Quantum Computing algorithms for thermal averages estimation: an analysis of sources of systematical error.

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

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DESY.

Thermal averages: why quantum?

In order to characterize the phase diagram of lattice QFT models, we are interested in computing **thermal averages** of observables $\mathcal{O}$ over a Gibbs ensamble at temperature T, i.e.

$$\langle \mathcal{O} \rangle_T = \mathrm{Tr}[\mathcal{O} e^{-H/kT}]/Z.$$

Often this is possible via the path-integral formulation and Monte Carlo techniques, but in many cases one incurs in the so called **sign problem**:

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

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It is possible to efficiently simulate at finite baryon density and with a topological θ term, both extremely valuables for phenomenology.

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Computing Gibbs ensembles

Many approaches have been proposed, to mention a few:

- quantum metropolis methods; [B. Terhal, D. Di Vincenzo (2000)]
- quantum simulated annealing; [R. D. Somma *et al.* (2008)]
- approaches based on variational methods; [J. Whitfield *et al.* (2011)]
- many others. . .

In [GC *et al.*, PRD **101** (2020) 7], we focused our analysis on the **Quantum Metropolis Sampling** (QMS) algorithm, first introduced 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.
Here we extend the discussion by considering another algorithm, in the simulated annealing class, called the **Quantum-Quantum Metropolis Algorithm** (Q^2MA), first introduced in [M.-H. Yung and A. Aspuru-Guzik, Proc. Natl. Acad. Sci. USA **109** (2012) 754]. In particular:

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Output of QMS and Q^2MA algorithm

Denoting eigenpairs as $(E_k, |\psi_k\rangle)$, the output is

QMS (Metropolis class)

- Generate sequence of eigenstates $\cdots \to |\psi_{k_i}\rangle \to |\psi_{k_{i+1}}\rangle \to \cdots$ sampled with probability $p_k \simeq e^{-\beta E_k}/Z$ for each $|\psi_k\rangle$;
- $\rho_{\text{QMS}} = \frac{1}{M}\sum_{i=1}^{M} |\psi_{k_i}\rangle \langle\psi_{k_i}|$

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- Generate coherent encoding of thermal state (**CETS**): $|\alpha\rangle \simeq \sum_k \sqrt{e^{-\beta E_k}/Z(\beta)}\, |\psi_k\rangle \otimes |\psi_k^*\rangle$
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In practice, both algorithms prepare states which get destroyed after each measurement.

We studied algorithm-specific systematical errors with our Simulator for Universal Quantum Algorithms (SUQA), completely neglecting quantum noise.

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[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.

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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$\implies$ basis elements: $\left|acc, E^{new}, E^{old}, \psi\right\rangle$

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Sources of systematical errors or performance criticalities

Common to both algorithms

- Digitalization artifacts: representing physics of continuum d.o.f. with a finite number of qubits n;
- Energy representation with finite number of qubits r: incommensurable differences in energy $\implies$ energy (phase-)estimation always inexact with a finite number of qubits in the energy register;
- Finite Trotter step-size in the phase-estimation procedure.

QMS specific

- Rethermalization steps between (destructive) measurements;
- Threshold in number of reversal attempts in case of reject.

Q^{2}MA specific

- Finite number of annealing steps;
- Finite QPE resolution for Szegedy projection.
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We considered a simple toy model devoid of the first three (common) sources of systematical errors: the Frustrated Triangle.

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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. $\langle 011| \, \mathrm{e}^{-\frac{\beta H}{N}} \, |000\rangle < 0$).

Useful as testbed to study algorithm-specific systematical errors: no discretization required (8 system states), exact energy representation (two distinct energy levels) and no trotter error.

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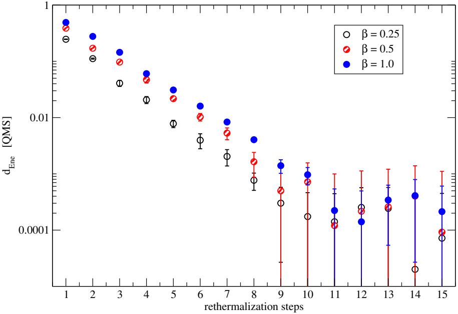
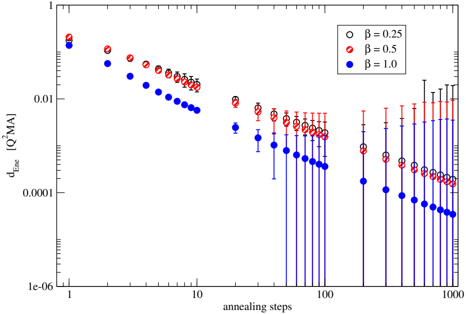
Results ideal case: QMS energy discrepancy

Denoting by $\{E_i\}_{i=1}^{N}$ the measurements of the energy for a sample of size N, the quantities $\bar{E} \equiv \frac{1}{N}\sum_i E_i$

$$d_{\mathrm{Ene}} \equiv \left|\bar{E} - \langle E \rangle_{\mathrm{exact}}\right|$$



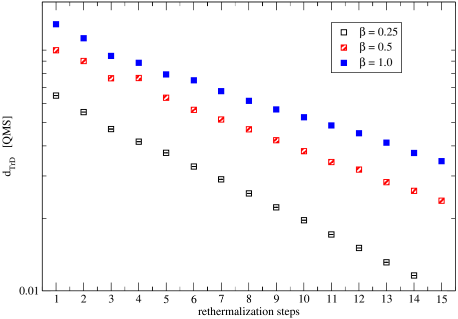
QMS



Q^2MA

Results ideal case: QMS rho discrepancy (trace distance)

$$d_{\mathrm{TrD}} \equiv \frac{1}{2} Tr|\bar{\rho} - \rho_{\mathrm{exact}}|$$



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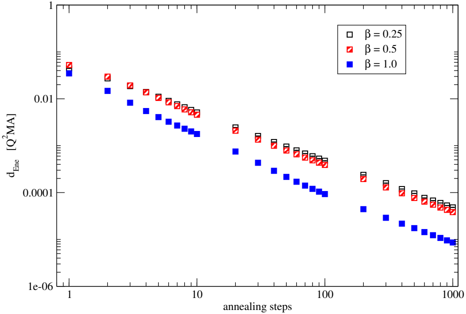


Q^2MA

Both energy and trace distance errors vanish exponentially with the number of (re-)thermalization steps for QMS, while as a power law for Q^2MA.

Slightly non-ideal case: wrong energy range

What happens if we perform an inexact energy QPE (choosing different range and qubit number)?

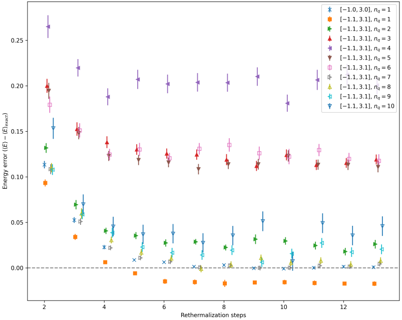
Quantum phase-estimation (QPE) requires fixing a uniform grid of 2^r levels in a certain range.

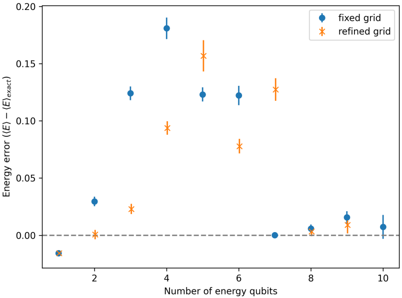
Considering exact eigenvalues $[E_m, E_M]$ and a deformation parameter δ we considered two grid prescriptions:

- *fixed (extrema) grid* with range $[E_m - \delta, E_M + \delta]$: by increasing r, resolution increases, but inner grid points move;
- *refined grid* with range $[E_m - \delta, E_M + \delta + (E_M - E_m + 2\delta)(1 - 2^{1-r})]$: new grid points at $r + 1$ are inserted between old ones at r (with some offshot on the right).

Non-ideal phase-estimation for QMS

QMS results of energy thermal average for Frustrated Triangle $\beta = 0.25$ and $\delta = 0.1$:

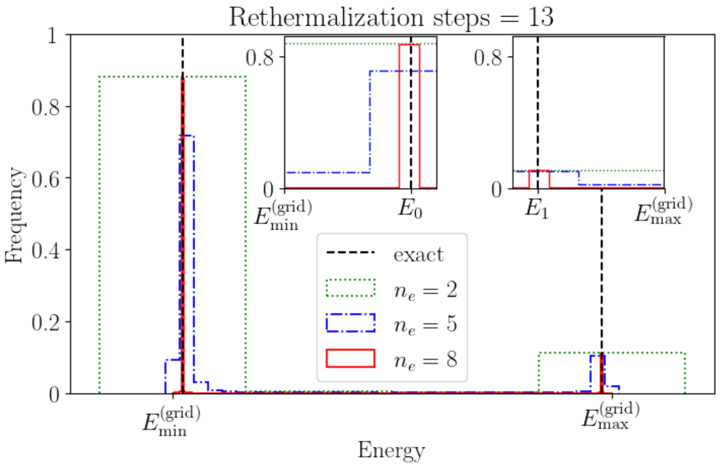




Results stabilize as function of rethermalization steps, but systematical error persists for wrong range QPE, no clear trend for small number of energy qubits.

Non-ideal phase-estimation for QMS: close-up

Close-up on convergence of the energy probability distribution for sufficient number of energy qubits:



Summary and Perspectives

To sum up:

- the sign problem, and the role of Quantum Computing as a solution, have been discussed;
- we briefly overviewed the QMS [K. Temme *et al.* (2011)] and the Q^2MA [M.-H. Yung and A. Aspuru-Guzik (2012)] algorithms, comparing sources of systematical errors;
- in the minimal systematical error case, the *QMS shows advantage* with exponential convergence, unlike power law convergence of Q^2MA.

Work in progress:

- we are applying these algorithms and systematical analysis beyond toy systems;
- in particular, implementing codes for non-abelian gauge systems, for which some modifications are in order, and the phase estimation requires preservation of gauge-invariance. [NuQS Collaboration, PRD **11**, 114501 (2019)]

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Additional slides

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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}

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

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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

Initialization: prepare $|0\rangle_{\text{acc}} |0\rangle_{E^{\text{new}}} |0\rangle_{E^{\text{old}}} |\psi_k\rangle_{\text{syst.}}$ with $|\psi_k\rangle$ 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}

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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.

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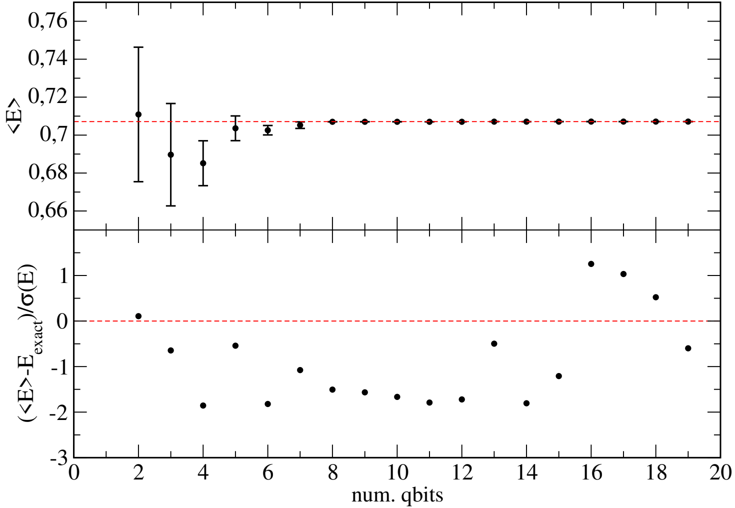
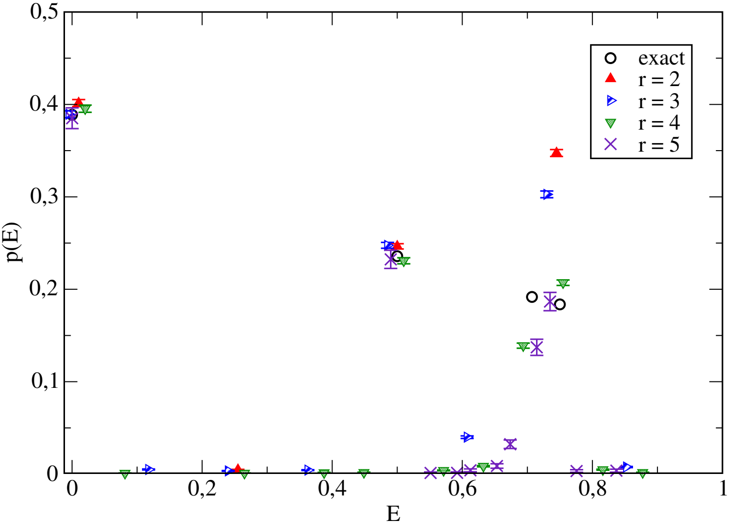
Fluctuation behavior of inexact phase estimation

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

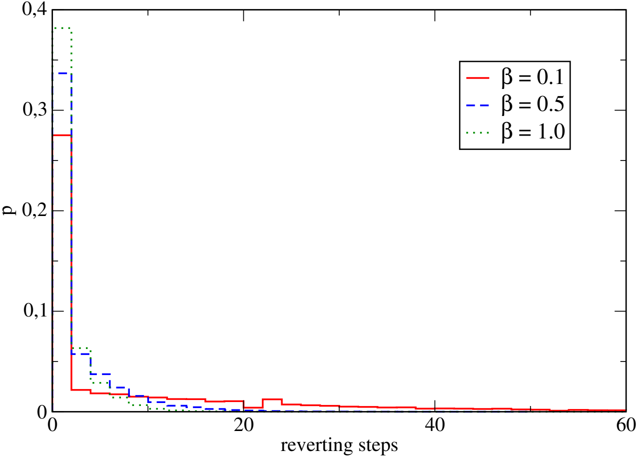


Phase estimation: QMS with incommensurable levels

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



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**.