Variational quantum simulation of the imaginary-time Lyapunov control for accelerating the ground-state preparation

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Quantum computers have been widely speculated to offer significant advantages in obtaining the ground state of difficult Hamiltonians in chemistry and physics. In this work, we first propose a Lyapunov control-inspired strategy to accelerate the well-established imaginary-time method for the ground-state preparation. Different from the typical setting of performing optimal control in the real-time domain, we extend the Lyapunov control method to the imaginary-time domain for the ground-state preparation. To make the method accessible in the noisy intermediate-scale quantum era, we further propose a variational form of the algorithm that could work with shallow quantum circuits. Through numerical examples, we show that the driven imaginary-time evolution can converge to the desired ground state exponentially faster than the standard imaginary-time evolution for some difficult physical systems involving small energy gaps, such as diatomic molecules HF with a large intra-molecular distance and spin models with long-range couplings. Finally, with a careful selection of the control Hamiltonians, the new variational algorithm does not incur additional measurements costs, compared to the variational imaginary-time algorithm.

Introduction.—Quantum computing holds great promises to accelerate essential computational tasks in many fields, such as cryptography, finance, chemistry, material science and machine learning[1–4]. Particularly, using a quantum computer to solve chemical problems is deemed one of the most promising areas to first witness a practical quantum advantage[4] against classical algorithms. For instance, many efforts have been invested in devising efficient algorithms for finding the ground state of molecular Hamiltonians. Some of the major approaches[5] include Variational Quantum Eigensolver (VQE)[6–8, 26], Quantum Phase Estimation (QPE)[10–13], and imaginary time evolution (ITE) [14–16, 37].

Among these approaches, variational algorithms have attracted much of the recent attention with their potential to prepare the ground state of a complex Hamiltonian with a shallow quantum circuit in the noisy intermediate-scale quantum (NISQ) era. However, the hybrid quantum-classical optimization loop of the variational algorithms has soon been pointed out to suffer a few prominent technical challenges. More specifically, the classical optimization not only faces a plethora of local minima on but also may encounter notorious barren plateau[24–28] on the energy landscape. One possible scheme to mitigate this challenge is to simulate the ITE with the time-dependent variational principle. While the variational simulation of the ITE avoids a deep quantum circuit and alleviates issues with optimizations, such as the barren plateau, it incurs additional costs associated with the ancillary measurements[16].

Apart from the ITE, another common strategy to prepare a ground state by utilizing the time-dependent Schrodinger’s function is adiabatic evolution in the real-time domain, though it is more commonly realized with a quantum annealer instead of a quantum circuit. Going beyond the adiabatic regime, the theory of optimal quantum control[29–32] provides a general tool and foundation for designing pulses to drive the desired state transitions in a finite time and in the presence of other constraints. Recently, the theory of Lyapunov quantum control has been used, in the context of hybrid quantum-classical algorithms, to solve classical optimization problems[33]. Under this formulation, one encodes the solutions to an optimization problem as the ground states of a classical spin system. To prepare a ground state (i.e. finding the solution to the original problem), one temporally modulates the structural form of a Hamiltonian, via pulse engineering, in order to achieve the desired state-to-state transition. With the Lyapunov control theory, one can simply use the system’s energy as the Lyapunov function to guide the pulse engineering. Through our demonstrative examples below, the control-theory-inspired variational methods clearly exhibit faster convergence as well as enhanced robustness against noises compared to the standard VQE. Despite these encouraging instances, real-time quantum control has hardly been regarded as a practical approach to prepare the ground state of strongly correlated many-body systems, because real-time control requires a careful analysis of the controllability of a given setup which is prohibitive to perform for complex systems. Without full controllability, one cannot successfully steer a quantum system towards a target state as illustrated in our numerical example presented later in the text.

Using a temporally modulated Hamiltonian to steer many-body quantum dynamics is not restricted to the real-time domain. In fact, an extensive body of literature proposed quantum simulation methods involving complex time variable. Specifically, in Ref.[37], it is found that an ITE under the alternating influences of two differ-
ent Hamiltonians may accelerate the convergence of the
ground-state preparation problems. The combination of
interesting observations on the accelerated convergence
of an open-loop control of a many-body ITE and the
real-time control based variational methods for shallow
quantum circuits provoke more thoughts on whether one
can efficiently prepare ground states based on a close-loop
control theory for shallow parametrized quantum circuits
in the imaginary-time domain.

To this end, we propose an imaginary-time Lyapunov
control theory for the ground-state preparation in this
work. Firstly, we discuss the essential differences between
the real- and imaginary-time versions of the control the-
ory. For the ground-state preparations, the imaginary
time control generally admits more lenient conditions on
the selection of control Hamiltonians to facilitate a given
state transition. Secondly, as expected, a properly driven
ITE can converge to the ground state faster than an un-
driven ITE. For small-gap systems reported in this work,
we show cases that a driven ITE can even converge expo-
entially faster. Finally, to make this method compatible
with the limitation of the NISQ hardware, we formulate
a time-dependent variational simulation of the driven
ITE. Hence, one derives a new set of equations for time-
dependent updates of parameters for an ansatz circuit. In
addition, through numerical examples, we demonstrate
that the newly proposed variational version of the driven
ITE not only converges faster than the standard vari-
tional ITE but also manifest higher robustness against
noises of moderate strength. With a properly chosen
set of driven Hamiltonian, the variational simulation of
the driven ITE does not incur many measurement over-
heads. For instance, if one chooses $H_d$ that commutes
with the constituting Pauli terms in $H_p$ then one can
significantly minimize the number of measurement over-
heads. As discussed before, imaginary-time control for
the ground-state preparation has admits a much more
relaxed conditions for the selection of $H_d$.

Quantum imaginary time control—A quantum sys-
tem’s dynamical evolution under a time-dependent
Hamiltonian in the imaginary-time domain is given by
the modified time-dependent Schrodinger’s equation,
\[
\frac{d\psi(\tau)}{d\tau} = -(H_p + \beta(\tau)H_d - E_r)\psi(\tau),
\]
where $\psi(\tau)$ is the system’s state vector, $H_p$ is the
problem Hamiltonian, and $H_d$ is the control Hamiltonian
coupled to a time-dependent control pulse $\beta(\tau)$. $E_r =
\langle\psi(\tau)| (H_p + \beta(\tau)H_d)\psi(\tau)\rangle$ is the state’s expected en-
ergy, and it is introduced in Eq. 1 to ensure the time-
evolved wave function will be properly normalized. Ac-
gording to the Lyapunov method and La Salle invariance
principle [45], the state preparation problem can be re-
formulated as an optimization problem in which the tar-
get state minimizes a Lyapunov function $V(\psi(\tau))$, which
must satisfy the following conditions. Consider a system
of differential equations $\dot{\psi}(\tau) = f(\psi(\tau))$ with a smooth $f$
and the state of the system satisfies the conservation
of probability $|\psi(\tau)|| = 1, \forall \tau \geq 0$, which means that $\psi$
is on the unit sphere $S = \{x \in \mathbb{C}^n : |x|| = 1\}$. Con-
sider a smooth function $V(\psi)$ on the phase space $\Omega$, such
that $V(\psi) \geq 0$ and $\frac{dV(\psi)}{d\tau} \leq 0$ for $\psi \in \Omega$. Let us define
$\mathcal{M}$ to be the set of points $\psi \in \Omega$ such that $\frac{dV(\psi)}{d\tau} = 0$, then
every solution of the time-dependent Schrodinger’s equa-
tion converges to $\mathcal{M}$ as $t \to \infty$. For the prepara-
tion of the ground state of a Hamiltonian, the Lyapunov
function can be chosen as follows,
\[
V(\psi(\tau)) = \langle\psi(\tau)|P|\psi(\tau)\rangle,
\]
where $P = H_p - \tilde{E}$ with $\tilde{E}$ a constant shift of energy
to ensure that $P$ is a semi-positive definite Hermitian
operator[42]. The time derivative of the Lyapunov func-
tion in Eq.(2) reads,
\[
\dot{V}(\psi) = 2\sigma_{H_p}^2(\tau) - \beta(\tau)D(\tau),
\]
where $\psi$ is an abbreviation for $\psi(\tau)$. The other variables
are given by
\[
\sigma_{H_p}^2(\tau) \equiv \langle\psi|H_p|\psi\rangle^2 - \langle\psi|H_p^2|\psi\rangle,
\]
\[
D(\tau) \equiv \langle\psi|[H_p,H_d]\psi\rangle - 2\langle\psi|H_p|\psi\rangle\langle\psi|H_d|\psi\rangle,
\]
where $\{,\}$ is the anti-commutator. In this case, the
Lyapunov-controlled quantum dynamics will be driven to
the asymptotically stable points, which form the ground-
state manifold, in $\mathcal{M}$. To the end of making $V(\psi) \leq 0$, it is
sufficient to enforce $\beta(\tau)D(\tau) \geq 0$ or $\sigma_{H_p}^2(\tau)$ is neces-
sarily less than or equal to zero. In summary, a successful
imaginary-time control to prepare the ground state of a
Hamiltonian is to design an appropriate $\beta(\tau)$ and suit-
able $H_d$ as well (see appendix A). For this work, we pro-
posed an imaginary time control strategy (see appendix
B) that is inspired from the approximate bang-bang Lyap-
unov control that can attain rapid state transitions for
quantum systems in the real-time domain[43].

Comparison to the real-time control for the ground-
state preparation—In this section, we comment on how
the imaginary-time control is fundamentally different
from the more familiar real-time control for the ground-
state preparation. An essential question for a driven state
preparation concerns the controllability for a given set of
control Hamiltonians $\{H_p^t, H_d^t, \ldots\}$, i.e. whether the quan-
tum system can be driven to the ground state of $H_p$ from
any given initial state when it is subjected to evolve un-
der the time-dependent Hamiltonian $H(\tau) = H_p + \beta(\tau)H_d$
in our context where $H_d = \sum_i \beta_i(\tau)H_d^i$. Without loss of
genreality, we write $\beta(\tau)H_d$ as opposed to the more gen-
eral form $\sum_i \beta_i(\tau)H_d^i$ throughout most parts of this work.
This simple question for the real-time control turns out to
be rather difficult to answer for a large quantum system.
A common technique involves analysis of the structure
and rank of corresponding Lie groups and algebra for the
propagators[39, 40, 44]. It is computationally demanding
to determine the controllability of a particular setup, and
it is unlikely that a random selection of control Hamilton-
ions can guarantee the complete controllability. The
FIG. 1. The numerical result of 2 qubits Hydrogen molecule (see appendix C), x-axis is serial number of the initial states, left y-axis is the convergent steps and right y-axis (corresponding to grey area) is overlap between initial state and ground state. The complete imaginary time control (red), the non-completely imaginary time control (green) and complete real time control (blue) could all converge in time. However, the non-completely real time control (yellow) cannot converge in limit time (>1000 steps).

challenge to select an appropriate set of control Hamiltonians (with respect to a given initial state) poses a severe challenge to derive a practical real-time control strategy to prepare a target ground state.

The same question regarding controllability admits a much clearer answer in the imaginary-time domain. As long as the imaginary-time-evolved state $\psi(\tau')$ and the ground state have a non-zero overlap, the system can always converge to ground state in sufficiently long evolution time. For instance, one can simply set $\beta(\tau') = 0$ when $\tau' > \tau$. Hence, a more crucial question is whether a set of control Hamiltonians along with the corresponding control strategy $\beta(\tau)$ (i.e. to ensure $\dot{V}(\psi) \leq 0$) can substantially accelerate the driving from a given initial state to the ground state of $H_p$. As discussed next, the imaginary-time Lyapunov control can indeed work with a broader range of control Hamiltonians for accelerating the ground-state preparations.

We further illustrate the differences between real-time and imaginary-time Lyapunov control with a numerical example involving $H_2$ molecule in Fig. 1. We randomly choose 100 initial states and examine how long the real-time and imaginary-time evolutions converge to the ground state under control Hamiltonians with various degrees of controllability. When the control Hamiltonian satisfying the strongly complete controllability[41], we expect that the driven dynamics (in both real and imaginary time) can converge to the ground state without difficulty. While this expectation holds in the numerical experiments, we find the imaginary-time evolution converges much faster (with roughly one-tenth of the time steps for the real-time evolution on average). We expect this performance gap to be further enlarged with the system size. For control Hamiltonians with incomplete controllability, the imaginary-time control can still lead to satisfactory convergence in a small number of time steps. In contrast, the real-time simulation under the same control Hamiltonians cannot converge for all 100 initial states in the pre-defined maximum number of steps allowed.

Comparison to imaginary time evolution—In this section, we justify why the imaginary-time control can generally accelerate the imaginary-time evolution. In fact, the imaginary-time controlled dynamics can even converge exponentially faster to the ground state for the small-gap systems investigated in this study.

Under an imaginary-time evolution, the incremental change of energy at time $\tau$ reads,

$$\Delta E_I(\tau) = 2 \sum_{i=0}^{n} |c_i|^2 \left( \sum_{j=0}^{n} |c_j|^2 \Delta_{i0}\Delta_{j0} - \Delta_{i0}^2 \right) \Delta \tau, \quad (5)$$

where $e_i$ is eigenvalue of $H_p$ and $|c_i|^2$ denotes the probability of the $i$-th eigenstate $|\psi_i\rangle$ of $H_p$ (see more details Appendix F). The instantaneous energy of the driven state $\psi(T)$ is given by $e_0 = \langle \psi(0) | H_p | \psi(0) \rangle + \int_0^T \frac{dE_I}{d\tau} d\tau + \epsilon$, where $\epsilon$ is the simulation accuracy. The convergence rate of $E_I(\tau)$ towards the exact ground-state energy de-
pends on the dynamical distribution of $|c_i(\tau)|^2$ and the energy gap $\Delta_{i0} = \varepsilon_i - \varepsilon_0$.

Under the imaginary-time control, the incremental change of energy at time $\tau$ reads,

$$
\Delta E_C(\tau) = \Delta E_I(\tau) + \sum_i \beta(\tau) \Delta \tau \sum_j \left( 2|c_i|^2 \sum_{jk} c_j^* c_k d_{jk} - \sum_j c_i^* c_j d_{ij} \right),
$$

where $d_{ij} = \langle \psi_i | H_d | \psi_j \rangle$. From this equation, it is clear that the driven ITE gains an extra contribution, which could facilitate a faster rate of change for the energy. As we can see, this extra term (contributed by $H_d$) to the energy convergence becomes more pronounced for a quantum system with a small energy gap $\Delta_{i0} \ll 1$ and $\Delta^2_{i0} \ll \Delta_{i0}$. Thus, with a proper design of $H_d$ and $\beta(\tau)$, we may realize a substantial acceleration of the ground-state preparation via quantum dynamics in the imaginary-time domain.

In addition, we may also interpret the overall effects of the imaginary-time control as modulating the instantaneous energy of the eigenstates of $H_p$ with $E_i(\tau) = \langle \psi_i | H(\tau) | \psi_i \rangle$. We presented the numerical analysis of the energy functions in Appendix D. The result implies that the control terms temporally adjust the energy gaps, and facilitate the population transfer from the high-energy to low-energy eigenstates of $H_p$.

In Fig. 2(a), we use a 4-qubit $H_2$ system as an example to illustrate the enhanced convergence efficiency for the driven ITE with 100 different initial states. These results also indicate that the convergence of the driven ITE does not sensitively depend on the initial states. In Fig. 2(b), we present the results of ground-state preparation for an 8-qubits HF system (frozen cores, see appendix C). The result shows that the driven ITE provides an exponential speedup in the rate of convergence with respect to the intra-molecular distance. Note that the $\Delta_{i0}$ energy gap reduces when the intra-molecular distance grows. This observed scaling trend certainly benefits the simulation of large complex systems with small energy gaps. To ensure this observed exponential speedup holds in a variety of model systems, we provide another eleven-qubits example in Appendix F that corresponds to a constrained optimization problem, 3-SAT.

A successful energy-gap modulation for the enhanced convergence depends strongly on the structural form of the control Hamiltonian and the design of control law, i.e. $\beta(\tau)$. More specifically, the dynamical controllability depends crucially on the selection of the control Hamiltonian. A completely controllable system implies that the entire energy spectrum $\{E_i(\tau)\}$ could be dynamically adjusted (See appendix D for more details) by pulse engineering. As for the design of control laws, it is not the case that stronger control pulses always lead to a faster convergence. In fact, a strongly driven ITE (with dynamics strongly dominated by $H_d$) may even lead to an unexpected slowdown towards the ground state. This is because that the entire set of the eigenstates of $H_p$ constitutes the critical points of the Lyapunov function $V(\psi) = \langle \psi | (H_p - \hat{E}) | \psi \rangle$[42]. Hence, a strongly driven ITE may end up trapping in an excited state of $H_p$. In practice, we recommend to maintain the strength of the control pulse weaker than the norm of $H_p$ (See appendix D for more details).

**Variational algorithm for NISQ simulations**—To utilize the proposed imaginary-time control to prepare a
ground state on a near-term quantum device, we rely on the time-dependent variational principle to approximate the evolutions of the driven ITE as sequential updates of parameters for an ansatz circuit, as first proposed by McArdle et al.\cite{16} for the undriven ITE. The modified algorithm proceeds as follows. Given a time-dependent Hamiltonian $H(\tau) = H_\rho + \beta(\tau)H_d$, we would invoke the McLachlan’s variational principle\cite{47, 48},

$$\delta\|\partial \tau + H(\tau) - E_\tau\| \psi(\tau)\| = 0,$$

which conducting the dynamic evolution $\partial \| \psi(\tau) \| / \partial \tau = -[H(\tau) - E_\tau] \psi(\tau)$ by deducing the incremental update (corresponding to one time step $\partial \tau$) of the parameters $\theta$ for an ansatz circuit. Following Ref.\cite{16}, we need to solve the following equations,

$$\sum_j A_{ij} \theta_j = C_i, \forall i$$

where,

$$A_{ij} = \text{Re} \left( \frac{\partial \langle \phi(\tau) | \partial \phi(\tau) \rangle}{\partial \theta_i} \right)$$

$$C_i = \text{Re} \left( - \sum_a \lambda_a \frac{\partial \langle \phi(\tau) | \partial \theta_i \rangle}{\partial \theta_a} h_a \phi(\tau) \right)$$

and $h_a$ and $\lambda_a$ are the Pauli terms and coefficients of the Hamiltonian $H = H_\rho + \beta(\tau)H_d = \sum_a \lambda_a(\tau) h_a$. With the new ansatz state, we can then evaluate the Lyapunov function and assign values to the pulse $\beta(\tau)$ via a predetermined control rule to keep $V(\psi) < 0$. The procedure of alternating updates of $\theta$ and $\beta$ is then repeated until a fixed point is reached.

In Fig. 3 we compare the results between the variational ansatz-based driven ITE and undriven ITE for the ground-state preparation of a 4-qubit $H_2$ system under both noise-free and noisy situations. We adopt the hardware-efficient ansatz with high expressibility\cite{23} initialized by the same random initial parameters for both methods (i.e. driven and undriven ITE). The results shows that the driven ITE converges faster than the undriven case for both the noisy and noise-free model.

**Conclusion**—In summary, we propose to utilize the imaginary-time Lyapunov control to prepare ground states. In the main text, we explain the advantages of driven ITE. First, comparing to real-time control, imaginary-time control admits more relaxed conditions for controllability (when the target is the ground state) and a broader range of control Hamiltonians to facilitate the desired state transitions in a finite time. Secondly, imaginary time control can speed up imaginary time evolution with the proper design of control Hamiltonian and control function $\beta(\tau)$. For the small-gap systems invested in this work, exponential speedup with respect to the gap size is clearly manifested in our numerical simulations. Finally, to make the present method accessible in the NISQ era, we propose a variational simulation of the driven ITE with an ansatz circuit. When the control Hamiltonian is chosen appropriately, it does not incur much additional measurement costs and exhibits higher robustness against noises. These merits make the present approach a natural replacement for the variational ground-state preparation. For future work, we aim to study imaginary time control for other challenging state preparation tasks, such as excited states simulation and Gibb state preparation, etc.

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[1] Monz, Thomas, et al. "Realization of a scalable Shor algorithm." Science 351.6277 (2016): 1068-1070.
[2] Schaden, Martin. "Quantum finance." Physica A: Statistical Mechanics and Its Applications 316.1-4 (2002): 511-538.
[3] Biamonte, Jacob, et al. "Quantum machine learning." Nature 549.7671 (2017): 195-202.
[4] McArdle, Sam, et al. "Quantum computational chem-
istry.” Reviews of Modern Physics 92.1 (2020): 015003.
[5] Bauer, Bela, et al. "Quantum algorithms for quantum
chemistry and quantum materials science.” Chemical
Reviews 120.22 (2020): 12685-12717.
[6] Peruzzo, Alberto, et al. "A variational eigenvalue solver
on a photonic quantum processor.” Nature communications
5.1 (2014): 1-7.
[7] Grimsley, Harper R., et al. "An adaptive variational
algorithm for exact molecular simulations on a quantum
computer.” Nature communications 10.1 (2019): 1-9.
[8] Childs, Andrew M., et al. "Theory of trotter error with
variational quantum computation of excited states.” Quantum
3 (2019): 156.
[9] Cerezo, Marco, et al. "Variational quantum algorithms.”
Nature Reviews Physics (2021): 1-20.
[10] Kitaev, A. Yu. "Quantum measurements and the Abelian
stabilizer problem.” arXiv preprint quant-ph/9511026
(1995).
[11] Dobsiček, Miroslav, et al. "Arbitrary accuracy iterative
quantum phase estimation algorithm using a single an-
cillary qubit: A two-qubit benchmark.” Physical Review
A 76.3 (2007): 032306.
[12] Wiebe, Nathan, and Chris Granade. "Efficient Bayesian
phase estimation.” Physical review letters 117.1 (2016):
010503.
[13] O’Brien, Thomas E., Brian Tarasinski, and Barbara M.
Terhal. "Quantum phase estimation of multiple eigenval-
ues for small-scale (noisy) experiments.” New Journal of
Physics 21.2 (2019): 023022.
[14] Gomes, Niladri, et al. "Efficient step-merged quantum
imaginary time evolution algorithm for quantum chem-
istry.” Journal of Chemical Theory and Computation
16.10 (2020): 6256-6266.
[15] Motta, Mario, et al. "Determining eigenstates and ther-
mal states on a quantum computer using quantum imagi-
ary time evolution.” Nature Physics 16.2 (2020): 205-
210.
[16] McArdle, Sam, et al. "Variational ansatz-based quantum
simulation of imaginary time evolution.” npj Quantum
Information 5.1 (2019): 1-6.
[17] Yuan, Xiao, et al. "Theory of variational quantum simu-
lation.” Quantum 3 (2019): 191.
[18] Beach, Matthew JS, et al. "Making trotters sprint: A
variational imaginary time ansatz for quantum many-
body systems.” Physical Review B 100.9 (2019): 094434.
[19] Childs, Andrew M., et al. "Theory of trotter error with
commutator scaling.” Physical Review X 11.1 (2021):
011020.
[20] Grimsley, Harper R., et al. "Is the trotterized uccsd
ansatz chemically well-defined?.” Journal of chemical
theory and computation 16.1 (2019): 1-6.
[21] Lee, Joonho, et al. "Generalized unitary coupled clus-
ter wave functions for quantum computation.” Journal of
chemical theory and computation 15.1 (2018): 311-324.
[22] Kandala, Abhinav, et al. "Hardware-efficient variational
quantum eigensolver for small molecules and quantum
magnets.” Nature 549.7671 (2017): 242-246.
[23] Sim, Sukin, Peter D. Johnson, and Álan Aspuru-Guzik.
"Expressibility and entangling capability of parameter-
ized quantum circuits for hybrid quantum-classical algo-
rithms.” Advanced Quantum Technologies 2.12 (2019):
1900070.
[24] McClean, Jarrod R., et al. "Barren plateaus in quantum
neural network training landscapes.” Nature communi-
cations 9.1 (2018): 1-6.
[25] Grant, Edward, et al. "An initialization strategy for ad-
dressing barren plateaus in parametrized quantum cir-
cuits.” Quantum 3 (2019): 214.
[26] Cerezo, Marco, et al. "Cost-function-dependent barren
plateaus in shallow quantum neural networks.” arXiv e-
prints (2020): arXiv-2001.
[27] Wang, Samson, et al. "Noise-induced barren plateaus
in variational quantum algorithms.” arXiv preprint
arXiv:2007.14384 (2020).
[28] Holmes, Zoë, et al. "Barren plateaus preclude learning
scramblers.” Physical Review Letters 126.19 (2021):
190501.
[29] Kuang, Sen, and Shuang Cong. "Lyapunov control meth-
ods of closed quantum systems.” Automatica 44.1 (2008):
98-108.
[30] Wang, Xiaoting, and Sophie G. Schirmer. "Analysis of
Lyapunov method for control of quantum states.” IEEE
Transactions on Automatic control 55.10 (2010): 2259-
2270.
[31] Dong, Daoyi, and Ian R. Petersen. "Quantum control
theory and applications: a survey.” IET Control Theory
& Applications 4.12 (2010): 2651-2671.
[32] Cong, Shuang, and Fangfang Meng. "A survey of quan-
tum lyapunov control methods.” The Scientific World
Journal 2013 (2013).
[33] Kuang, Alicıa B., et al. "Feedback-based quantum op-
timization.” arXiv preprint arXiv:2103.08619 (2021).
[34] Mañag, Alicıa B., et al. "Digital quantum simulation of
molecular dynamics and control.” Physical Review Re-
search 3.2 (2021): 023165.
[35] Ramakrishna, Viswanath, et al. "Controllability of
molecular systems.” Physical Review A 51.2 (1995): 960.
[36] Chen, Yu-Qin, et al. "Optimizing quantum anneal-
ing schedules: From monte carlo tree search to quan-
tumzero.” arXiv preprint arXiv:2004.02836 (2020).
[37] Beach, Matthew JS, et al. "Making trotters sprint: A
variational imaginary time ansatz for quantum many-
body systems.” Physical Review B 100.9 (2019): 094434.
[38] Ran, Du, et al. "Speeding up adiabatic passage by adling
Lyapunov control.” Physical Review A 96.3 (2017):
033803.
[39] Schirmer, Sonia G., H. Fu, and Allan I. Solomon. "Com-
plete controllability of quantum systems.” Physical Re-
vies A 63.6 (2001): 063410.
[40] Albertini, Francesca, and Domenico D’Alessandro. "No-
tions of controllability for bilinear multilevel systems.”
IEEE Transactions on Automatic Control 48.8
(2003): 1399-1403.
[41] Zhang, Chen-Bin, Dao-Yi Dong, and Zong-Hai Chen.
"Control of non-controllable quantum systems: a quan-
tum control algorithm based on Grover iteration.” Jour-
nal of Optics B: Quantum and Semiclassical Optics
7.10 (2005): S313.
[42] Grivopoulos, S., & Bamieh, B. (2003, December).
Lyapunov-based control of quantum systems. In 42nd
IEEE International Conference on Decision and Control
(IEEE Cat. No. 03CH37475) (Vol. 1, pp. 434-438).
IEEE.
[43] Kuang, S., Dong, D., & Petersen, I. R. (2014, Novem-
ber). Approximate bang-bang Lyapunov control for closed
quantum systems. In 2014 4th Australian Control Con-
ference (AUCC) (pp. 124-129). IEEE.
[44] Huang, Garng M., Tzyh J. Tarn, and John W. Clark.
"On the controllability of quantum-mechanical systems.”
Journal of Mathematical Physics 24.11 (1983): 2608-2618.
[45] d’Alessandro, D. (2021). Introduction to quantum control and dynamics. Chapman and hall/CRC.
[46] Schuld, Maria, et al. "Evaluating analytic gradients on quantum hardware." Physical Review A 99.3 (2019): 032331.
[47] McLachlan, A. D. "A variational solution of the time-dependent Schrödinger equation." Molecular Physics 8.1 (1964): 39-44.
[48] Broeckhove, J., et al. "On the equivalence of time-dependent variational principles." Chemical physics letters 149.5-6 (1988): 547-550.

Appendix A: Control Hamiltonian Selection

In this section we discuss the selection of control Hamiltonian from the perspective of the controllability and the cost of computational resources for the ground-state preparation. In this case, we deal with the Lyapunov functions of the form $V(\psi) = \langle \psi | H_p | \psi \rangle$, the time derivatives of $V(\psi)$ for the real-time and imaginary-time control reads,

$$V_{\text{imag}}(\psi) = 2(\langle \psi | H_p | \psi \rangle^2 - \langle \psi | H_p^2 | \psi \rangle),$$

$$V_{\text{real}}(\psi) = \beta(t)(\langle \psi | H_d, H_p | \psi \rangle).$$

In the absence of the control Hamiltonian, $V_{\text{imag}} \leq 0$ still holds since the time derivative of the Lyapunov function reduces to $V_{\text{imag}}(\psi) = 2(\langle \psi | H_p | \psi \rangle^2 - \langle \psi | H_p^2 | \psi \rangle)$, and $(\langle \psi | H_p | \psi \rangle^2 - \langle \psi | H_p^2 | \psi \rangle)$ only equals to zero when the current state $\psi(\tau)$ is one of the eigenstates of $H_p$ otherwise it is always negative-valued. Thus, the selection of the control Hamiltonian largely impacts the convergence rate but not the eigenstate convergence as long as the controls are turned off when the system is close to an eigenstate. However, for the real-time Lyapunov control, one needs to ensure for any states it satisfies the condition that $V_{\text{real}}$ will be controllable unless the state $\psi(t)$ is one of the eigenstates. To ascertain the condition, a straightforward method is to adopt a structurally more complex control Hamiltonian in order to achieve the strongly complete controllability or complete controllability[41], which implies an ability to perfectly steer any initial state towards the target state under an appropriate control strategy.

Usually, it is difficult to choose a set of control Hamiltonians that gives strongly complete controllability or complete controllability. The most trivial way is to take the control set to cover all possible combinations of Pauli matrices and Identity $\{P_0, P_1, \ldots, P_n\}$, where $P_k = \{I, X, Y, Z\}$. This selection strategy will lead to an exponentially increasing size of the control set as the system size scales up. Another way is to examine if the dimension of the Lie algebra $L_0$ generated by the drift and control Hamiltonian is $N^2$, where $N$ is the number of qubit. In this work, we examining the span of the Hamiltonians according to the algorithm purposed by Schirmer et al.[39], the algorithm’s runtime scales exponentially with the number of qubit. Therefore, for an arbitrarily selected set of control Hamiltonians, the controllability is unknown. Compares to the real-time control, the imaginary time control possess lower requirements for the control Hamiltonian or controllability.

On the other hands, from the perspective of the resource requirements. Since the imaginary time control is not strongly affected by the controllability of the control Hamiltonian for the ground state problem. We can use the control Hamiltonian $H_d$ with the less measurement like simple ones $ZIII$ or a subset of Paulis from $H_p$ or Paulis that commutes with subsets of Pauli strings appearing in $H_p$ etc., then the $\langle \psi | H_d | \psi \rangle$ can be obtained when measuring $\langle \psi | \{H_d, H_p \} | \psi \rangle$. For measuring  $\langle \psi | \{H_d, H_p \} | \psi \rangle$, using this type of selection, one can significant refrain the needs for extra measurements for the imaginary-time control based variational algorithms.

Appendix B: The Bang-Bang and Approximate Bang-Bang Control Strategy

Here we use both approximate bang-bang control and bang-bang control laws to design the $\beta(t)$ as shown in Fig. 4 to avoid staying on excited states. To be appreciate our approach, we first review some typical real-time control strategies designed to guarantee $\dot{V} \leq 0$. Following a standard convention [43], we refer to the following choice as the standard Lyapunov control,

$$u_k(t) = -K_k T_k(t),$$

where $u_k(t)$ is an external real-valued control field, $K > 0$ is the control gain used to adjust the amplitude of the control field and $T_k(t) \equiv (\langle \psi | i[H_d, H_p] | \psi \rangle)$ for the real-time control. Another commonly used strategy is the bang-bang Lyapunov control,

$$u_k(t) = \begin{cases} -S, & (T_k > 0) \\ S, & (T_k < 0) \\ 0, & (T_k = 0) \end{cases} \quad k = 1, ..., m,$$
where $S > 0$ is the maximum strength of the control field. In order to achieve a good trade-off between convergence and the rapidity of control, Kuang et al. propose an approximate bang-bang control as follows,

$$u_k(t) = \frac{2S}{1 + e^{-\gamma T_k}} - S,$$

where $\gamma > 0$ is a parameter used to adjust the hardness of the control strategy.

For the imaginary-time case, we adopt idea from both strategies introduced above. First, let us generalize the standard Lyapunov control such that it could work with the imaginary-time evolution. We redefine

$$T_k = 2 \langle \psi |H_p| \psi \rangle \langle \psi |H_d| \psi \rangle - \langle \psi |(H_p, H_d)| \psi \rangle$$

in this case. The $H_d$ related terms in $T_k(\tau)$ may entail lots of extra measurements if it cannot be obtained by measuring the Pauli terms appearing in $\langle \psi |H_p| \psi \rangle$. To reduce the measurement cost and still maintain a powerful $H_d$ to provide an enhanced convergence, we propose the following strategy. We first decide if the state in the quantum circuit has high overlap with any eigenstate of $H_p$ or $H_d$ by checking the value of $T_k$, if $T_k < L$ then we do not apply any control pulses, otherwise we use a similar control strategy for the real-time case introduced above. More precisely, the proposed imaginary-time control strategy is

$$\beta_k(\tau) = \begin{cases} -K_k T_k(\tau), & (T_k \geq L) \\ 0, & (T_k < L) \end{cases}$$

where $L$ is some pre-defined threshold value. If the state is close to an eigenstate (i.e. $T_k(\tau) < L$), we should turn off the control field and let the system evolves under $H_p$ in the imaginary-time domain. This truncation can greatly reduce the measurement costs (for the implementation of the corresponding variational algorithm) in the region that the state will linearly converge to the eigenstate.

We also consider the approximate bang-bang control strategy to accelerate the control. In our test, given a large $S$, one can speed up the convergence but it may sometime lead to non-convergence when the differential time step $d\tau$ is too large or the scale of $u_k(\tau)$ is to big in some region (see appendix D). We proposed that by using a large $S$ with the modified bang-bang law according to $A(\tau)$, one should only activate the control field when the current state is not close to any eigenstates of $H_p$. This overall strategy should prevent the algorithm from converging towards an excited state of $H_p$, reduce the measurement costs near any eigenstate and greatly accelerate the convergence. In summary, we propose the following control strategy,

$$\beta_k(\tau) = \begin{cases} \frac{2S}{1 + e^{-\gamma T_k}} - S, & (T_k \geq L) \\ 0, & else \end{cases}$$

FIG. 4. The flow chart of imaginary time bang-bang control
Finally, we test how the truncation (i.e. setting $\beta_k(\tau) = 0$ when $T_k(\tau) < L$) will affect the precision of the converged results given by truncating the control pulse in the middle of the convergence. For physical system with a large energy gap between the first-excited state and the ground state, it only requires few control steps at the beginning then the result of convergence will very close to the result without truncation. For systems with a small energy gap, the truncation will significantly affect the precision of the converged results.

Appendix C: Molecule Hamiltonian

1. Hydrogen

In our simulations, we consider the Hydrogen molecule in the minimal STO-3G basis. Each Hydrogen atom contributes a single 1S orbital. As a result of spin, there are four spin-orbitals in total. By using the function of the Qiskit, the qubit Hamiltonian for JW representation can be obtained. This 4 qubit Hamiltonian is given by:

$$H = h_0 I + h_1 Z_0 + h_2 Z_1 + h_3 Z_2 + h_4 Z_3 + h_5 Z_0 Z_1 + h_6 Z_0 Z_2 + h_7 Z_0 Z_3 + h_8 Z_1 Z_2 + h_9 Z_1 Z_3 + h_{10} Z_2 Z_3 + h_{11} Y_0 Y_1 Y_2 Y_3 + h_{12} Y_0 Y_1 Y_2 Y_3 + h_{13} X_0 X_1 X_2 X_3 + h_{14} X_0 Y_1 Y_2 Y_3 + h_{15} X_0 X_1 Y_2 Y_3$$

By using the function of the Qiskit, the 2 qubit Hamiltonian of Hydrogen molecule can be obtained from parity representation with $Z_2$ symmetry reduction. This 2 qubit Hamiltonian is given by:

$$H = h_0 I + h_1 Z_0 + h_2 Z_1 + h_3 Z_2 + h_4 Z_3 + h_5 X_0 X_1$$

And the circuit for Variational-based ansatz simulation used in the main text.

For update the parameters of Variational-based ansatz, we calculate the gradient of the circuit from using parameter shift rule to obtain the numerical differential result of the circuit.

2. Hydrogen Fluoride

In our simulations, we consider the Hydrogen fluoride molecule in the minimal STO-3G basis. The Fluoride atom has 9 electrons, and so contributes a 1S, 2S, 2$P_x$, 2$P_y$ and 2$P_z$ orbital to the basis, while the Hydrogen atom contributes
a single 1S orbital. By freezing the core two 1S orbitals, we can reduce the system from 12 orbitals with 10 electrons to 8 orbitals with 6 electrons on 2S and 2P orbitals. By using the Qiskit, the qubit Hamiltonian for Jordan-Wigner representation can be obtained. This 8 qubit Hamiltonian is given by 145 different Pauli terms and coefficients.

Appendix D: Dynamic of Imaginary Time Control

Let us comment on how the energy gap changes with time under control. For the case of the non-driven imaginary time evolution, since the $H_p$ is time-independent Hamiltonian, the energy gap between the ground state and the first excited state remains fixed in time. For the driven imaginary time evolution, on the other hand, the energy gap between the ground state and the first excited state of $H_p$ will change with time as,

$$\Delta E(\tau) = \langle \psi_0 | H(\tau) | \psi_0 \rangle - \langle \psi_1 | H(\tau) | \psi_1 \rangle.$$  

where $H(\tau) = H_p + \beta(\tau) H_d$, $| \psi_0 \rangle$ and $| \psi_1 \rangle$ correspond to the ground state and first excited state of drift Hamiltonian $H_p$, respectively. In Fig. 5 we show the simulated result of using a driven ITE to prepare the ground state for a 2-qubit hydrogen model. In this case, we adopt a set of control Hamiltonians that yield strongly complete controllability on the 2-qubit dynamics. As clearly illustrated in the figure, the driven ITE temporally modulates the entire spectrum of $H(\tau)$ during the evolution and return back to the original spectrum of $H_p$ when time $t >> 1$ as $\beta(t >> 1) \to 0$. Thus, we conclude that the controlled system can evolve towards the ground state of $H_p$ in fewer time steps with enlarged energy gaps.

![Fig. 5](image_url)

**FIG. 5.** The result of 2 qubits hydrogen with strongly complete control. The left figure shows how the energy levels change with time, as the solid line is the original energy level and the dashed line is the controlled energy level. The right figure is convergence of imaginary time models. The left y-axis corresponding to the energy for red solid line and blue solid line. The right y-axis corresponding to the energy gap between the ground state and the first excited state, and the $\beta(\tau) = \frac{1}{\hbar} \sum_{i=1}^{\infty} \beta_i(\tau)$. The result shows that all energy level will change with time.
Next, we attempt a different experiment. If the control Hamiltonian does not guarantee strongly complete controlability or complete controllability, the imaginary-time control will not be able to enlarge all energy gaps but just few of them. In this case, it can still speed up the convergence of the driven ITE but may not be as fast as the previous case with complete controllability. In Fig. 6, the 2-qubit Hydrogen is driven by a non-complete controllable Hamiltonian $H_d$, the increase of energy gap only occurs between the ground state and the highest excited state. This control will only be beneficial when the initialized quantum state has an appreciable overlap with the highest excited state.

![Graph](image1.png)

**FIG. 6.** The result of 2 qubits hydrogen with non-complete control shows that the highest excited state and the ground state will both change with time.

However, when the control Hamiltonian is not completely controllable and the control strategy $\beta(\tau)$ is too aggressive, then the driven ITE may actually compromise the rate of convergence. This is because the ground state has been inverted to the highest excited state in some time steps, and the system will be temporarily driven away from the target state (i.e. the ground state of $H_p$) when its energy has been shifted upwards. In Fig. 7, during the period $\tau \in (0.5, 1.0)$, the order of the ground state and the highest excited state are swap. Clearly, as shown in the right panel of Fig. 7, the undriven ITE converges to the desired ground state faster in this case.

![Graph](image2.png)

**FIG. 7.** The result of 2 qubits hydrogen with aggressive control strategy shows that the control pulses is able to rearrange energy level.
To avoid the unintended eigenstate re-ordering by the control field, it is crucial to confine the magnitude of $\beta$ to some proper range. In our test, it is better to set $|\beta|$ to be equal to or less than the magnitude of the energy $\langle \psi(\tau) | H_p | \psi(\tau) \rangle$ which can be obtained from measuring the norm of the matrix problem Hamiltonian. In Fig. 8 we illustrate the effects of choosing different $\beta$ on the time-evolved energy levels of $H_p$, which is the Hamiltonian for a 2-qubit Hydrogen. In this test, we adopt two different approximate bang-bang control strategies $\beta(\tau) = \frac{2S}{1 + e^{-\gamma T_k}} - S$, introduced in appendix B. These two control strategies share the same $\gamma$ but $S = 1$ and $S = 10$, respectively. From Fig. 8, it is clear that, under the condition of non-complete controllability, bigger $|\beta|$ may enlarge energy gaps between eigenstates of $H_p$ but also increases the likelihood of state re-ordering.

![Fig. 8. The result of 2 qubits hydrogen with different admissible maximum strength S. It shows that the large admissible maximum strength might decrease the energy gap.](image)

**Appendix E: The simulation result of 3-SAT problem**

In the main text, we show that driven ITE can provide an exponential speedup over the undriven ITE when the energy gap is small for molecular systems. While we succinctly elucidate the source of this superior performance of driven ITE, it is also deriable to verify whether such a superior advantage can hold for other scenarios. To this end, we compare the driven and undriven ITEs for solving a spin model that is closely related to the 3-SAT problems, another ground-state preparation task that is sufficiently distinct from the molecular systems considered in the main text. Let us first introduce the 3-SAT problem, which is defined by a logical statement involving $n$ boolean variables $b_i$. The logical statement consists of $m$ clauses $C_i$ in conjunction: $C_1 \land C_2 \land \ldots \land C_m$. Each clause is a disjunction of 3 literals, where a literal is a boolean variable $b_i$ or its negation $\neg b_i$. For instance, a clause may read $(b_j \lor b_k \lor b_l)$. The task is to first decide whether a given 3-SAT problem is satisfiable; if so, then assign appropriate binary values to satisfy the logical statement. We can map a 3-SAT problem to a Hamiltonian for a set of qubits. Under this mapping, each binary variable $b_i$ is represented as a qubit state. Thus, an $n$-variable 3-SAT problem is mapped into a Hilbert space of dimension $N = 2^n$. Furthermore, each clause of the logical statement is translated to a projector acting on this $n$-qubit system. Hence, a logical statement with $m$ clauses may be translated to the following Hamiltonian,

$$H_{final} = \sum_{\alpha=1}^{m} \left( b_j^\dagger b_k^\dagger b_l \right)^\alpha \left( b_j^\alpha b_k^\alpha b_l \right)^\alpha.$$

A common approach to solve this type of constraint satisfaction problems is to use the adiabatic quantum computations (AQC). One first prepares the ground states of an easy-to-solve Hamiltonian $H_{init}$. Next, one slowly evolve the Hamiltonian such that it adiabatically connects $H_{init}$ and $H_{final}$. In other words, the adiabatically evolved Hamiltonian reads

$$H(s) = (1 - s)H_{init} + sH_{final}, \quad s \in [0, 1].$$
where $H_{init}$ is typically chosen to be a sum of one-qubit Hamiltonians $H_i$ acting on the $i$-th qubit,

$$H_{init} = \frac{1}{2} \sum_{i=1}^{n} h_i, \quad h_i = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$ 

The energy gap $\Delta E(s)$ between the instantaneous ground state and first-excited state of $H(s)$ will vary with time $s$ as shown in Fig. 9. Based on the well-established theoretical studies, it is also clear that the instantaneous energy gap of interest can get very small along the adiabatic path when the system size is large.

Inspired by the facts given above, we consider an 11-qubit 3-SAT problem with the linear schedule for $H(s)$ above. We then implement and compare the variational simulations of the driven and undriven ITEs in order to prepare the ground states for a series of $H(s)$ chosen along the adiabatic path.

In Fig. 10, we show the result of the simulations. We again numerically verify the exponential speedup of the driven ITE as the instantaneous energy gap $\Delta E(s)$ shrinks.

**FIG. 9.** The energy gap between the ground state and first excited state of the time-dependent Hamiltonian $H(s)$.

**Appendix F: Energy evolution analysis**

In this section, we analyze how the Quantum Imaginary Time Control (QITC) can speedup the convergence dramatically for systems with small energy gaps, in comparison to the Quantum Imaginary Time Evolution (QITE). First, we recall the imaginary time evolution,

$$|\psi(\tau)\rangle = A(\tau)e^{-H_{p}\tau}|\psi(0)\rangle,$$

$$A(\tau) = (\langle\psi(0)\rangle e^{-2H_{p}\tau}|\psi(0)\rangle)^{-\frac{1}{2}}.$$ 

The mean energy change with time step $\Delta \tau$ can be written as,

$$\Delta E(\tau) = (\frac{\partial(\langle H \rangle)}{\partial \tau})\Delta \tau = 2(\langle H \rangle^2 - \langle H^2 \rangle)\Delta \tau.$$ 

Spanning the problem Hamiltonian in the eigenbasis $H_p = e_0 H_0 + e_1 H_1 + \ldots + e_n H_n$, where $H_i = |\psi_i\rangle \langle \psi_i|$ with $H_p |\psi_i\rangle = e_i |\psi_i\rangle$ and eigenvalues $e_i$, and express $|\psi(\tau)\rangle = \sum_i c_i |\psi_i(\tau)\rangle$. The mean energy change for QITE can be
FIG. 10. The log-log plot result of 3-SAT quantum annealing problem. The x-axis is energy gap between the ground state and the first excited state. The y-axis is the converge steps difference between the ITE and imaginary time control. The fitted curved is $f(x) = 1065.6 \cdot x^{40.93} + 1.3$

written as,

$$\langle H_p \rangle = \sum_i e_i |c_i|^2$$
$$\langle H_p^2 \rangle = \sum_i e_i^2 |c_i|^2$$
$$\Delta E_I(\tau) = 2(\langle H_p \rangle^2 - \langle H_p^2 \rangle) = 2 \left( \sum_{i,j} e_i e_j |c_i|^2 |c_j|^2 - \sum_i e_i^2 |c_i|^2 \right) \Delta \tau$$

We can further rewrite the function above with $\Delta_{ij} = e_i - e_j$ as,

$$\Delta E_I(\tau) = 2 \left( \sum_{i,j} e_i e_j |c_i|^2 |c_j|^2 - \sum_i e_i^2 |c_i|^2 \right) \Delta \tau = 2 \left( \sum_i |c_i|^2 (e_0 + \Delta_{i0}) \left( \sum_j |c_j|^2 (e_0 + \Delta_{j0}) - (e_0 + \Delta_{i0}) \right) \right) \Delta \tau = 2 \left( \sum_i |c_i|^2 \left( \sum_j |c_j|^2 \Delta_{i0} \Delta_{j0} - \Delta_{i0}^2 \right) \right) \Delta \tau$$

For QITC, the imaginary time evolution is governed by the driven Hamiltonian $H_p + \beta(\tau)H_d$ where the $\beta(\tau)$ is the control law. By replacing original QITE Hamiltonian with the QITC Hamiltonian, the mean energy change rate can be written as

$$\Delta E_C(\tau) = 2(\langle H_p \rangle^2 - \langle H_p^2 \rangle) + \beta(\tau)(2\langle H_d \rangle \langle H_p \rangle - \langle \{H_p, H_d\} \rangle) \Delta \tau.$$
Terms like $\langle H_d \rangle$ and $\langle [H_d, H_p] \rangle$ etc can be more easily analyze if we decompose them in the $H_p$ eigenbasis (using $d_{ij} = \langle \psi_i | H_d | \psi_j \rangle$ and $d_{ij} = d_{ji}^*$), the $H_d$-related expectation value can be written as,

$$
\langle H_d \rangle = \sum_{ij} c_i^* c_j d_{ij}
$$

$$
\langle H_p H_d \rangle = \sum_{ij} c_j^* c_i e_i d_{ji}
$$

$$
\langle H_d H_p \rangle = \sum_{ij} c_i^* c_j e_i d_{ij}.
$$

The energy change can be rewritten as,

$$
\Delta E_C (\tau) = \frac{2}{\Delta \tau} [\langle H_p \rangle^2 - \langle H_p^2 \rangle] + \beta (\tau) \langle \Delta H_p \rangle (2 \langle H_d \rangle \langle H_p \rangle - \langle [H_p, H_d] \rangle)\Delta \tau
$$

$$
= \Delta E_I (\tau) + \beta (\tau) \left[ 2 \sum_i e_i |c_i|^2 \sum_{jk} c_j^* c_k d_{jk} - \sum_{ij} c_j^* c_i e_i d_{ji} - \sum_{ij} c_i^* c_j e_i d_{ij} \right] \Delta \tau
$$

$$
= \Delta E_I (\tau) + \beta (\tau) \left[ \sum_i \Delta \tau_0 (2 |c_i|^2 \sum_{jk} c_j^* c_k d_{jk} - \sum_{i} c_j^* c_i d_{ji} - \sum_{i} c_i^* c_j d_{ij} \right] \Delta \tau
$$

$$
= \Delta E_I (\tau) + \beta (\tau) \left[ \sum_i \Delta \tau_0 \left( 2 |c_i|^2 \sum_{jk} c_j^* c_k d_{jk} - \sum_{j} c_j^* c_i d_{ji} - \sum_{j} c_j^* c_j d_{ij} \right) \right] \Delta \tau
$$

In conclusion, the rate of energy change under QITE is proportional to $\Delta \tau_0^2$ while the rate of energy change is boosted with an extra contribution proportional to $\Delta \tau_0$ under QITC. It is easy to see that when $\Delta \tau_0$ is small, the additional control might provide some speedup with proper designs of the control Hamiltonian and the control law.