Quantum computing algorithms for the investigation of the thermodynamic properties of physical systems

K. Zambello[†,1]

C. Bonati[1] G. Clemente[2] M. D'Elia[1] L. Maio[1] R. Pariente[1]

[†] Speaker

[1] University of Pisa, INFN Sez. di Pisa [2] Deutsches Elektronen-Synchrotron (DESY)

SM&FT 2022, Bari, 20/12/2022

- Numerical solutions for interesting physical problems are hindered by the infamous sign problem

- A noteworthy example is QCD at finite density. In lattice QCD expectation values

$$\langle O \rangle = \frac{1}{Z} \int DU \; O[U] \; e^{-S[U]}$$

are computed by importance sampling, sampling gauge configurations $\propto e^{-S}$.

At finite density S is complex: the theory is affected by a sign problem which hinders the investigation of the QCD phase diagram.

- Quantum computing has been proposed as a possible solution to tackle the sign problem.

  Here we are interested in the application of quantum computing for calculating thermal averages.

- Quantum algorithms useful for our case:
  - Quantum Metropolis Algorithm [K. Temme et al., 2011]
  - Quantum-Quantum Metropolis Algorithm [M. H. Yung et al., 2012]

    QMA seems to be advantageous (yesterday talk by G. Clemente)

- Idea: sample the energy eigenstates $|\psi_i\rangle$ according to the Boltzmann weight $e^{-\beta H}$ using a quantum Markov chain.

The quantum Metropolis algorithm

QMA in a nutshell (I)

- Required quantum registers:

Global state: $|acc, E_f, E_i, \psi\rangle$

  - System state, n qbits
  - Energy at previous and next step, $r + r$ qbits
  - Acceptance, 1 qbit

- Steps (continues...):

1. Start from eigenstate $|\psi_i\rangle$ of energy E_i

$$|0, 0, 0, \psi_i\rangle$$

2. Measure energy E_i

$$|0, 0, 0, \psi_i\rangle \rightarrow |0, 0, E_i, \psi_i\rangle \text{ (QPE)}$$

Measure E_i

3. Metropolis proposal

$$|0, 0, E_i, \psi_i\rangle \rightarrow C|0, 0, E_i, \psi_i\rangle = \sum_p \alpha^c_{ip}|0, 0, E_i, \psi_p\rangle$$

The quantum Metropolis algorithm

QMA in a nutshell (II)

- Steps (...continued):

4. Metropolis accept-reject step $[f(\Delta E_{pi}) = exp(-\beta \Delta E_{pi})]$

$$\sum_p \alpha^c_{pi} |0, 0, E_i, \psi_p\rangle \rightarrow \sum_p \alpha^c_{ip} |0, E_p, E_i, \psi_p\rangle \text{ (QPE)}$$
$$\rightarrow \sum_p \alpha^c_{ip} (\sqrt{f(\Delta E_{pi})}|1\rangle + \sqrt{1 - f(\Delta E_{pi})}|0\rangle) \otimes |E_p, E_i, \psi_p\rangle \text{ (W)}$$

Measure *acc*

If *acc* $= 1$, measure E_p to obtain the new eigenstate. If *acc* $= 0$, the state has to be reverted to the previous eigenstate.

No cloning theorem $\rightarrow$ try to revert the state
[we might fail, reset chain after N_{max} attempts]

5. Measure observable

Measuring non-H-commutating observables destroys equilibration
$\rightarrow$ some extra *rethermalization* steps are needed.

6. Iterate

- Sources of systematics: finite number of qbits for energy/state representation, thermalization/rethermalization, Trotterization for QPE

- QMA applied to a frustrated triangle using a simulator

  [G. Clemente et al., 2020]

- Now we consider the one-dimensional Hubbard model as a prototype for more complex theories

$$H = -t \sum_{\langle i,j \rangle \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i\sigma} n_{i\sigma}$$

  t term $\leftrightarrow$ interaction between fermions at different sites

  U term $\leftrightarrow$ interaction between fermions with different spin

  μ is the chemical potential

- The theory is affected by a sign problem.

- Mapping the physical state requires 2 qbits per site:

  occupation number of a given fermionic mode $\leftrightarrow$ qbit state

- The Hamiltonian dynamics is encoded by anti-commutating operators, but can be mapped to a quantum computer using the Jordan-Wigner representation. This yields

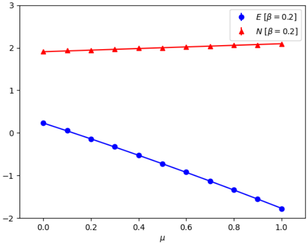
$$H = -t \left(\sum_{j=0}^{N-2} + \sum_{j=N}^{2N-2} \right) (\sigma_j^- \sigma_{j+1}^+ + \sigma_{j+1}^- \sigma_j^+)$$

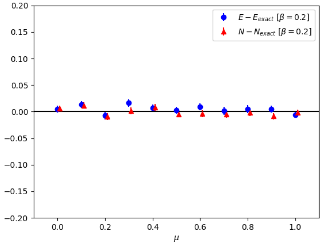
$$+ \frac{U}{4} \sum_{j=0}^{N-1} (1_j - \sigma_j^z)(1_{j+N} - \sigma_{j+N}^z) - \mu \sum_{j=0}^{2N-1} (1_j - \sigma_j^z) \ ,$$

were $\sigma^\pm = \frac{1}{2}(\sigma^x \pm i\sigma^y)$.

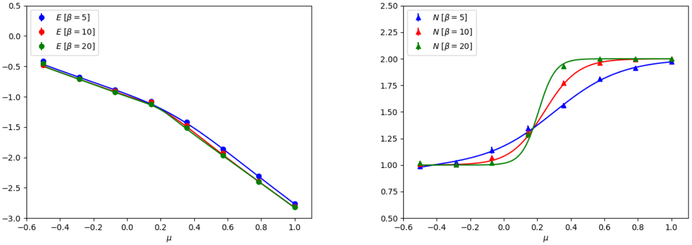
- We have considered the 2 sites case, i.e. the *minimal* case that preserves the full structure of the Hamiltonian.
- Quantum registers:

  $2 \cdot 2$ qbits (system) + $2 \cdot 7$ qbits (energy) + 1 qbit (acceptance)
- Hadamard gates were used as unitary operators for the Metropolis proposal.

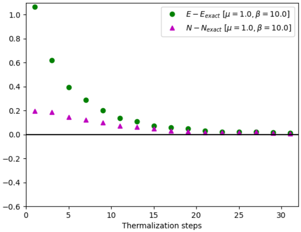




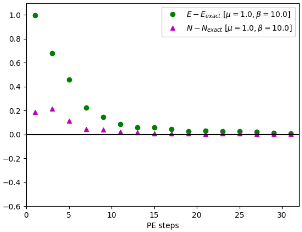
- The simulations have been repeated at different β.
  Numerical results are in agreement with the exact results.



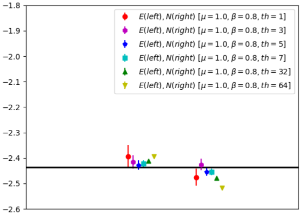
Thermalization steps

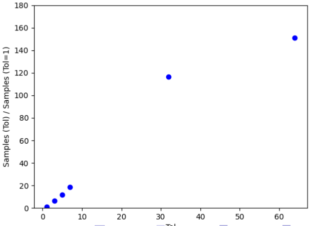


Trotter steps



Tolerance bins

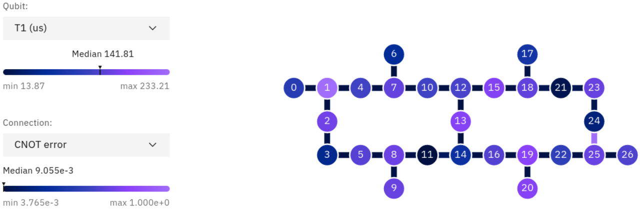




Hamiltonian evolution on IBM Quantum hardware

IBM Quantum Hardware

- As part of the INFN-CERN agreement we had access to a 27-qbit premium IBM machine (`ibmq_kolkata`).



- relaxation time $\approx 100\mu s$, gate time $\approx 400ns$, $cx\ err \approx 10^{-2}$

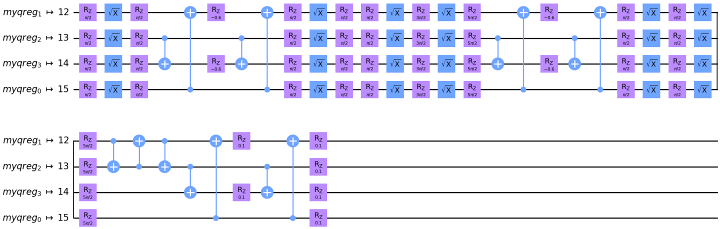
  But notice the high variability in the qbit quality metrics.

  $\rightarrow$ circuits with $O(100)$ circuit depth and number of cx gates
- QMA circuit depth too large to run on current generation machines, but we can test the Hamiltonian evolution which is a key ingredient of the QPE and the QMA

Hamiltonian evolution on IBM Quantum hardware

Hamiltonian evolution operator

- Hamiltonian evolution operator decomposed to native gates



- No all-to-all connectivity, a series of swap gates is required to apply 2-qbit gates between unconnected qbits.

  On `ibmq_kolkata` with an optimal selection of the qbits the evolution operator requires 2 swap gates per Trotter step.

  Each trotter step: circuit depth ≈ 30, number of cx gates ≈ 20. Evolution performed using 4 Trotter steps at each t.

Noise is present due to unintended interaction between the qbits and the environment. Quantum error mitigation strategies:

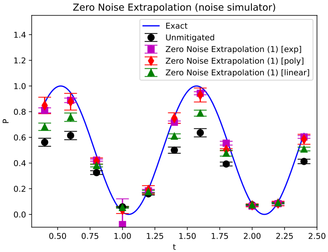
- Zero noise extrapolation [K. Temme et al., 2017]
- General error mitigation [M. S. Jattana et al., 2020]
- Self-mitigation [S. A. Rahman et al., 2022]
- ...

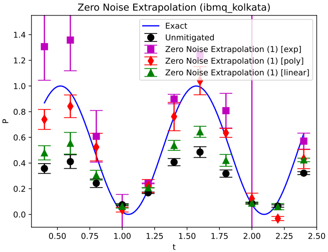
1. Zero noise extrapolation

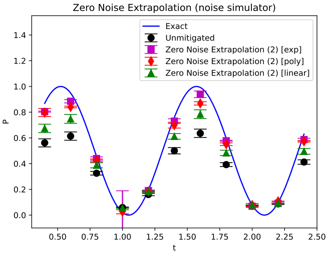
   Artificially inflate noise by replacing a subset of cx gates with a larger odd number of cx gates, then extrapolate the results in the limit of zero noise.

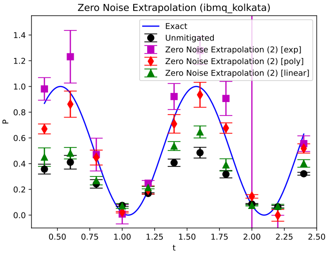
Hamiltonian evolution on IBM Quantum hardware

Error mitigation strategies - ZNE (II)









2. General error mitigation

Postulate the existence of a $2^N \times 2^N$ calibration matrix M such that $MV = E$, where E are the exact data and V are the data from the machine.

The columns of M can be reconstructed by running a calibration circuit starting from all the 2^N possible initial states for the qbits.

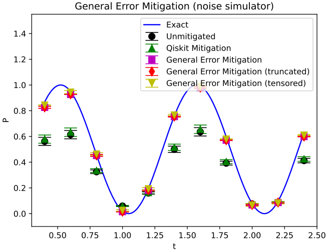
Calibration circuit: 2 trot. step for dt + 2 trot. steps for $-dt$.

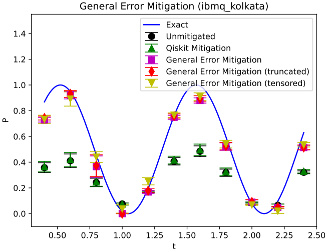
We tested 2 possible workarounds to address the scalability concerns:

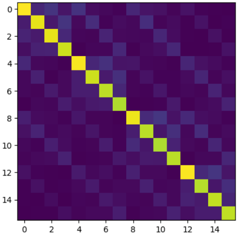
- Use only partial information. Start from the identity matrix and reconstruct only a few columns.
- Construct N 2×2 calibration matrices for the individual qbits and then build a tensored $2^N \times 2^N$ calibration matrix out of those.

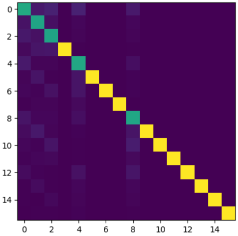
Hamiltonian evolution on IBM Quantum hardware

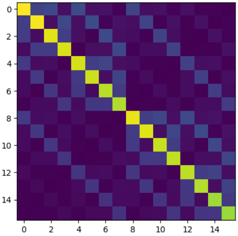
Error mitigation strategies - GEM (II)









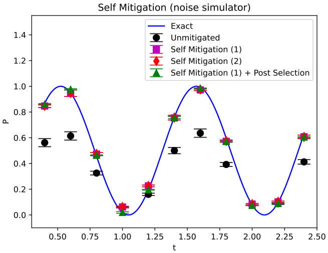


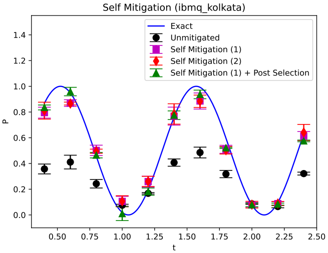
3. Self-mitigation

Describe the noise by a global incoherent depolarizing noise model, $\epsilon(\rho) = (1-p)\rho + p\ \frac{I}{2^N}$.

The parameter p can be estimated by running a parner circuit with known ouputs. Randomized compiling is used to convert coherent noise to incoherent noise.

Partner circuit: 2 trot. step for dt + 2 trot. steps for $-dt$.





Conclusions

In conclusion:

- we have applied the Quantum Metropolis algorithm to the one-dimensional Hubbard model using a simulator and we were able to recover the expected results at different β
- using the same model as a test bench we tested and compared the effectiveness of various quantum error mitigation strategies on real hardware
- we found it hard to keep systematic uncertainties under control with Zero-noise extrapolation
- General error mitigation is more reliable and works better than ZNE; the workarounds that we tested to lessen the scalability concerns do not seem too detrimental to the final results
- Self-mitigation works better than GEM

Thank you for listening!