Hybrid Quantum Estimation of Thermal Averages via Partial Mixed States Preparation.

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HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

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Table of Contents

Challenges of the classical paradigm

> *"Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."* – *Richard Feynman*

Markov Chain Monte Carlo (MCMC) proved **successful** in computing particle spectrum and vacuum structure, **but unsuccessful** for some specific systems or tasks:

- real-time dynamics;
- thermal equilibrium with non-zero baryonic chemical potential $\mu > 0$;
- non-zero topological theta term $\theta \neq 0$ (or external fields in general);
- computation of transport coefficients (such as conductivities);
- frustrated systems.

The **quantum to classical mapping** is not always viable in some cases: either missing statistical interpretation or expensive inversions show up.

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 $\frac{1}{\beta}$

$$\langle \mathcal{O} \rangle_\beta = \mathrm{Tr}[\mathcal{O} e^{-\beta \hat{H}}]/Z,$$
$$Z = \lim_{N\to\infty} \sum_{\{x_\tau\}} \langle x_0 | e^{-\hat{H}\frac{\beta}{N}} | x_1 \rangle \langle x_1 | \ldots | x_N \rangle \langle x_N | e^{-\hat{H}\frac{\beta}{N}} | x_0 \rangle .$$

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**:

If exists $\langle x_\tau | e^{-\hat{H}\frac{\beta}{N}} | x_{\tau+1} \rangle \notin \mathbb{R}_{\geq 0} \implies$ exist paths with Euclidean *action* $S[\{x_\tau\}] \notin \mathbb{R}$ $\implies$ weight $e^{-S} \not> 0$ in the path-integral $\implies$ no statistical intepretation

Unlike traditional Monte Carlo, quantum computing shows no sign problem:

In principle, it is possible to efficiently simulate at finite baryon density and with a topological θ term at thermal equilibrium, both extremely valuables for phenomenology.

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Computing Gibbs ensembles: overview of main approaches

Many approaches have been proposed, to mention a few:

- quantum metropolis methods; [B. Terhal, D. Di Vincenzo (2000), K. Temme *et al.*, Nature **471** (2011) 87,...] [GC *et al.*, PRD **101** (2020) 7][E. Ballini, GC, M. D'Elia, L. Maio, and K. Zambello (2023, coming soon)] **(see Lorenzo Maio's talk Today)**
- quantum simulated annealing; [R.D. Somma *et al.* (2008), M.-H. Yung and A. Aspuru-Guzik, Proc. Natl. Acad. Sci. USA **109** (2012) 754,...] [R. Aiudi, C. Bonanno, C. Bonati, GC, M. D'Elia, L. Maio, D. Rossini, S. Tirone, and K. Zambello (2023, on arXiv today!)]
- approaches based on Variational Quantum Eigensolver (VQE) techniques; [J. Whitfield *et al.* (2011), J. Selisko *et al.* (2022),...] [M. Consiglio *et al.* (2023)] **(see Xiaoyang's talks)**
- approaches based on Quantum Imaginary Time Evolution (QITE); [A. Tan Teck Keng (2023)] **(see Juan William's talks)**
- others...

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Sketch of the algorithm

The algorithm can be roughly decomposed in two stages:

1. **prepare a fiducial mixed state** approximating a fiducial truncated density matrix through Variational Quantum Eigensolving (VQE);
2. **reweight and measure observables** using the auxiliary register as a quantum channel for postselection.

Working in vectorized form of a truncated density matrix ($K = \dim \mathcal{H}_{\text{aux}} \leq \dim \mathcal{H}_{\text{sys}}$)

$$\left|\Psi^{(K)}_{\vec{\theta}}\right\rangle = \sum_{k=0}^{K-1} \gamma_k \left|k\right\rangle \otimes \left|\psi_k(\vec{\theta})\right\rangle \in \mathcal{H}_{\text{tot}} = \mathcal{H}_{\text{aux}} \otimes \mathcal{H}_{\text{sys}}$$

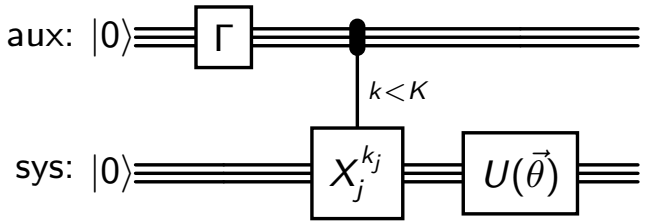
$$\uparrow \textit{ vectorization } \uparrow$$

$$\hat{\rho}_{\text{mix}}\left[\left|\Psi^{(K)}_{\vec{\theta}}\right\rangle\right] \equiv \text{Tr}_{\mathcal{H}_{\text{aux}}}\left[\left|\Psi^{(K)}_{\vec{\theta}}\right\rangle\left\langle\Psi^{(K)}_{\vec{\theta}}\right|\right] = \sum_{k=0}^{K-1} |\gamma_k|^2 \left|\psi_k(\vec{\theta})\right\rangle\left\langle\psi_k(\vec{\theta})\right|$$

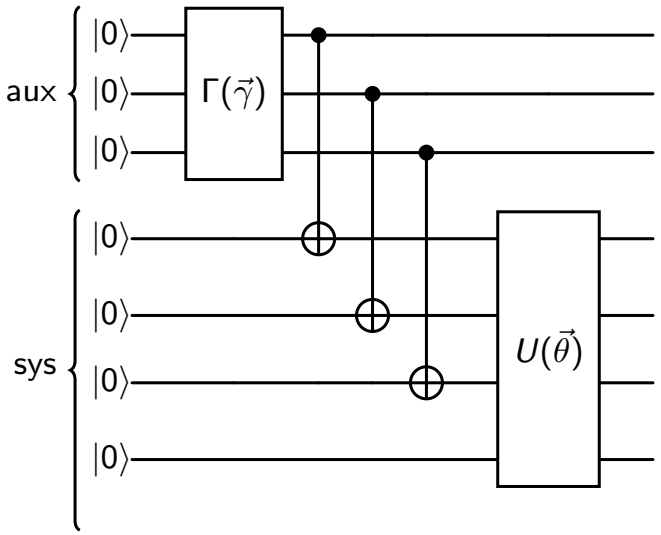
At this stage, $\{\gamma_k\}$ are completely arbitrary and chosen by the user, while $\psi_k(\vec{\theta})$ are prepared via VQE to approximate the lowest K Hamiltonian eigenstates $\{\phi_k\}$.

Sketch of the algorithm: VQE stage

- Approximate eigenstates $\left|\psi_k(\vec{\theta})\right\rangle \equiv U(\vec{\theta})\left|k\right\rangle_{\text{sys}}$ automatically orthonormal;
- Cost functional (for example): $C\left[\left|\Psi(\vec{\theta})\right\rangle\right] = \left\langle\Psi(\vec{\theta})\right|\mathbb{1}\otimes H_0\left|\Psi(\vec{\theta})\right\rangle$;
- with decreasing mixing coefficients $\gamma_k > \gamma_{k+1} > 0$, a variational minimization of the cost function forces the first K columns of $U(\vec{\theta})$ to converge to the exact eigenstates $\left|\psi_k(\vec{\theta})\right\rangle \to |\phi_k\rangle$ (a bit subtler than this, actually).



(a) Condensed form



(b) Example of explicit form $q_A = 3$ and $q_S = 4$

(a similar ansatz structure is used also in [M. Consiglio *et al.* (2023)])

the VQE convergence performance appears to depend heavily on the structure of the ansatz, especially for larger systems. Notice that $U(\vec{\theta})$ **must represent the full low-energy physics, with accuracy decreasing as** $|\gamma_k|^2$**.**

Sketch of the algorithm: reweighting stage

Once a mixed state $\left|\Psi^{(K)}\right\rangle$ is prepared for a certain $\vec{\gamma}$, the information about temperature and observables is introduced through reweighting.

For any observable $\hat{\mathcal{O}}$, the target expectation value we want to measure is

$$\left\langle \hat{\mathcal{O}}(\beta) \right\rangle_{\mathcal{H}_{\mathbf{sys}}} = \mathrm{Tr}_{\mathcal{H}_{\mathbf{sys}}} \left[\hat{\mathcal{O}} \hat{\rho}(\beta) \right] = \lim_{K \to D} \frac{1}{Z^{(K)}(\beta)} \sum_{k=0}^{K-1} e^{-\beta E_k} \langle \phi_k | \hat{\mathcal{O}} | \phi_k \rangle \,,$$

this must must **match** the measurement of some functional $\mathcal{F}[\hat{\mathcal{O}}]$ on the extended space:

$$\begin{aligned} \left\langle \hat{\mathcal{O}}(\beta) \right\rangle_{\mathcal{H}_{\mathbf{sys}}} &= \lim_{K \to D} \frac{\left\langle \Psi^{(K)} \middle| \mathcal{F}[\hat{\mathcal{O}}] \middle| \Psi^{(K)} \right\rangle}{\langle \Psi^{(K)} | \mathcal{F}[\hat{\mathbb{1}}] | \Psi^{(K)} \rangle} = \lim_{K \to D} \frac{\mathrm{Tr}_{\mathcal{H}_{\mathbf{tot}}} \left[\mathcal{F}[\hat{\mathcal{O}}] \left| \Psi^{(K)} \right\rangle \left\langle \Psi^{(K)} \right| \right]}{\mathrm{Tr}_{\mathcal{H}_{\mathbf{tot}}} \left[\mathcal{F}[\hat{\mathbb{1}}] \left| \Psi^{(K)} \right\rangle \left\langle \Psi^{(K)} \right| \right]} \\ &= \lim_{K \to D} \frac{\sum_{k,p=0}^{K-1} \gamma_k \gamma_p^* \, \mathrm{Tr}_{\mathcal{H}_{\mathbf{tot}}} \left[\mathcal{F}[\hat{\mathcal{O}}] \left| k \right\rangle \left\langle p \right| \otimes \left| \phi_k \right\rangle \left\langle \phi_p \right| \right]}{\sum_{k,p=0}^{K-1} \gamma_k \gamma_p^* \, \mathrm{Tr}_{\mathcal{H}_{\mathbf{tot}}} \left[\mathcal{F}[\hat{\mathbb{1}}] \left| k \right\rangle \left\langle p \right| \otimes \left| \phi_k \right\rangle \left\langle \phi_p \right| \right]} , \end{aligned}$$

Therefore:

$$\mathcal{N} e^{-\beta E_k} \delta_{k,p} \langle \phi_k | \hat{\mathcal{O}} | \phi_p \rangle \stackrel{!}{=} \gamma_k \gamma_p^* \langle k, \phi_k | \mathcal{F}[\hat{\mathcal{O}}] | p, \phi_p \rangle \,, \quad (1)$$

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Sketch of the algorithm: reweighting stage (cont.d)

The functional on the extended space can then be chosen of the form:

$$\mathcal{F}[\hat{\mathcal{O}}] \equiv \mathcal{N}\hat{A} \otimes \hat{\mathcal{O}}, \quad \text{where } \hat{A} \equiv \sum_{k=0}^{K-1} \frac{e^{-\beta E_k}}{|\gamma_k|^2} |k\rangle\langle k|_{\text{aux}} .$$

Many strategies for the actual measurements can be used. One possibility is to introduce a **vectorial measurement**, which we define through a vector valued Hermitian operator

$$\hat{\vec{\mathcal{E}}} \equiv \sum_{k=0}^{K-1} \hat{e}_k \frac{1}{|\gamma_k|^2} |k\rangle\langle k|_{\text{aux}} \otimes \hat{H}_0$$

$$= \sum_{i=0}^{M^{(\hat{H}_0)}-1} (\hat{\mathbb{1}} \otimes \hat{S}_i^{(\hat{H}_0)})^\dagger \left[\sum_{k=0}^{K-1} \hat{e}_k \frac{1}{|\gamma_k|^2} |k\rangle\langle k|_{\text{aux}} \otimes \hat{\Lambda}_i^{(\hat{H}_0)} \right] (\hat{\mathbb{1}} \otimes \hat{S}_i^{(\hat{H}_0)}),$$

where we use a diagonal-circuit decomposition for any Hermitian operator of interest $\hat{D} \equiv \sum_{i=0}^{M^{(\hat{D})}-1} \hat{S}_i^{(\hat{D})\dagger} \hat{\Lambda}_i^{(\hat{D})} \hat{S}_i^{(\hat{D})} \to \{(\hat{\Lambda}_i^{(\hat{D})}, \hat{S}_i^{(\hat{D})})\}_{i=0}^{M^{(\hat{D})}-1}$.
The previous vectorial measurement can then be used to define the functional as approximation to the spectrum (errors are assess via a bootstrap procedure):

$$\mathcal{F}[\hat{\mathcal{O}}] \simeq \sum_{m=0}^{M^{(\hat{\mathcal{O}})}-1} (\mathbb{1} \otimes \hat{S}_m^{(\hat{\mathcal{O}})})^\dagger \left[\sum_{k=0}^{K-1} \frac{e^{-\beta \mathcal{E}^k}}{|\gamma_k|^2} |k\rangle\langle k| \otimes \hat{\Lambda}_m^{(\hat{\mathcal{O}})} \right] (\mathbb{1} \otimes \hat{S}_m^{(\hat{\mathcal{O}})}).$$

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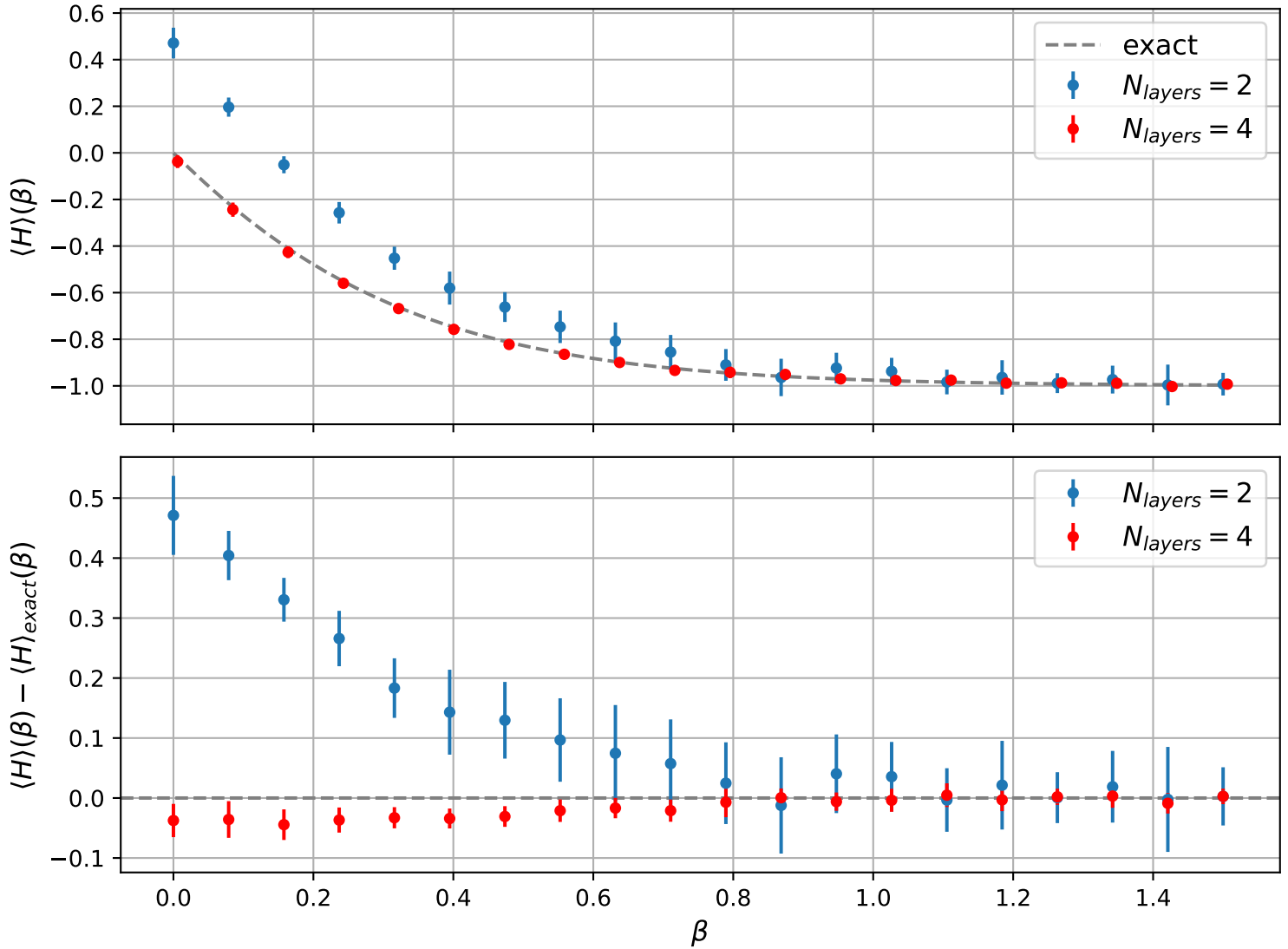
Some preliminary numerical results: frustrated triangle

Application to geometrically frustrated Ising model ($J > 0$), affected by sign problem



Conclusions

To summarize:

- I presented a novel quantum algorithm for the estimation of thermal averages based on VQE mixed state preparation followed by reweighted measurements;
- I sketched a basic construction of the algorithm, emphasizing the freedom available at each stage, and opportunities for improvement;
- the two stages presented can be merged and iterated, and different cost functions and reweightings can be considered. E.g., if efficient computation of entropy is available, one can use that in the cost function to build directly a thermal density matrix, as done by [M. Consiglio *et al.* (2023)].

Current challenges and future perspectives:

- I am currently exploring different variants and hyperparameterization of this algorithm, whose quality of VQE convergence appears to depend heavily on the structure of the ansatz, especially for larger systems. Reweighting is also noisier for observables with many non-commuting pieces;
- with some collaborators, we aim to study and develop algorithms for thermal average estimation, to be applied in cases with sign-problem and lattice gauge theories, in a path towards the investigation of the QCD phase diagram on a quantum computer.

Thank you for the attention!

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Additional slides

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 Trotterization error.

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