QITE implementation of quantum models using qiskit

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Contents

- What is QITE?
- QITE vs ITE in Transverse Ising Model
- Why QITE ?
- Ground State Energy of H_2 $using\ QITE \& VQE$
- Possible Problems with QITE?
- Importance of Selecting Parameter
- Pulse Calibration

What is QITE?

QITE = Quantum Imaginary Time Evolution

Idea: linearization to compute generators of unitary of step n+1, from measured expectation values at step n

$$|\bar{\Psi}'\rangle \equiv c^{-1/2}\, e^{-\Delta\tau \hat{h}[l]}|\Psi\rangle = e^{-i\Delta\tau \hat{A}[l]}|\Psi\rangle$$

$$\hat{A}[l] = \sum_{i_1 i_2 \dots i_D} a[l]_{i_1 i_2 \dots i_D} \hat{\sigma}_{i_1}\hat{\sigma}_{i_2}\dots\hat{\sigma}_{i_D} = \sum_I a[l]_I \hat{\sigma}_I$$

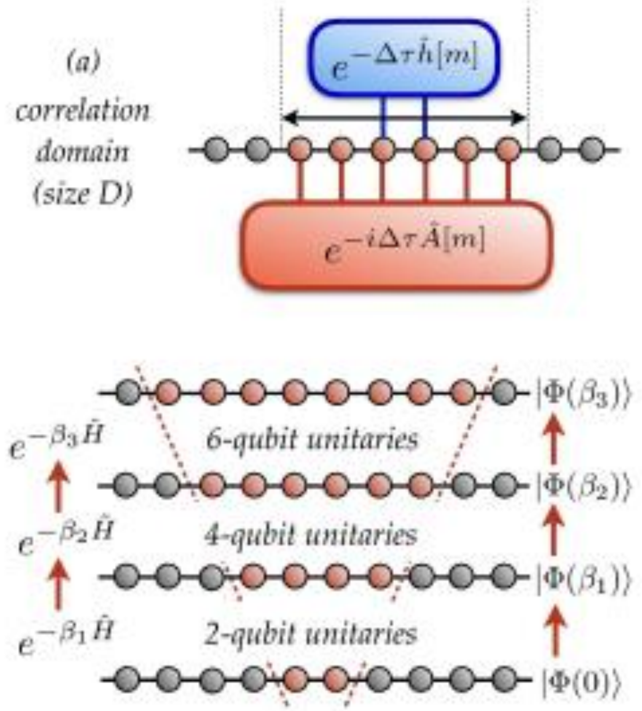
$$|\Delta_0\rangle = \frac{|\bar{\Psi}'\rangle - |\Psi\rangle}{\Delta\tau}\ ,\ |\Delta\rangle = -i\hat{A}[l]|\Psi\rangle\ .$$

$$f(a[l]) = f_0 + \sum_I b_I a[l]_I + \sum_{IJ} a[l]_I S_{IJ} a[l]_J$$

$$f_0 = \langle\Delta_0|\Delta_0\rangle \quad ,$$
$$S_{IJ} = \langle\Psi|\hat{\sigma}_I^\dagger \hat{\sigma}_J|\Psi\rangle \quad ,$$
$$b_I = i\,\langle\Psi|\hat{\sigma}_I^\dagger|\Delta_0\rangle - i\,\langle\Delta_0|\hat{\sigma}_I|\Psi\rangle \quad ,$$

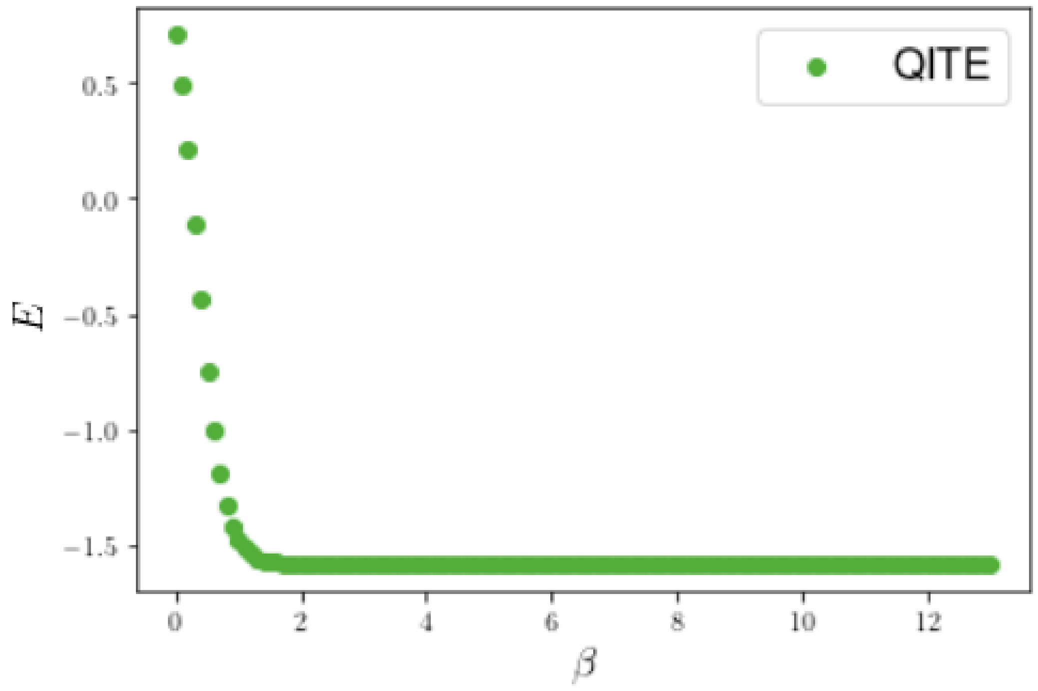
$$\left(\mathbf{S} + \mathbf{S}^T\right)\mathbf{a}[l] = -\mathbf{b}$$

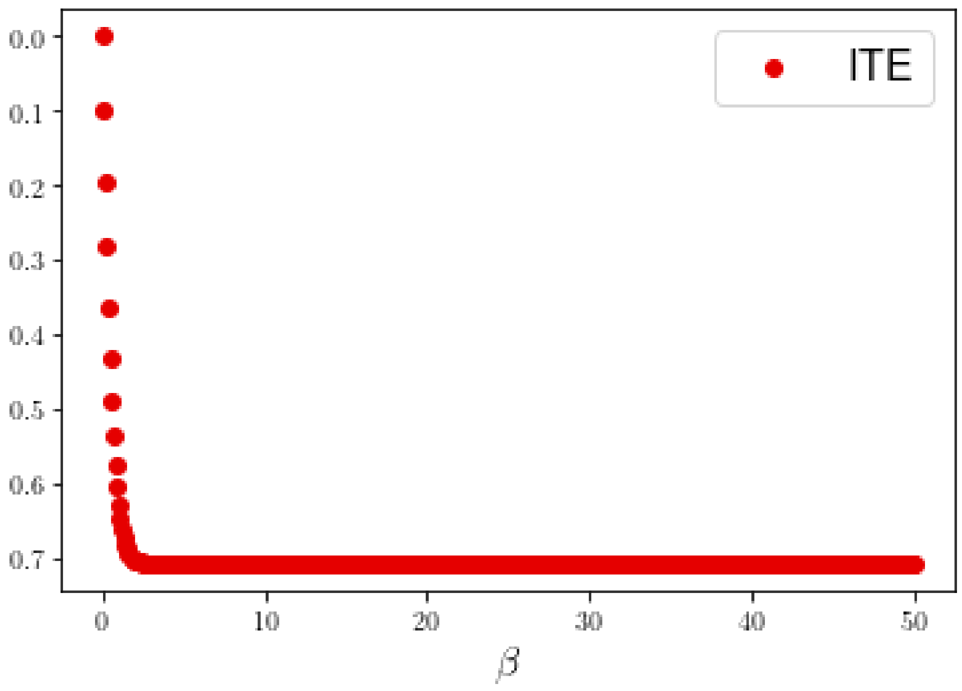
$$|\psi_n\rangle := \frac{\left(e^{-\Delta\tau\hat{h}[1]}\dots e^{-\Delta\tau\hat{h}[m]}\right)^n|\Psi_0\rangle}{\|\left(e^{\ \Delta\tau\hat{h}[1]}\dots e^{\ \Delta\tau\hat{h}[m]}\right)^n|\Psi_0\rangle\|}.$$



Motta et al. Nature Physics(2020): Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution

QITE vs ITE in Transverse Ising Model

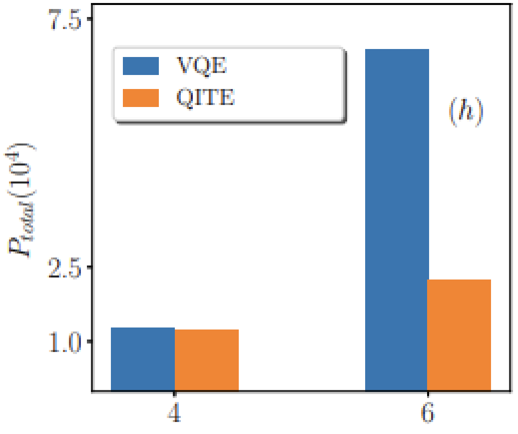




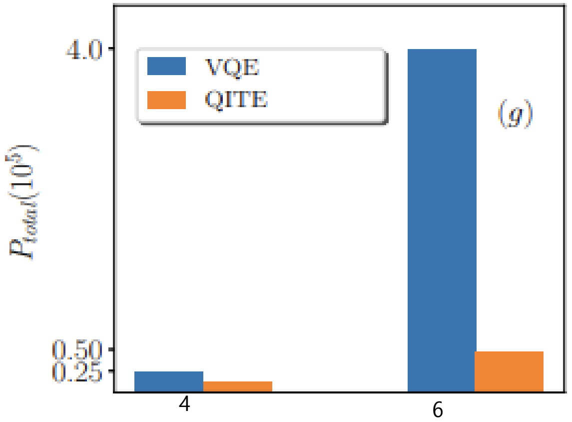
Why QITE ?

- When using VQE algorithm, creating ansatz is a complicated problem, and the classical part of the algorithm also requires optimization.

- QITE algorithm needs no ansatz.



Estimate of the number of Pauli string expectation values (Ptotal) needed for QITE and VQE to converge within 1% of the exact energy for a 4-site (left) and 6-site (right) 1D Heisenberg model



Estimate of the number of Pauli string expectation values (Ptotal) needed for QITE and VQE to converge within 1% (2%) of the exact energy for a 4-site (6-site) 1D AFM transverse-field Ising model.

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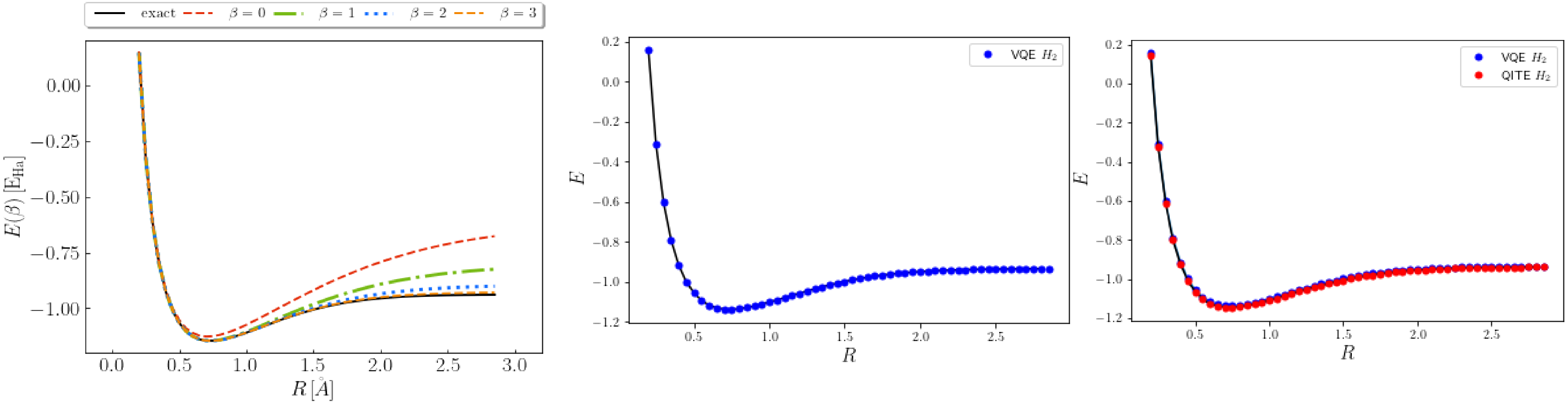
Ground State Energy of H_2 using $QITE\&VQE$

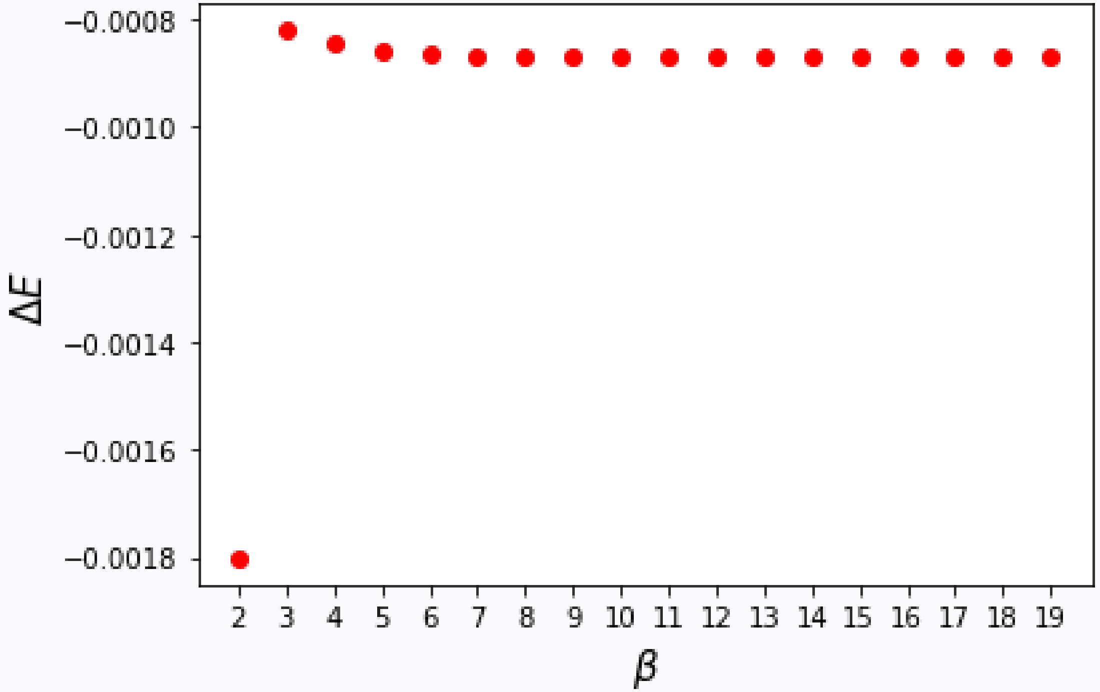


Possible Problems with QITE

$$e^{-\beta\hat{H}} = (e^{-\Delta\tau\,\hat{h}[1]}e^{-\Delta\tau\,\hat{h}[2]}\ldots)^n + \mathcal{O}(\Delta\tau);\; n = \frac{\beta}{\Delta\tau}$$

- As the beta increases, the circuit repeats more, so noise of hardware is increased.
- Also, the accuracy of Trotterization decreases.

Importance of Selecting Parameter



- Due to the hardware noise, proper $\Delta\tau$ must be set.

Pulse Calibration

- Additionally, to solve the basic problem of noise in hardware, we should apply an algorithm such as pulse-level QITE.