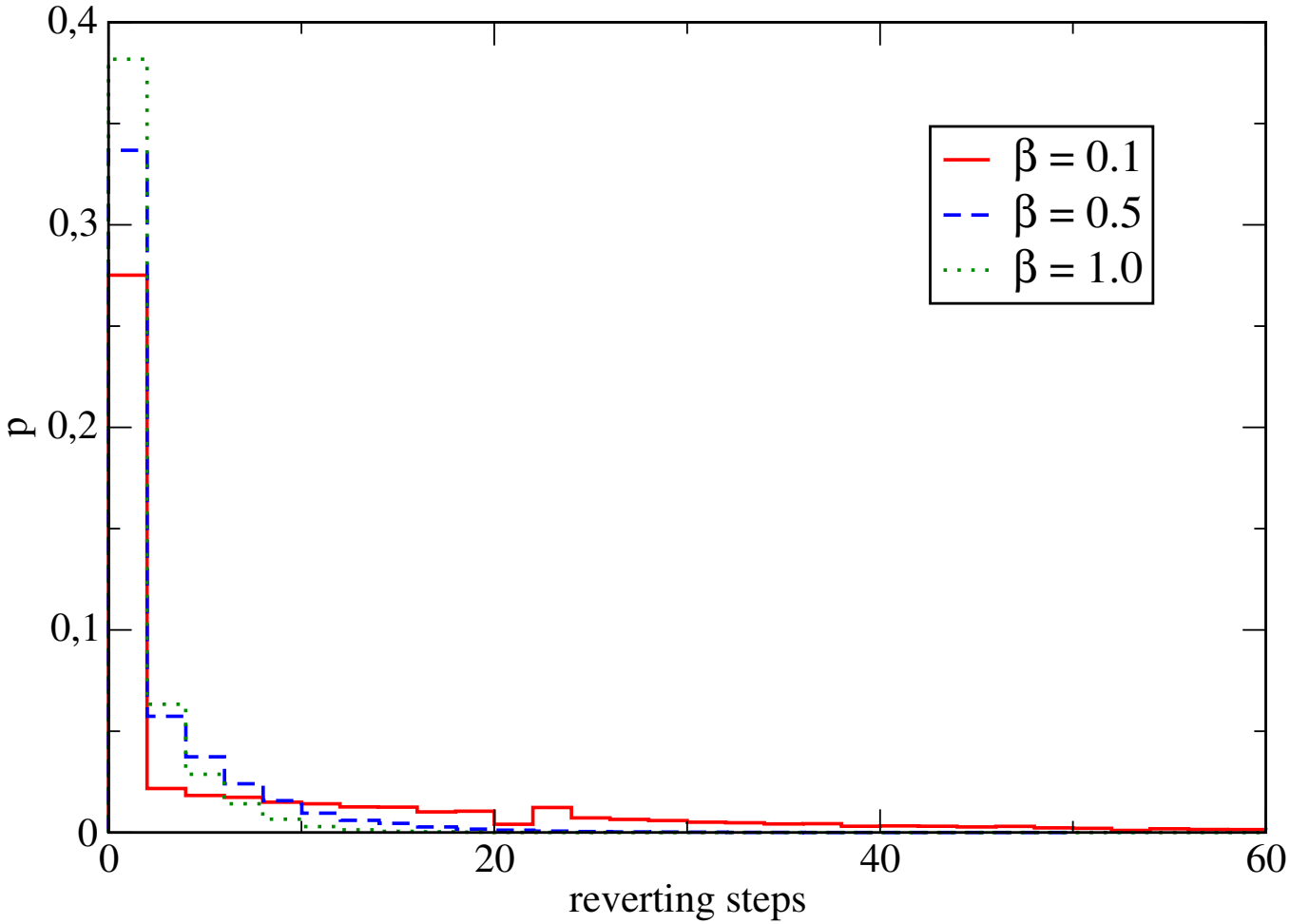
Phase estimation: QMS with incommensurable levels

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.

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**.