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InQubator for Quantum Simulation

U.S. DEPARTMENT OF ENERGY

IMAGINARY TIME PROPAGATION ON A QUANTUM CHIP

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Quantum computing for Many-Body problems

IJCLab, Orsay, 23 November 2022

Imaginary Time propagation

We move the time from real to imaginary:

$$|\psi(t)\rangle = e^{-i\,(H-E_T)\,t}\;|\psi(0)\rangle \quad \xrightarrow[t\to -i\tau]{} \quad |\psi(\tau)\rangle = e^{-(H-E_T)\,\tau}\;|\psi(0)\rangle$$

$$e^{-\tau\,(H-E_T)}\;|\psi(0)\rangle = \sum_n e^{-\tau(E_n-E_T)} c_n\,|\phi_n\rangle$$

$$\xrightarrow{\tau\to\infty} c_0\,e^{-\tau(E_0-E_T)}\;|\phi_0\rangle$$

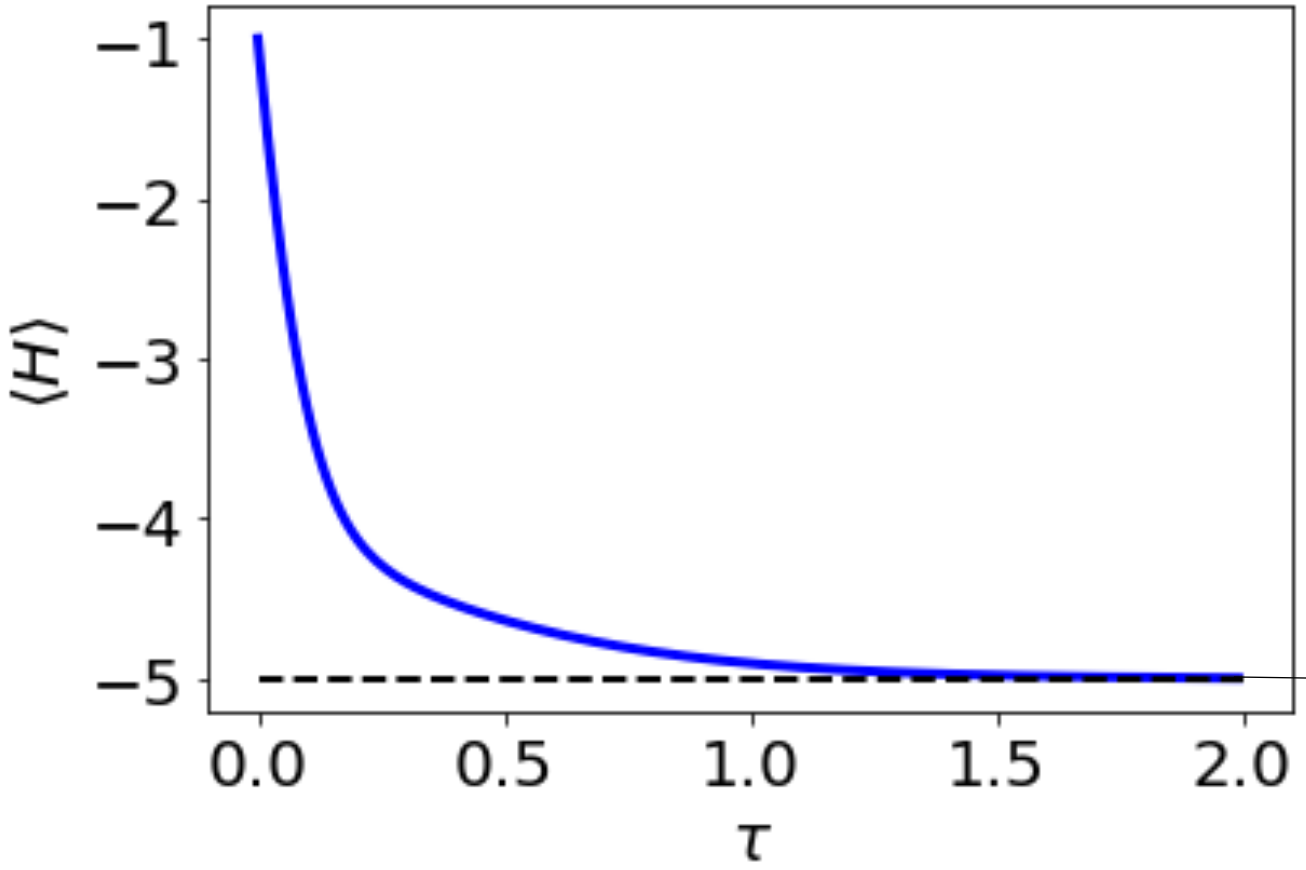
E_T is an algorithm parameter that stabilizes the normalization

E_0 is the actual ground energy

Ground state

With the (classical) Imaginary Time Propagation we get the ground state:

$$e^{-\tau\,(H-E_T)}\;|\psi(0)\rangle \xrightarrow{\tau\to+\infty} c_0\,e^{-\tau(E_0-E_T)}\;|\phi_0\rangle$$



Ground energy

Can we **directly** port this algorithm to a quantum computer?

NO

$$e^{-\tau(H-E_T)}$$

It is <u>not a unitary operator</u>

It cannot be described as a quantum gate

Our Solution: extend the Hilbert Space

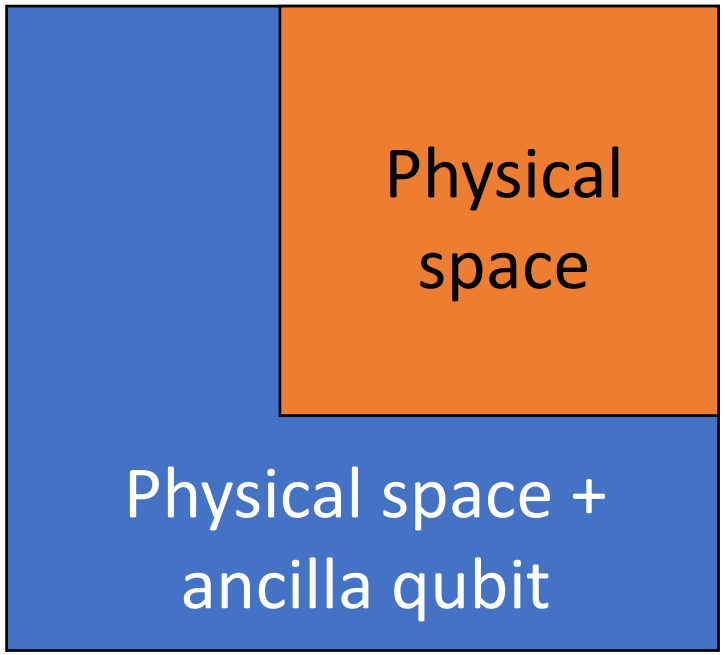
Add an external qubit (called ancilla qubit) to my simulation.

For instance, we prepare the ancilla qubit in the $|0\rangle$ state

$$|0\rangle \otimes |\psi_{init}\rangle$$

Ancilla qubit

Wavefunction of qubits for the physical system



Ancilla: Z. B. Walters (2015); H. Terashima and M. Ueda (2005); D. B. Kaplan et al (2017); Choi et al (2021)

QITP: M. Motta et al (2020); McArdle et al (2019)

We can define in this extended Hilbert space:

$$U_{QITP} = \begin{pmatrix} \frac{e^{-\tau(H-E_T)}}{\sqrt{1+e^{-2(H-E_T)\tau}}} & \frac{1}{\sqrt{1+e^{-2(H-E_T)\tau}}} \\ \frac{1}{\sqrt{1+e^{-2(H-E_T)\tau}}} & -\frac{e^{-\tau(H-E_T)}}{\sqrt{1+e^{-2(H-E_T)\tau}}} \end{pmatrix}$$

This operator is unitary $\Longrightarrow$ it can be described by a **quantum gate**

Turro et al, Phys. Rev. A 105, 022440 (2022)

$$U_{QITP}\left|0\right\rangle \otimes \left|\psi_{init}\right\rangle = \left|0\right\rangle \otimes \frac{e^{-(H-E_T)\tau}}{\sqrt{1+e^{-2(H-E_T)\tau}}}\left|\psi_{init}\right\rangle + \left|1\right\rangle \otimes \frac{1}{\sqrt{1+e^{-2(H-E_T)\tau}}}\left|\psi_{init}\right\rangle$$

This final state is **always closer** to ground state than the initial one

$$U_{QITP}\,|0\rangle \otimes |\psi_{init}\rangle = |0\rangle \otimes \boxed{\frac{e^{-(H-E_T)\tau}}{\sqrt{1+e^{-2(H-E_T)\tau}}}\,|\psi_{init}\rangle}$$

$$+\,|1\rangle \otimes \frac{1}{\sqrt{1+e^{-2(H-E_T)\tau}}}\,|\psi_{init}\rangle$$

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$$+\,|1\rangle \otimes \frac{1}{\sqrt{1+e^{-2(H-E_T)\tau}}}\,|\psi_{init}\rangle$$

Measuring the ancilla state in $|0\rangle$:

$$P_0\,U_{QITP}\,|0\rangle \otimes |\psi_{init}\rangle = \;C\;|0\rangle \otimes \frac{e^{-\tau(H-E_T)}}{\sqrt{1+e^{-2\tau(H-E_T)}}}\,|\psi_{init}\rangle$$

- Success probability is the probability of measuring the ancilla in $|0\rangle$

Quantum Imaginary Time Propagation (QITP) algorithm in a nutshell

Algorithm:

1. Insert an ancilla qubit in $|0\rangle$
2. Apply U_{QITP}
3. Measure the ancilla qubit in $|0\rangle$

$$U_{QITP} = \begin{pmatrix} \frac{e^{-(H-E_T)\tau}}{\sqrt{1+e^{-2(H-E_T)\tau}}} & \frac{1}{\sqrt{1+e^{-2(H-E_T)\tau}}} \\ \frac{1}{\sqrt{1+e^{-2(H-E_T)\tau}}} & -\frac{e^{-(H-E_T)\tau}}{\sqrt{1+e^{-2(H-E_T)\tau}}} \end{pmatrix}$$

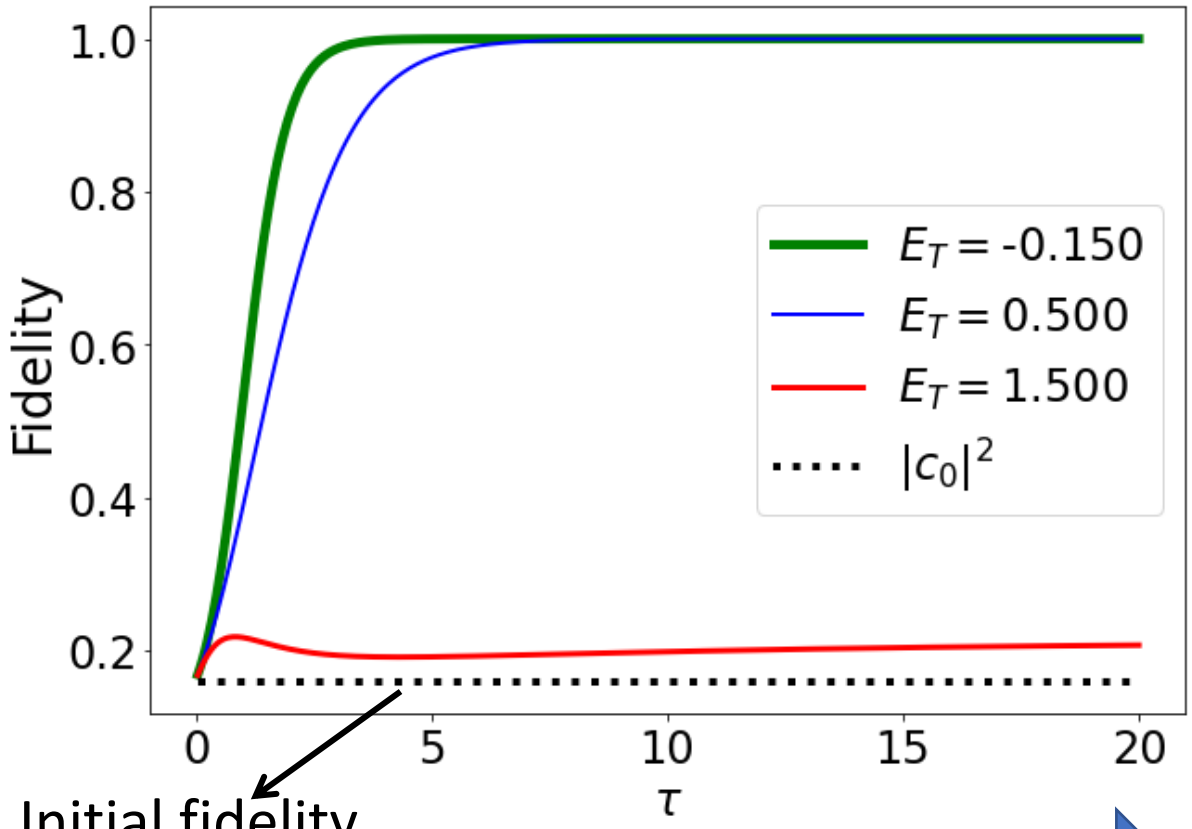
The result is a new state for the physical system closer to Ground State

- Two tunable parameters τ and E_T

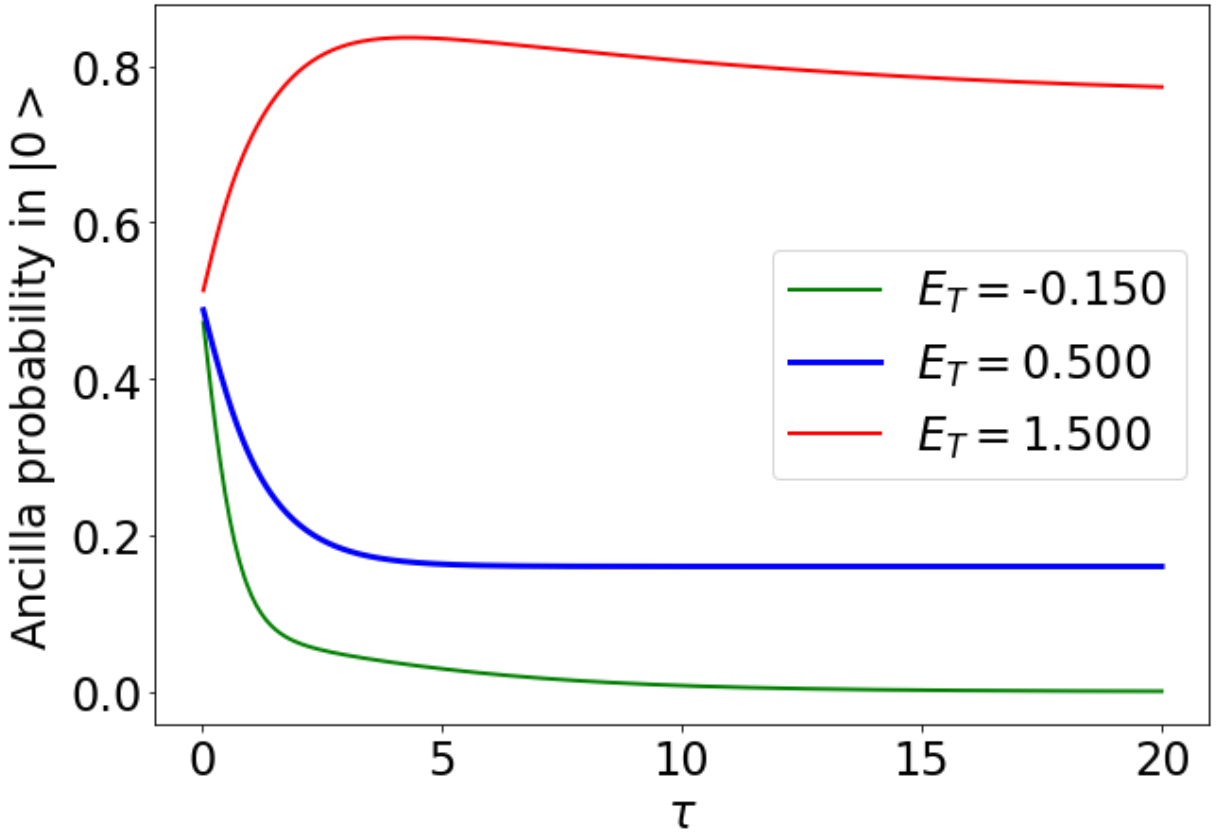
State Fidelity and Success Probability of QITP

Simple system with spectra E = $\left[0, 1, \frac{\pi}{2}\right]$

Fidelity definition: $F = |\langle \phi_0 | \psi_{fin} \rangle|^2$



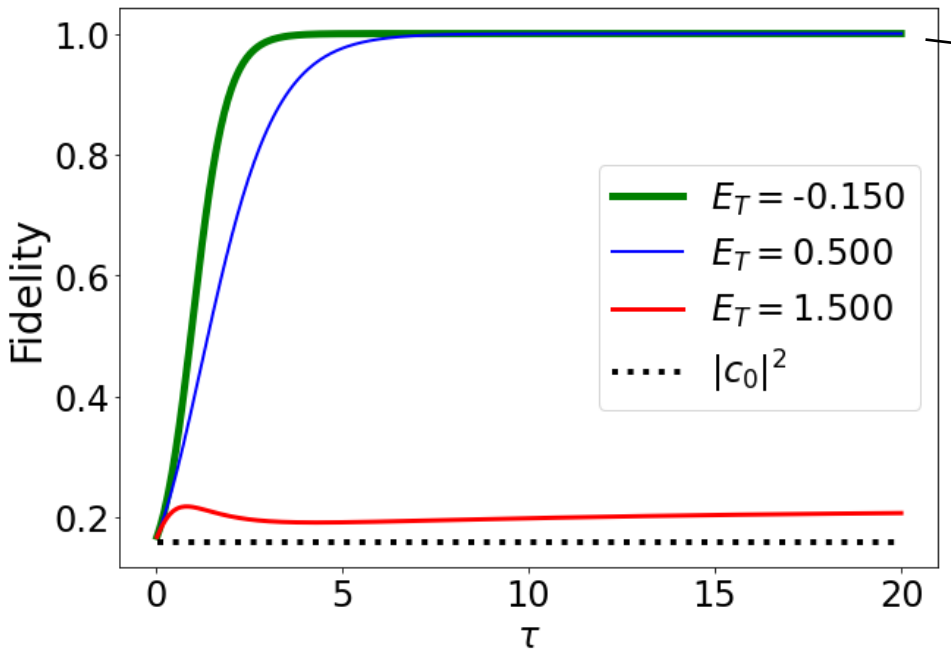
Initial fidelity



Optimal interval: $E_0 \leq E_T \leq E_1$

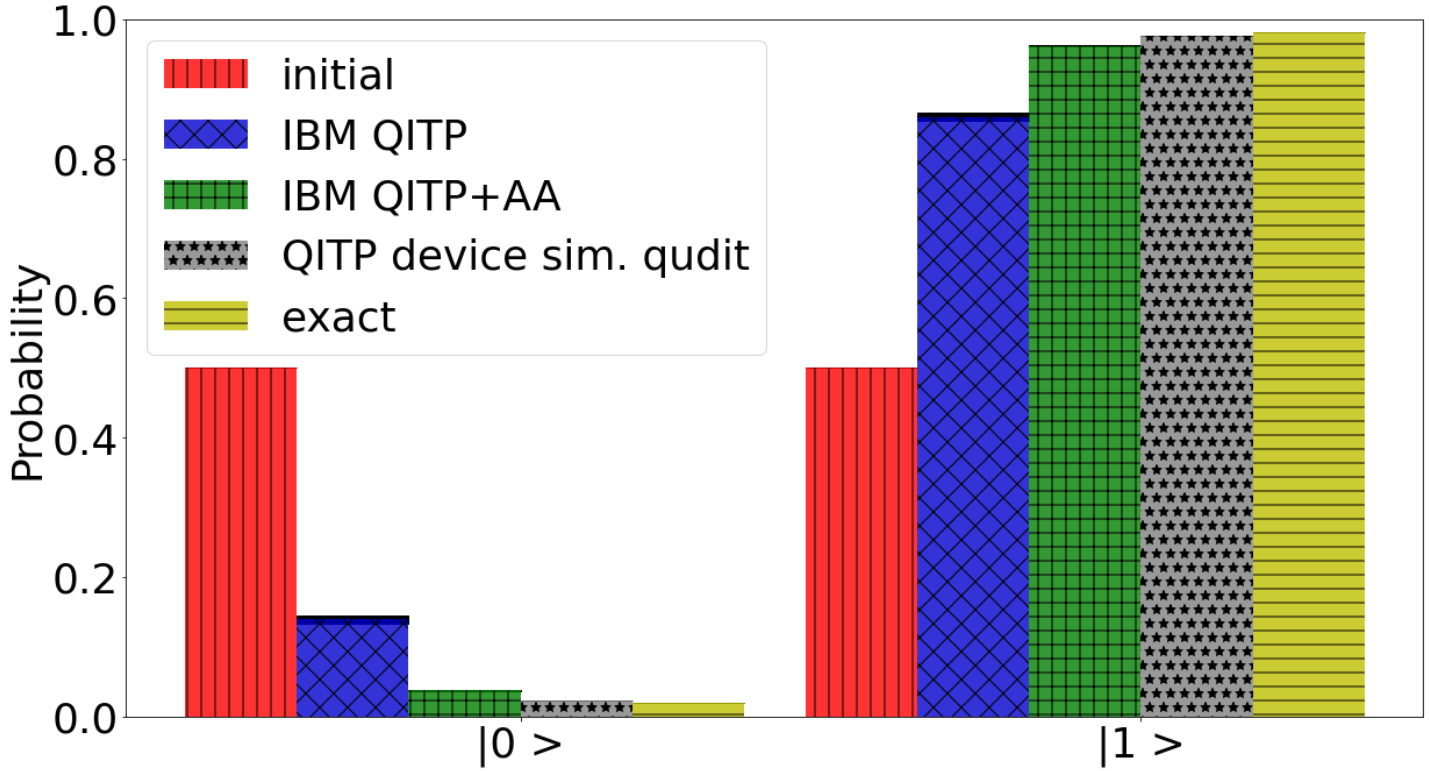
Test: Ground State of Hydrogen atom

- We expand the Hydrogen atom Hamiltonian using two Gaussians, using the STO-2G basis.
- We can use a single qubit to describe the Hydrogen system



Tuning the time step $\tau \gg 1$, we can get the Ground State

QITP result of STO-2G Hydrogen atom when $\tau \to +\infty$



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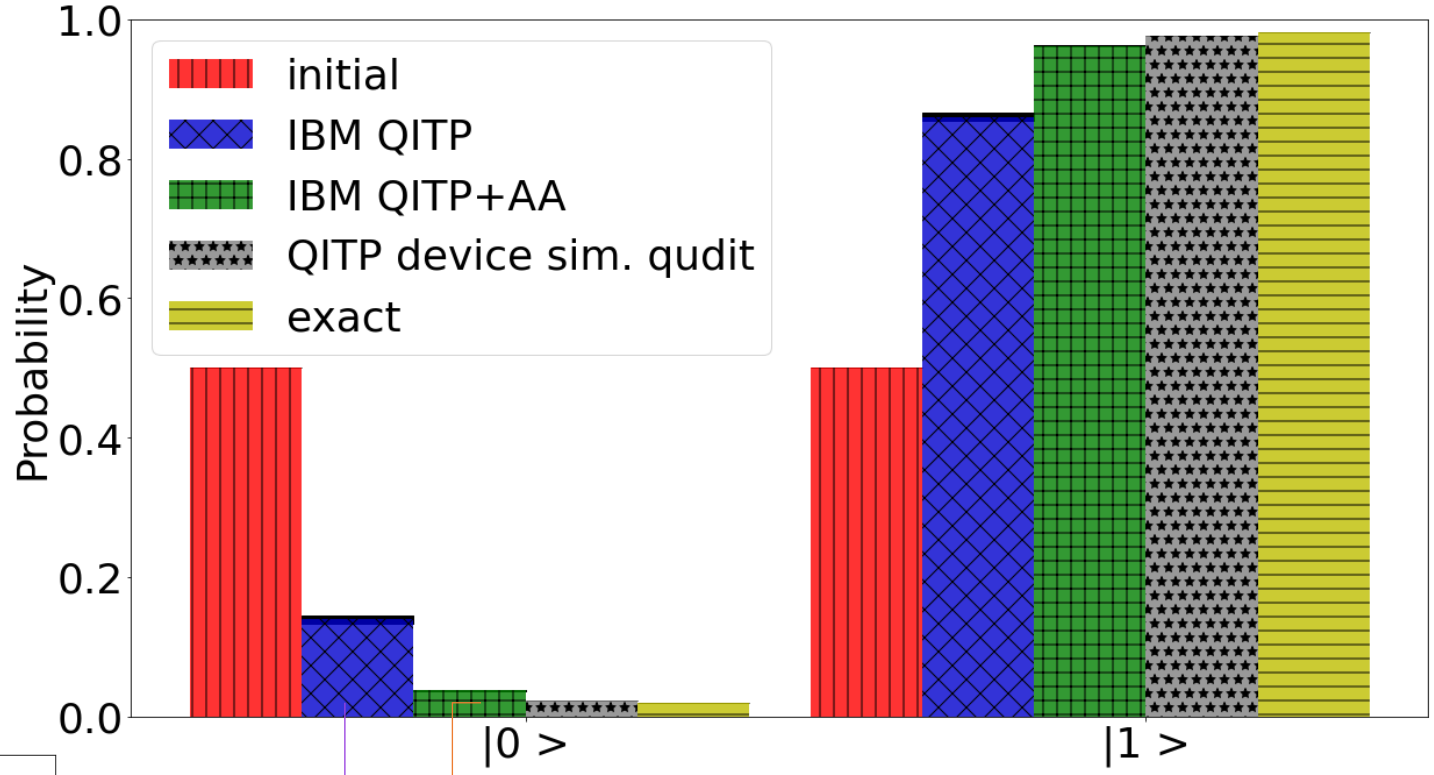
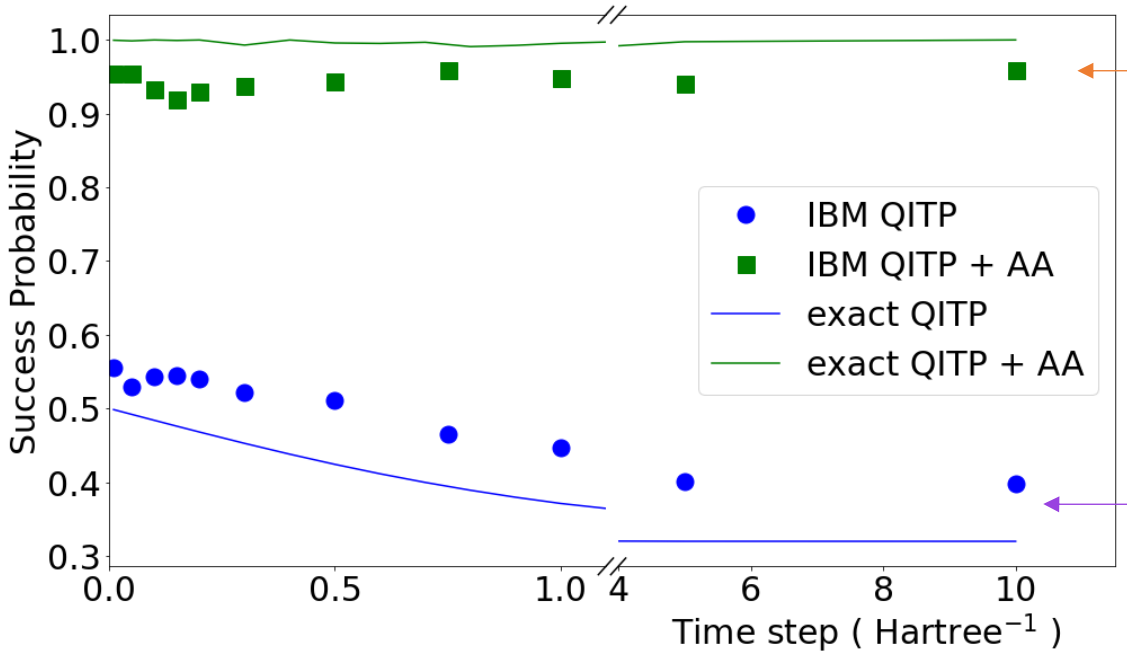
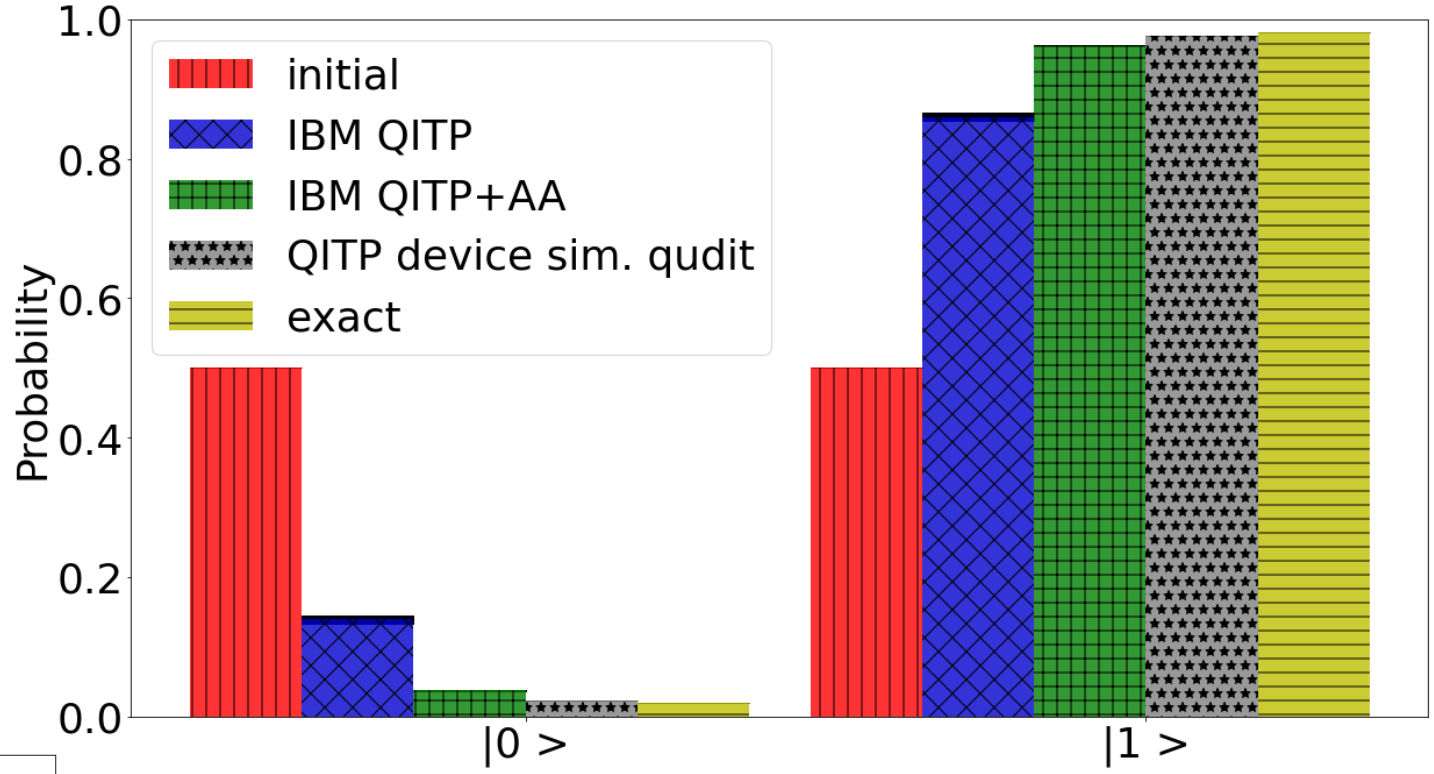
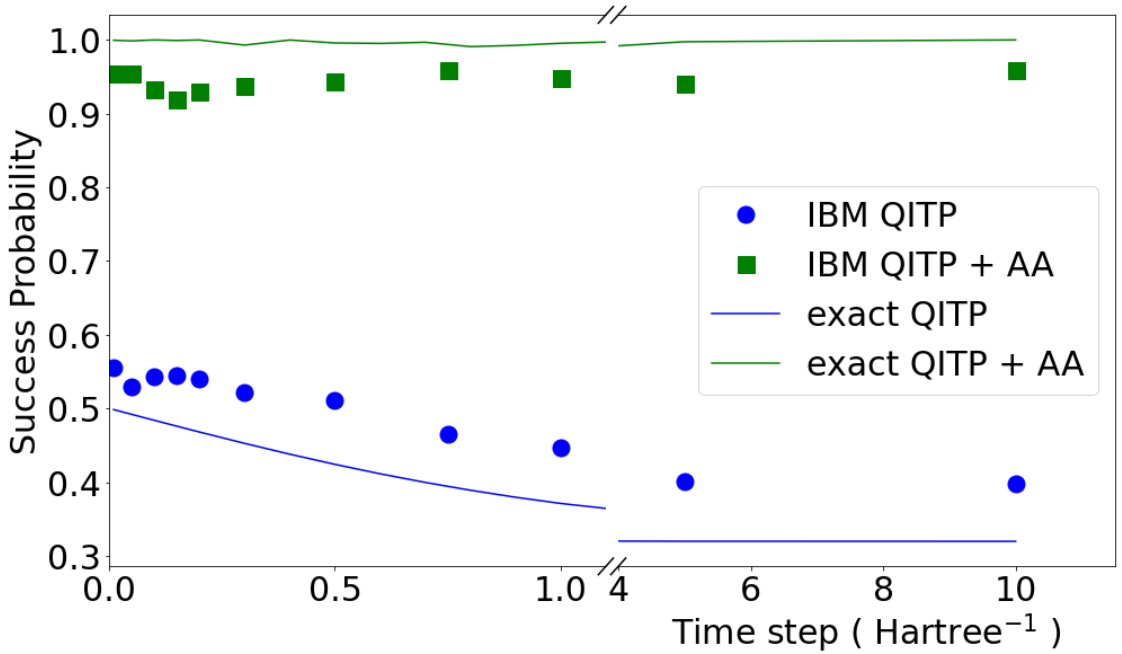




The amplitude amplification (AA) can increase the probability of measuring the ancilla in |0>.
The AA is based on reflections and rotations

QITP result of STO-2G Hydrogen atom when $\tau \to +\infty$





	Fidelity
Initial state	0.361
IBM QITP	0.942(4)
IBM QITP+Amplitude Amplification	0.9968(4)
Device simulation of LLNL testbed	0.9978

Short-time imaginary time propagation

We can reach the ground state with a sequence of short-time imaginary propagators, which can be approximated via Trotter decomposition

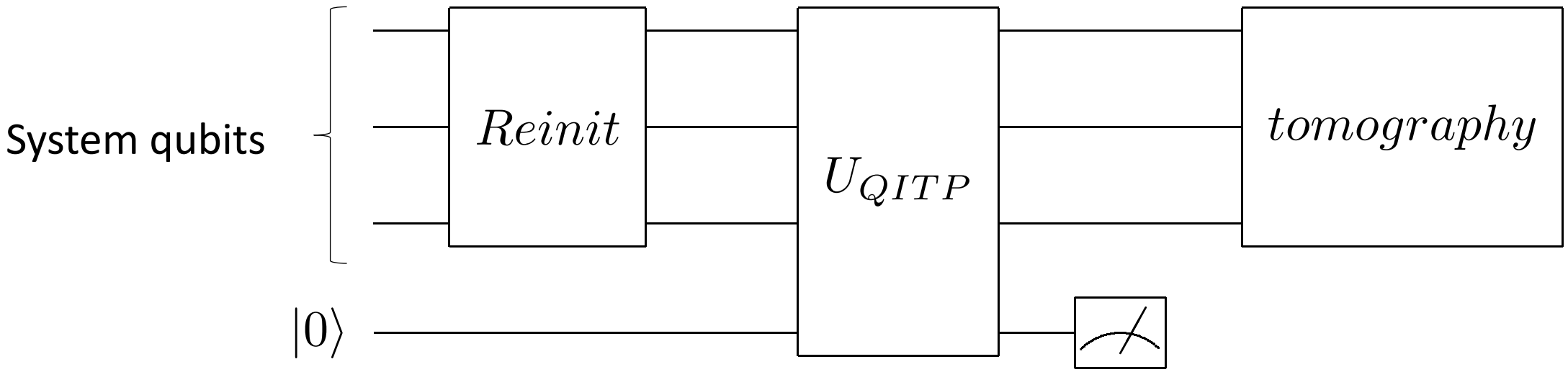
$$\left[P_0\, U_{QITP}\left(\frac{\tau}{r}\right)\right]^r |0\rangle \otimes |\psi_{init}\rangle \xrightarrow{r \to +\infty} c\, |0\rangle \otimes |\phi_0\rangle$$

Measure the ancilla qubit in $|0\rangle$

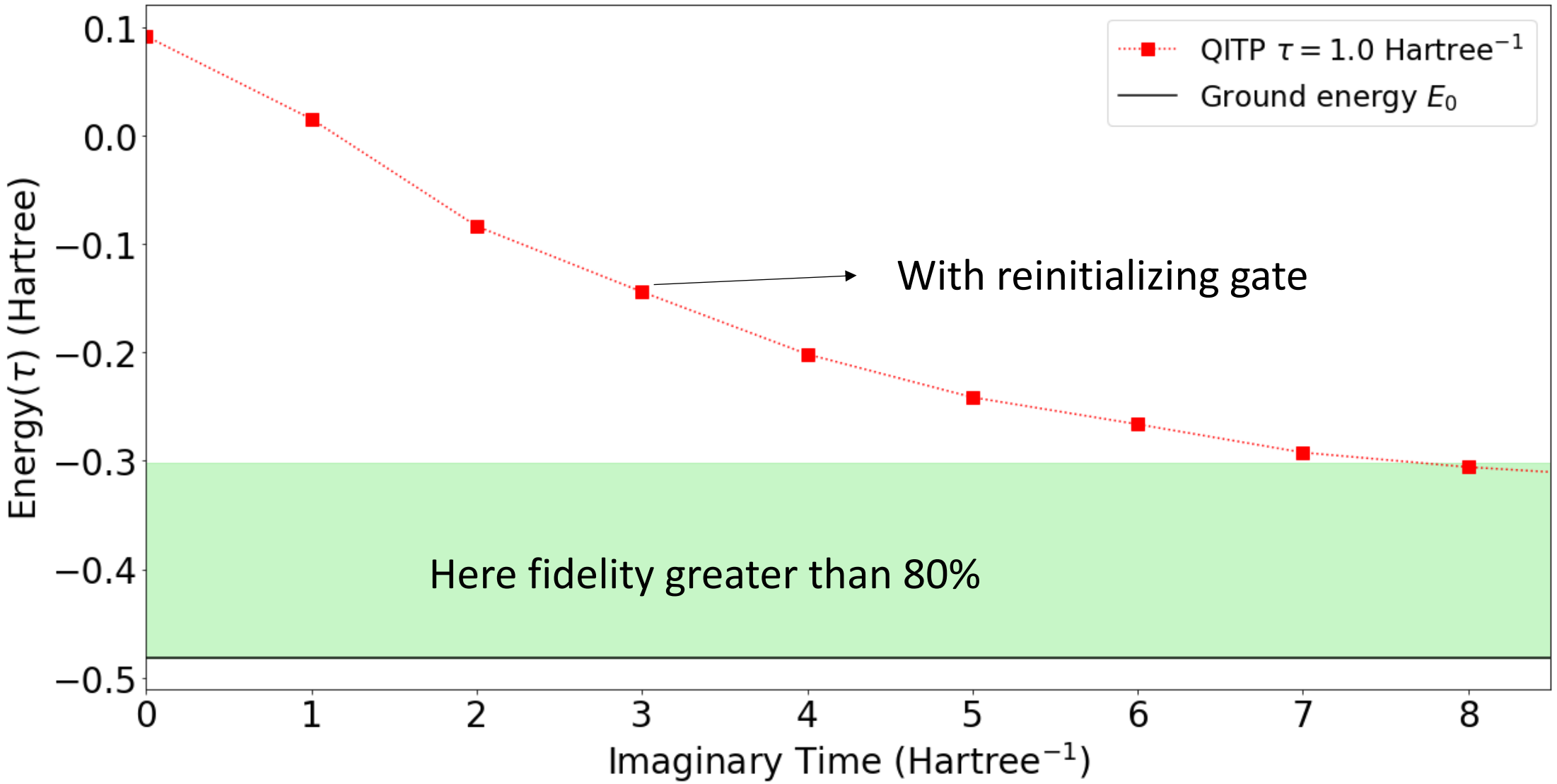
QITP operator

Possible implementations of short-time QITP

- **Reinitializing procedure**: after some step QITP we identify the state and we restart from it

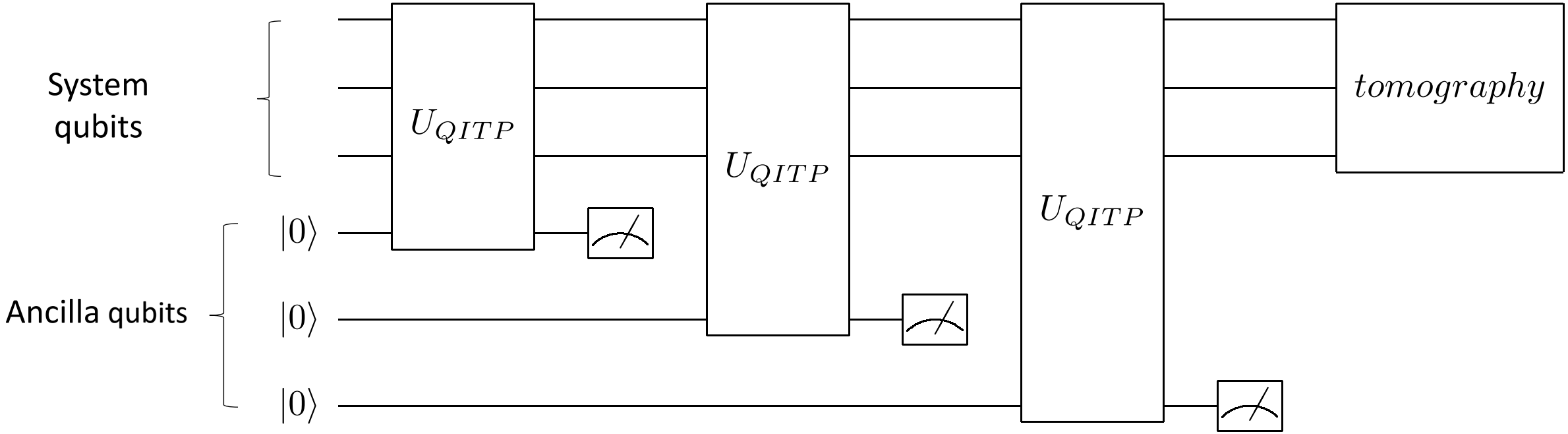


Imaginary Time Evolution



Possible implementations of short-time QITP

- Reinitializing procedure
- **Using N ancilla qubits** to propagate in N time steps:



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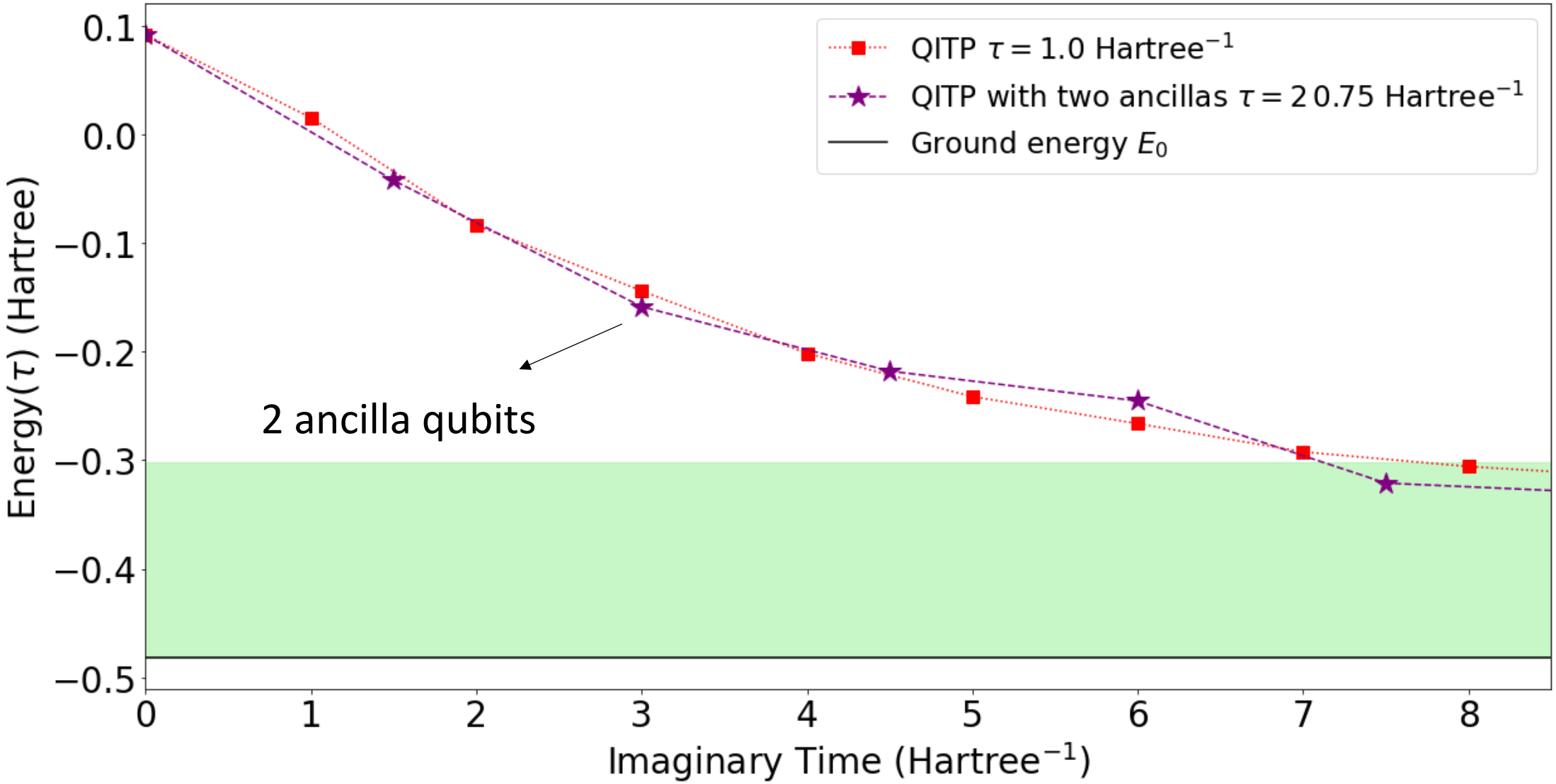

Possible implementations of short-time QITP

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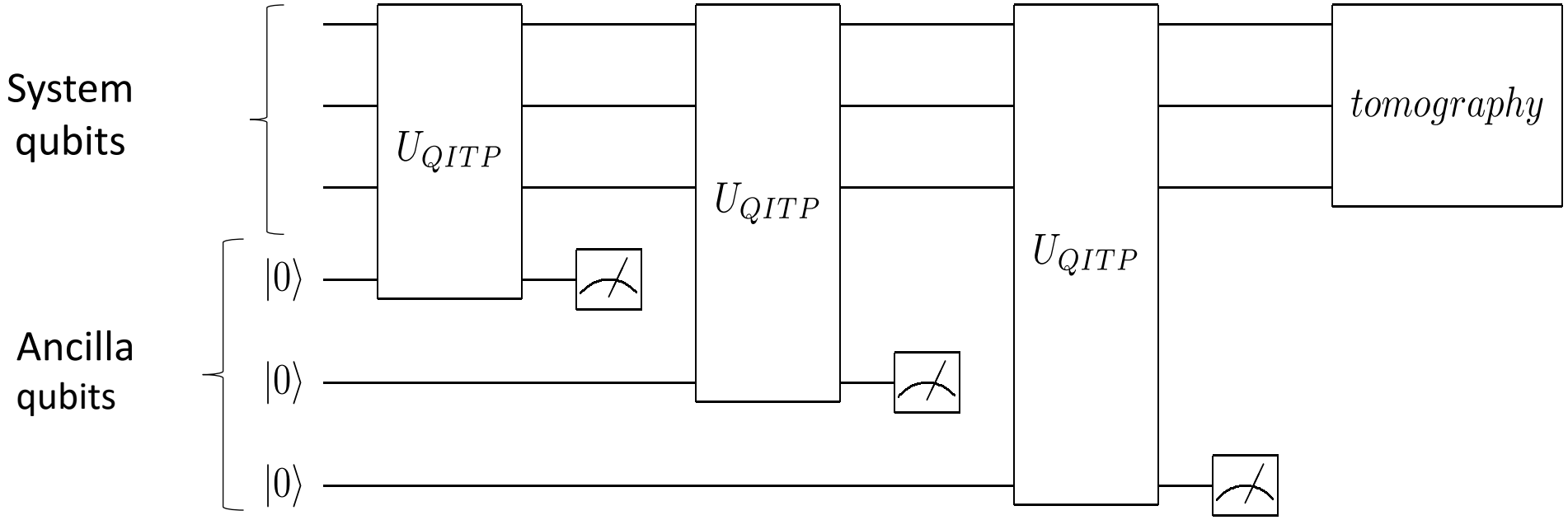
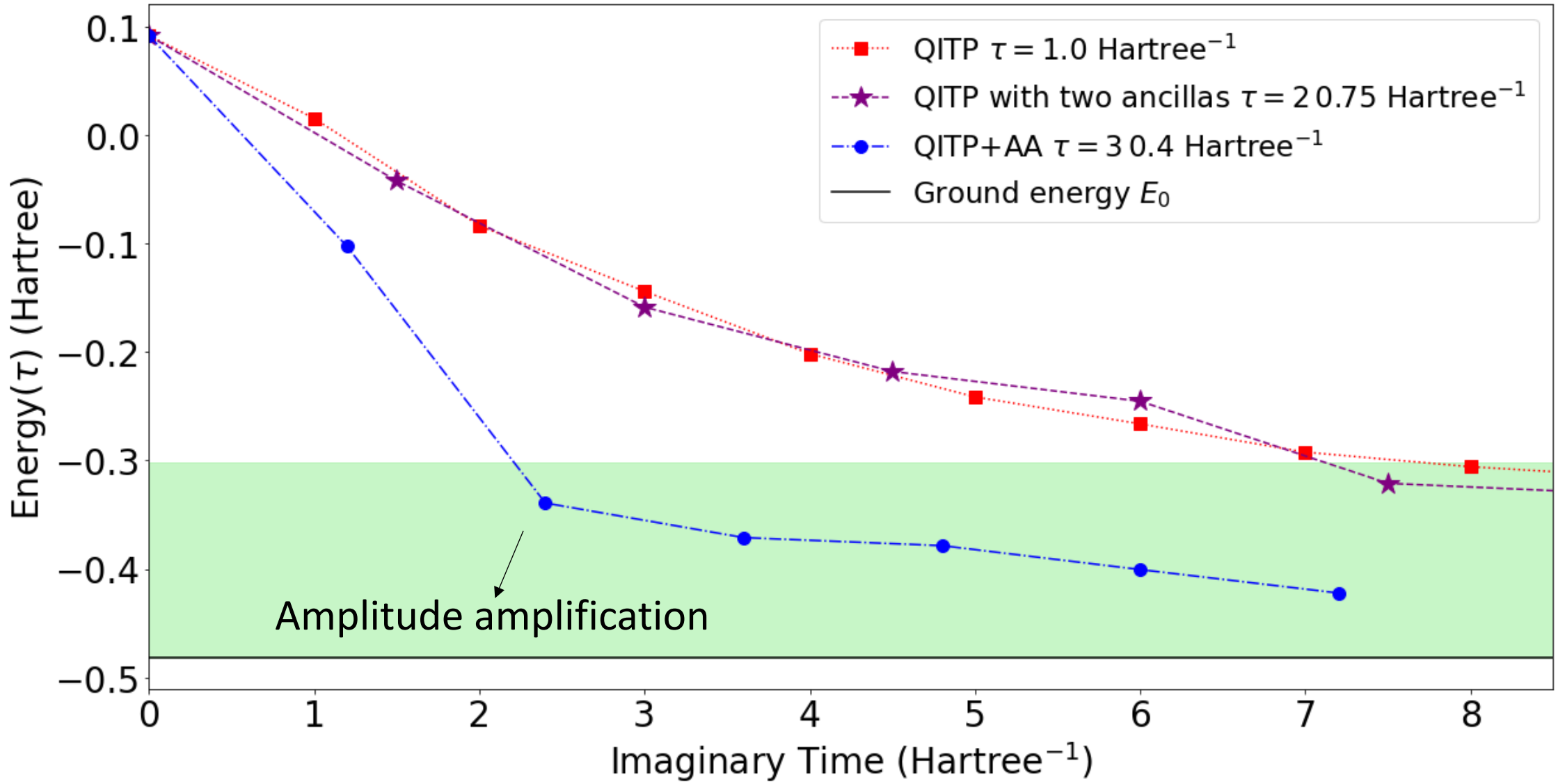


- **Amplitude amplification**: we increase the probability of measuring the ancilla qubit state in the $|0\rangle$ state to 1 without touching the information contained in the physical qubits

Imaginary Time Evolution



Scaling: there is no free lunch …

- The success probability may drop to 0 exponentially after r time steps

$$P_s(r) \geq \frac{|c_0|^2}{\left(e^{2\delta\tau(E_0-E_T)}+1\right)^r} \xrightarrow[\tau\to+\infty]{} 0$$

- We found that the fidelity goes to 1 subexponentially in r

$$F = |\langle\phi_0|\psi_{fin}\rangle|^2 \geq \frac{1}{1+\sum_n \frac{1-|c_0|^2}{|c_0|^2} e^{-\frac{1}{2}\delta\tau(r)\Delta}} \xrightarrow[r\to+\infty]{} 1$$

Scaling: there is no free lunch …

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The QITP algorithm can be used for few time steps as ***preconditioner*** for other state preparation methods that require a good initial fidelity

Lin, and Tong, *Quantum* 4 (2020)

Future Application: Preparing Quantum Thermal States on a quantum computer

The density matrix of a canonical ensemble is given by:

$$\rho = e^{-\beta(H-E_T)} \qquad \langle O \rangle = \frac{Tr\left[Oe^{-\beta(H-E_T)}\right]}{Tr\left[e^{-\beta(H-E_T)}\right]}$$

Future Application: Preparing Quantum Thermal States on a quantum computer

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a) We must consider that we work with density matrix not rather with operator

b) We should modify the operator in the QITP

$$U_{QITP} = \begin{pmatrix} \frac{e^{-(H-E_T)\beta}}{\sqrt{1+e^{-2(H-E_T)\beta}}} & \frac{1}{\sqrt{1+e^{-2(H-E_T)\beta}}} \\ \frac{1}{\sqrt{1+e^{-2(H-E_T)\beta}}} & -\frac{e^{-(H-E_T)\beta}}{\sqrt{1+e^{-2(H-E_T)\beta}}} \end{pmatrix}$$

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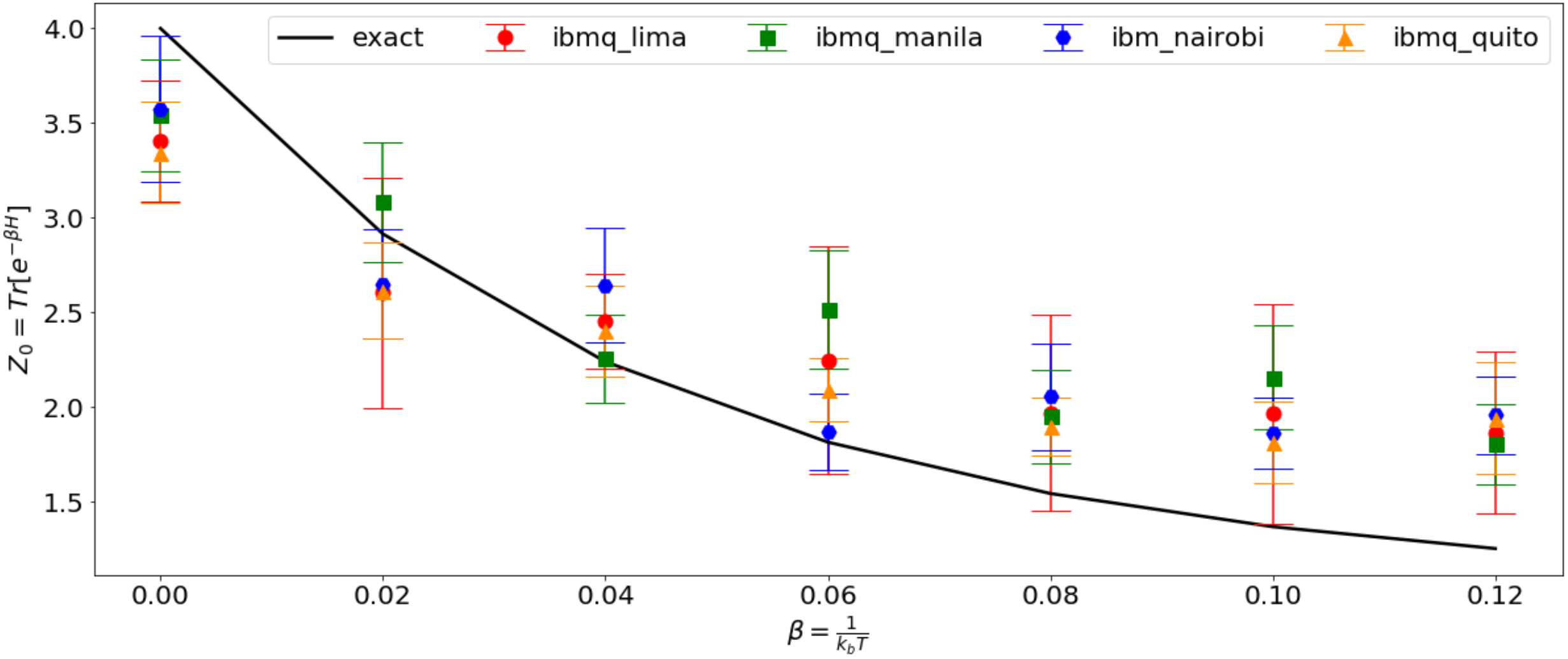
a) We must consider that we work with density matrix not rather with operator ⇒ We prepare the state in quantum processors in the "classical" state

b) We should modify the operator in the QITP

$$U_{QITP} = \begin{pmatrix} \frac{e^{-(H-E_T)\beta}}{\sqrt{1+e^{-2(H-E_T)\beta}}} & \frac{1}{\sqrt{1+e^{-2(H-E_T)\beta}}} \\ \frac{1}{\sqrt{1+e^{-2(H-E_T)\beta}}} & -\frac{e^{-(H-E_T)\beta}}{\sqrt{1+e^{-2(H-E_T)\beta}}} \end{pmatrix} \Rightarrow U^{th}_{QITP} = \begin{pmatrix} \sqrt{P_s e^{-(H-E_T)\beta}} & x \\ x & -\sqrt{P_s e^{-(H-E_T)\beta}} \end{pmatrix}$$

Preliminary result: Thermal distribution of two spin neutrons



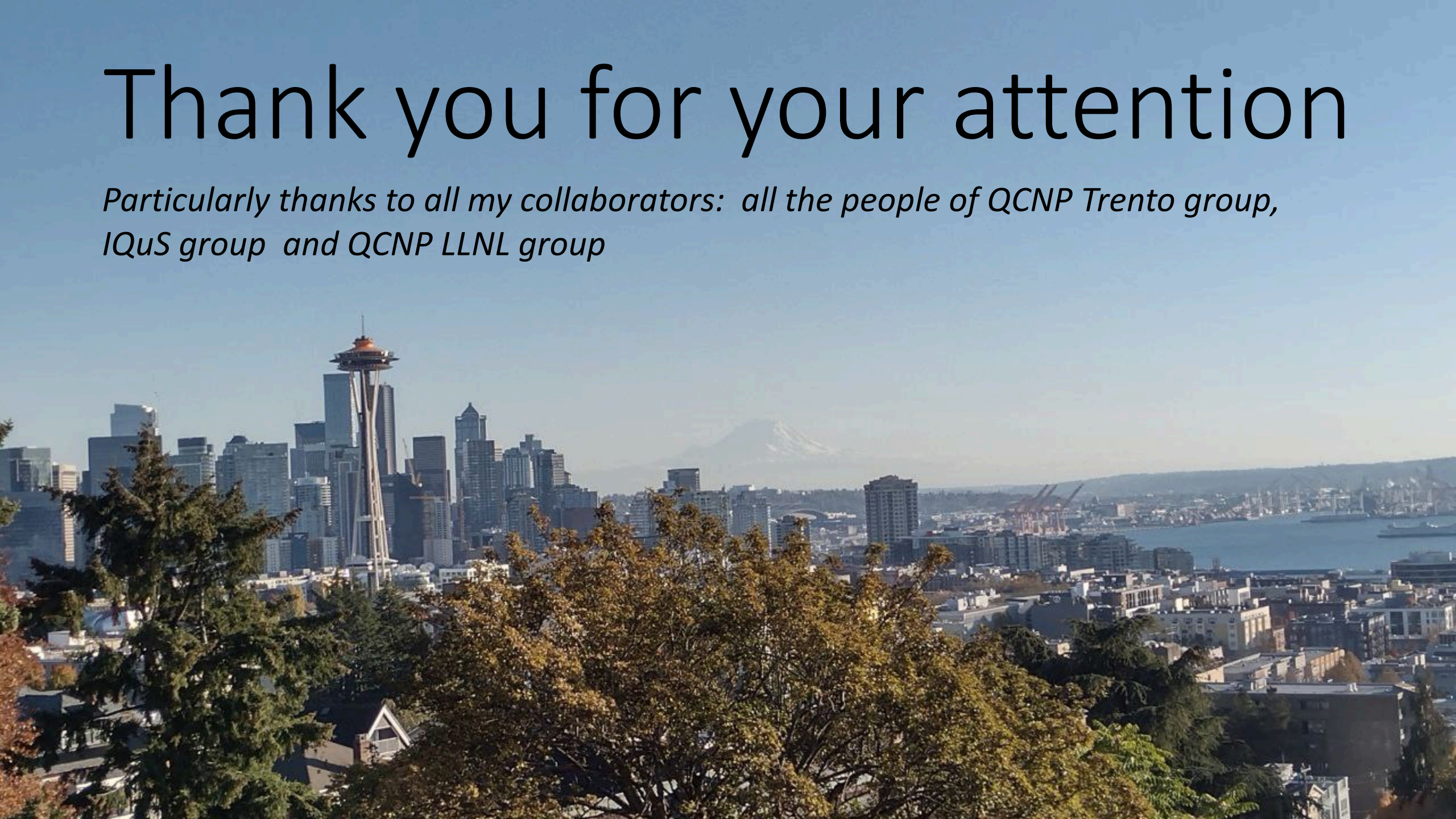
What to take home for QITP

What we have discussed:

- Implementation of non-unitary operator with a unitary gate with an ancilla qubit
- Theory of QITP:
  - Imaginary time evolution to prepare the Ground State
  - Fidelity with GS
  - Success Probability
- QITP simulations work
- Possible applications: Preparing thermal states in quantum processors

Thank you for your attention

Particularly thanks to all my collaborators: all the people of QCNP Trento group, IQuS group and QCNP LLNL group



Quantum Amplitude Amplification

Initial state of the quantum amplitude amplification:

$$|\psi_{init}\rangle = \cos(\theta)\,|\psi_b\rangle + \sin(\theta)\,|\psi_g\rangle$$

Generator of the undesired subspace

Generator of the desired subspace with probability P_s

θ is connected to the success probability: $P_s = \sin(\theta)^2$

How could we raise the probability of measuring the desired subspace?

Brassard and Hoyer, Proceedings of the Fifth Israeli Symposium on Theory of Computing and Systems (1997) 10.1109/ISTCS.1997.595153
Brassard et al, Quantum Amplitude Amplification and Estimation, arXiv:quant-ph/0005055

Quantum Amplitude amplification

Initial state:

$$|\psi_{init}\rangle = \cos(\theta)\,|\psi_b\rangle + \sin(\theta)\,|\psi_g\rangle$$

We define the Amplification operator:

$$Q = -(1 - 2\,P_{init})\,(1 - 2\,P_g)$$

$$P_{init} = |\psi_{init}\rangle\,\langle\psi_{init}| \qquad P_g = |\psi_g\rangle\,\langle\psi_g|$$

One finds that:

$$Q\begin{pmatrix}|\psi_b\rangle\\|\psi_g\rangle\end{pmatrix} = \begin{pmatrix}\cos(2\theta) & \sin(2\theta)\\-\sin(2\theta) & \cos(2\theta)\end{pmatrix}\begin{pmatrix}|\psi_b\rangle\\|\psi_g\rangle\end{pmatrix}$$

$$\Longrightarrow \quad Q^n\,|\psi_{init}\rangle = \cos((2n+1)\theta)\,|\psi_b\rangle + \sin((2n+1)\theta)\,|\psi_g\rangle$$

Brassard and Hoyer, Proceedings of the Fifth Israeli Symposium on Theory of Computing and Systems (1997) 10.1109/ISTCS.1997.595153
Brassard et al, Quantum Amplitude Amplification and Estimation, arXiv:quant-ph/0005055

Quantum Amplitude amplification

Initial state: $$|\psi_{init}\rangle = \cos(\theta)\,|\psi_b\rangle + \sin(\theta)\,|\psi_g\rangle$$

The Amplification operator: $$Q = -(1 - 2\,P_{init})\,(1 - 2\,P_g)$$

$$P_{init} = |\psi_{init}\rangle\,\langle\psi_{init}| \qquad P_g = |\psi_g\rangle\,\langle\psi_g|$$

We write Q in the basis of generators:

$$\begin{aligned} Q &= -(1 - 2P_i)(1 - P_g) \\ &= -\left[1 - 2\left(\sin(\theta)\,|\psi_g\rangle + \cos(\theta)\,|\psi_b\rangle\right)\left(\sin(\theta)\,\langle\psi_g| + \cos(\theta)\,\langle\psi_b|\ \right)\right] \\ &\quad \left[1 - 2\,|\psi_g\rangle\,\langle\psi_g|\right] \end{aligned}$$

The action of Q on the two generators:

$$Q\,|\psi_b\rangle \;=\; (2\cos(\theta)^2 - 1)\;|\psi_b\rangle + 2\,\sin(\theta)\,\cos(\theta)\;|\psi_g\rangle$$

$$Q\,|\psi_g\rangle \;=\; -2\,\sin(\theta)\,\cos(\theta)\;|\psi_b\rangle \;+\; (1 - 2\,\sin(\theta)^2)\;|\psi_g\rangle\;.$$

$$\Longrightarrow\; Q\begin{pmatrix}|\psi_b\rangle\\ |\psi_g\rangle\end{pmatrix} = \begin{pmatrix}\cos(2\theta) & \sin(2\theta)\\ -\sin(2\theta) & \cos(2\theta)\end{pmatrix}\begin{pmatrix}|\psi_b\rangle\\ |\psi_g\rangle\end{pmatrix}$$

Applying n times Q to the initial state:

$$Q^n\,|\psi_{init}\rangle \;=\; \cos((2n+1)\theta)\,|\psi_b\rangle + \underbrace{\sin((2n+1)\theta)}\,|\psi_g\rangle$$

We can tune *n* s. t. it is 1.
The probability would be 1

Consider now working in two Hilbert space (ancilla + physical system):

$$|\psi_{init}\rangle = \cos(\theta)\,|\psi_b\rangle\,|\phi_b\rangle + \sin(\theta)\,|\psi_g\rangle\,|\phi_g\rangle$$

The amplitude amplificator now is given by:

$$\begin{aligned} Q &= -(1-2P_i)(1-P_g) \\ &= -\left[1 - 2\left(\sin(\theta)\,|\psi_g\rangle\,|\phi_g\rangle + \cos(\theta)\,|\psi_b\rangle\,|\phi_b\rangle\right)\left(\sin(\theta)\,\langle\psi_g|\,\langle\phi_g| + \cos(\theta)\,\langle\psi_b|\,\langle\phi_b|\right)\right] \\ &\quad [1 - 2\,|\psi_g\rangle\,\langle\psi_g| \otimes 1] \end{aligned}$$

So, we obtain that

$$Q\,|\psi_b\rangle\,|\phi_b\rangle = (2\cos(\theta)^2 - 1)\,|\psi_g\rangle\,|\phi_g\rangle + 2\cos(\theta)\sin(\theta)\,|\psi_b\rangle\,|\phi_b\rangle$$

$$Q\,|\psi_g\rangle\,|\phi_g\rangle = 2\cos(\theta)\sin(\theta)\,|\psi_g\rangle\,|\phi_g\rangle + (2\cos(\theta)^2 - 1)\,|\psi_b\rangle\,|\phi_b\rangle$$

We see that the action of Q **<u>does not change the physical states</u>**, but just the probability

Quantum Amplitude Amplification for QITP

Desired subspace: Ancilla in the $|0\rangle$ state. Projector to desired subspace:

$$P_g = |0\rangle_A \langle 0|_A \otimes 1$$

Initial state of Amplitude Amplification: is the state after the implementation of $U_{QITP}(\tau)$

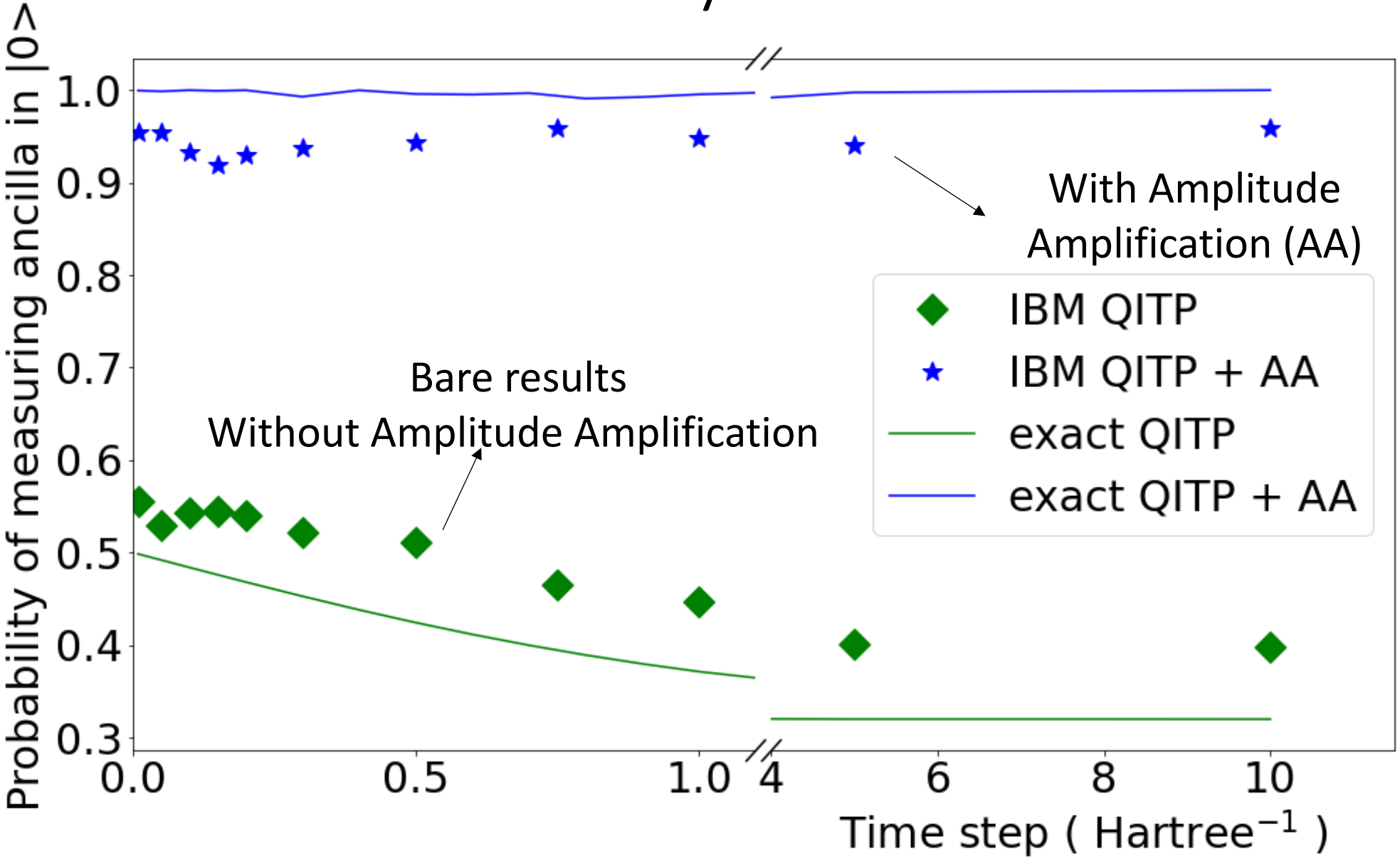
$$P_{init} = |\Psi_{fin}\rangle \langle \Psi_{fin}| = U(\tau) |\Psi_{init}\rangle \langle \Psi_{init}| U(\tau)$$

Therefore, the total QITP amplitude amplificatory is given by:

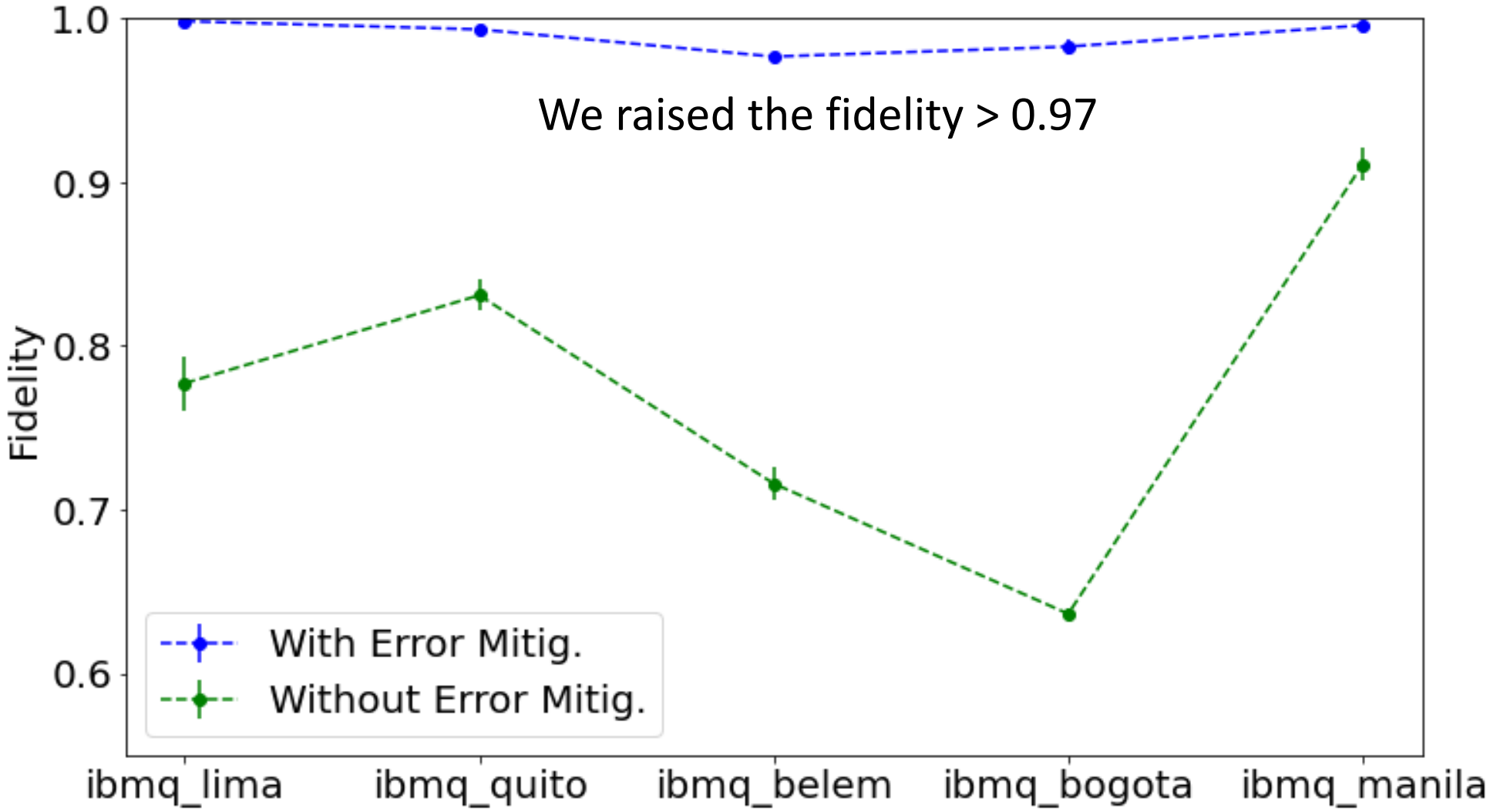
$$\begin{aligned} Q &= -(1 - |\Psi_{fin}\rangle \langle \Psi_{fin}|)(1 - 2P_A^0) \\ &= -(1 - 2U_{QITP} |\Psi_{ini}\rangle \langle \Psi_{ini}| U_{QITP}(\tau)^\dagger)(1 - 2P_A^0) \end{aligned}$$

With Q we can raise the probability of measuring the ancilla in 0 without touching the information contained in the physical system qubits

The Success Probability can be increased to 1



(New) IBM results with Readout Mitigation



We can show:

A. Limit for $\tau \to \infty$

$$U_{QITP}\,|0\rangle \otimes |\psi_{init}\rangle \xrightarrow{\tau\to\infty} |0\rangle \otimes c_0 \frac{e^{-\tau(E_0-E_T)}}{\sqrt{1+e^{-2\,\tau(E_0-E_T)}}}\,|\phi_0\rangle + |1\rangle \otimes |\psi_s^1\rangle$$

B. Limit for $\tau \to 0$. At first order we get

$$U_{QITP}\,|0\rangle \otimes |\psi_{init}\rangle \xrightarrow{\tau\to 0} \underbrace{\frac{1}{\sqrt{2}}\,|0\rangle \otimes e^{-\frac{1}{2}(H-E_T)\,\tau}}_{\text{In this case the success probability goes to 0.5}}\,|\psi_{init}\rangle + |1\rangle \otimes |\psi_s^1\rangle$$

One can also prove the **final state is always closer to ground state** than the initial one

- Success probability:

$$P_s = \left\| \frac{e^{-(H-E_T)\tau}}{\sqrt{1+e^{-2(H-E_T)\tau}}} |\psi_{init}\rangle \right\|^2 \geq |c_0|^2 \frac{1}{1+e^{2(E_0-E_T)\tau}}$$

Lower bounds

- State Fidelity for the Ground State:

$$F = |\langle \phi_0 | \Psi_{fin} \rangle|^2 \geq \left(1 + \sum_n \frac{1-|c_0|^2}{|c_0|^2} \frac{\left(e^{2\,\tau\,(E_0-E_T)}+1\right)}{\left(e^{2\,\tau\,(E_1-E_T)}+1\right)} \right)^{-1}$$

- In the interval $E_0 \leq E_T \leq E_1$, we have:

$$P_s \xrightarrow[\tau\to\infty]{} |c_0|^2 \qquad F \xrightarrow[\tau\to\infty]{} 1$$

Success probability

$$
\begin{aligned}
P_s &= \left\| \frac{e^{-(H-E_T)\tau}}{\sqrt{1+e^{-2(H-E_T)\tau}}} \left|\psi_{ini}\right\rangle \right\|^2 \\
&= \left\| \sum_n c_n \frac{e^{-(E_n-E_T)\tau}}{\sqrt{1+e^{-2(E_n-E_T)\tau}}} \left|\phi_n\right\rangle \right\|^2 \\
&= \sum_n \left|c_n\right|^2 \frac{e^{-2(E_n-E_T)\tau}}{1+e^{-2(E_n-E_T)\tau}} = \sum_n \left|c_n\right|^2 \frac{1}{1+e^{2\tau(E_n-E_T)}} \\
&\geq \left|c_0\right|^2 \frac{1}{1+e^{2(E_0-E_T)\tau}}
\end{aligned}
$$

Fidelity with Ground state

$$F = \left|\langle\phi_0|\Psi_{fin}\rangle\right|^2 = \left|\langle\phi_0| \frac{e^{-\tau(H-E_T)}}{\sqrt{1+e^{-2\tau(H-E_T)}}} |\psi_{ini}\rangle \frac{1}{P_s}\right|^2 = \frac{|c_0|^2 e^{-2\tau(E_0-E_T)}}{1+e^{-2\tau(E_0-E_T)}} \frac{1}{P_s^2}$$

$$= \frac{|c_0|^2}{\sum_n |c_n|^2 \frac{1+e^{2\tau(E_0-E_T)}}{1+e^{2\tau(E_n-E_T)}}}$$

$$\geq \left(1 + \sum_n \frac{1-|c_0|^2}{|c_0|^2} \frac{\left(e^{2\tau(E_0-E_T)}+1\right)}{\left(e^{2\tau(E_1-E_T)}+1\right)}\right)^{-1}$$

For lower bound: the maximum of denominator

At fixed c_0,
maximum when the quantum system is in the first eigenstate
With probability 1-c c_0^2

Scaling: for r time steps?

We use r ancilla qubits to propagate in r time steps and each qubit is measured

Success probability after r time steps:

$$P(0;r) = \left\| \frac{e^{-(H-E_T)\tau}}{\sqrt{1+e^{-2(H-E_T)\tau}}} |\psi_{ini}\rangle \right\|^{2r}$$

$$\geq |c_0|^2 \langle\phi_0| \left(\frac{e^{-(H-E_T)\tau}}{\sqrt{1+e^{-2(H-E_T)\tau}}} \right)^{2r} |\phi_0\rangle$$

$$\geq \frac{|c_0|^2}{(e^{2\delta\tau(E_0-E_T)}+1)^r}$$

Fidelity with Ground State after r time steps:

$$F = \left(1 + \sum_n \frac{|c_n|^2}{|c_0|^2} \frac{\left(e^{2\,\delta\tau\,(E_0 - E_T)} + 1\right)^r}{\left(e^{2\,\delta\tau\,r\,(E_n - E_T)} + 1\right)^r}\right)^{-1}$$

$$\leq \left(1 + \sum_n \frac{1 - |c_0|^2}{|c_0|^2} \frac{\left(e^{2\,\delta\tau\,(E_0 - E_T)} + 1\right)^r}{\left(e^{2\,\delta\tau\,r\,(E_1 - E_T)} + 1\right)^r}\right)^{-1}$$

Considering a small enough error ϵ or large r to be in the limit $2\delta\tau\,\Delta < 1$, one can prove when $E_0 \leq E_T \leq E_1$ and $\Delta = E_1 - E_0$ that

$$\left(\frac{e^{2\delta\tau(E_0 - E_T)} + 1}{e^{2\delta\tau(E_1 - E_T)} + 1}\right)^r \leq \left(1 - \frac{1}{2}\frac{2\delta\tau\Delta}{1 + 2\delta\tau\Delta}\right)^r$$

$$\leq \left(1 - \frac{1}{2}\delta\tau\Delta\right)^r \leq \exp\left(-\frac{1}{2}r\delta\tau\Delta\right)$$

Trotter decomposition of QITP

Let H be a Hermitian operator expressed as the sum of L Hermitian operators $\{\hat{H}_1, .., \hat{H}_L\}$ as $\hat{H} = \sum_l^L \hat{H}_l$ and $\Lambda_T = \max_j \left\| \hat{H}_j - E_T \right\|_\infty$. Then,

$$\left\| \hat{Q}_{ITP}(\eta, \tau) - \prod_k^L \hat{Q}_{ITP}^{(k)}(\eta, \tau) \right\| \leq L^2 \Lambda_T^2 \tau^2 \,,$$

where

$$\hat{Q}_{ITP}^{(k)}(\eta, \tau) \;=\; \frac{e^{-\tau\left(\hat{H}_k - \frac{E_T}{L}\right)}}{\sqrt{\eta^2 + e^{-2\tau\left(\hat{H}_k - \frac{E_T}{L}\right)}}}.$$

Unitarity of QITP

$$U^\dagger U = \left[\begin{pmatrix} \frac{e^{-\tau(H-E_T)}}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} & \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} \\ \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} & -\frac{e^{\tau(-(H-E_T)}}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} \end{pmatrix}\right]^\dagger \begin{pmatrix} \frac{e^{-\tau(H-E_T)}}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} & \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} \\ \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} & -\frac{e^{\tau(-(H-E_T)}}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{e^{-\tau(H-E_T)}}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} & \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} \\ \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} & -\frac{e^{\tau(-(H-E_T)}}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} \end{pmatrix}^2$$

$$= \begin{pmatrix} \left(\frac{e^{-\tau(H-E_T)}}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}}\right)^2 + \left(\frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}}\right)^2 & \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} - \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} \\ \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} - \frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}} & \left(-\frac{e^{\tau(-(H-E_T)}}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}}\right)^2 + \left(\frac{1}{\sqrt{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}}\right)^2 \end{pmatrix}$$

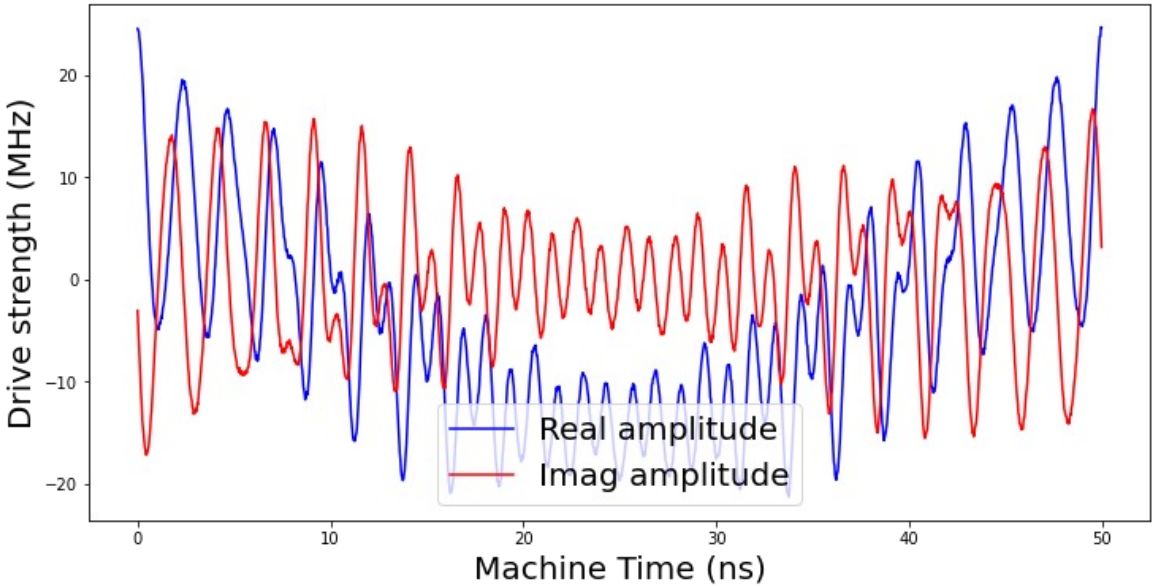
$$= \begin{pmatrix} \frac{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}} & 0 \\ 0 & \frac{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}}{\mathbb{1}+e^{-2(\hat{H}-E_T)\tau}} \quad 0 \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix} = \mathbb{1} \otimes \mathbb{1}$$

QITP for Hydrogen atom

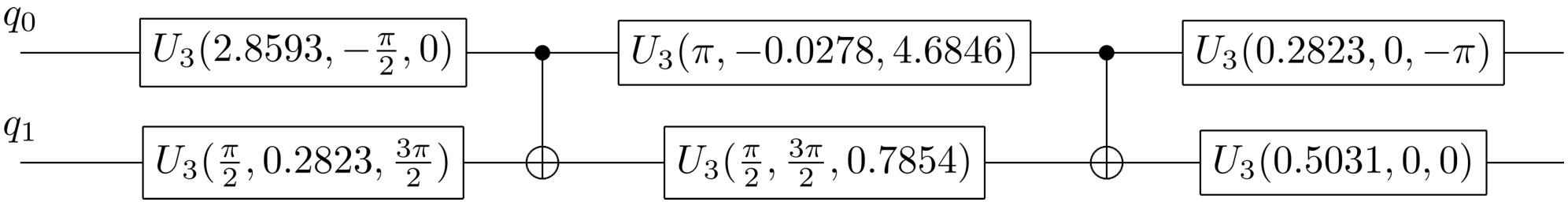
We expand the Hydrogen atom Hamiltonian with two Gaussians (STO-2G)

We implement the QITP algorithm in the limit $\tau \to \infty$

1. Optimal control through a transmon qudit



2. IBM quantum circuit:



QITP results for 2 frozen neutron spin system