Double-bracket quantum algorithms for quantum imaginary-time evolution

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Efficiently preparing approximate ground-states of large, strongly correlated systems on quantum hardware is challenging and yet nature is innately adept at this. This has motivated the study of thermodynamically inspired approaches to ground-state preparation that aim to replicate cooling processes via imaginary-time evolution. However, synthesizing quantum circuits that efficiently implement imaginary-time evolution is itself difficult, with prior proposals generally adopting heuristic variational approaches or using deep block encodings. Here, we use the insight that quantum imaginary-time evolution is a solution of Brockett's double-bracket flow and synthesize circuits that implement double-bracket flows coherently on the quantum computer. We prove that our Double-Bracket Quantum Imaginary-Time Evolution (DB-QITE) algorithm inherits the cooling guarantees of imaginary-time evolution. Concretely, each step is guaranteed to i) decrease the energy of an initial approximate ground-state by an amount proportion to the energy fluctuations of the initial state and ii) increase the fidelity with the ground-state. Thus DB-QITE provides a means to systematically improve the approximation of a ground-state using shallow circuits.

Introduction.—Preparing ground-states of Hamiltonians is a fundamental task in quantum computation with wide-ranging applications from studying properties of materials [1] and chemicals [2] to solving optimization problems [3]. However, ground-state preparation is not only NP-hard [4] but also QMA-complete [5–8], and thus is a challenging problem even for quantum computers [9–12], let alone classical ones. Nevertheless, improvements on the computational efficiency over classical simulation is anticipated to be feasible with quantum processors [13–15]. In other words, the shift to quantum computing could offer a pathway to overcoming practical [16], conceptual [17] and fundamental [18, 19] challenges to the classical simulation of ground-states.

To date, various quantum algorithms have been proposed for ground-state preparation both for fault-tolerant [20–35] and near-term quantum computers [36–56]. Among these a promising family of protocols take a thermodynamic-inspired approach and use imaginary-time evolution (ITE) to cool an initial state $|\Psi_0\rangle$ with respect to a Hamiltonian $\hat{H}$ via

$$|\Psi(\tau)\rangle = \frac{e^{-\tau\hat{H}}|\Psi_0\rangle}{\|e^{-\tau\hat{H}}|\Psi_0\rangle\|} \, . \tag{1}$$

Here τ is the ITE duration and the normalization involves the norm defined for any vector $|\Omega\rangle$ by $\||\Omega\rangle\| = \sqrt{\langle\Omega|\Omega\rangle}$. ITE is guaranteed to converge to the ground-state $|\lambda_0\rangle$ of $\hat{H}$ in case the initial overlap with the ground-state is non-zero [57].

We make a distinction between ITE and *quantum imaginary-time evolution (QITE)* [21, 34, 36–42] in that ITE is defined by the normalized action of a non-unitary propagator and QITE is the implementation of ITE by explicitly using a unitary Q_τ such that $|\Psi(\tau)\rangle = Q_\tau|\Psi_0\rangle$. Finding the unitaries that implement the ITE states $|\Psi(\tau)\rangle$ is not straightforward.

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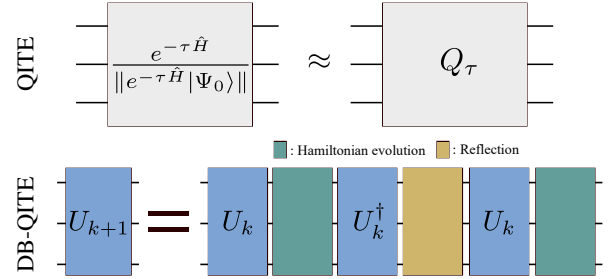
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FIG. 1. **Double-bracket Quantum Imaginary-Time Evolution (DB-QITE).** We propose a new quantum algorithm to implement imaginary-time evolution (ITE). To implement the Quantum Imaginary-Time Evolution (QITE) unitary Q_τ, we utilize a Double-Bracket Quantum Algorithm (DBQA) and show that QITE can be recursively compiled using Hamiltonian evolution and reflection gates.

One family of approaches use a hybrid quantum-classical optimization loop to learn Q_τ [34, 36–41]. This can yield compressed circuits by fine-tuning to individual input instances, but scaling to large problem sizes is generally inhibited by growing requirements on measurement precision [58, 59]. Another approach is to extend the system size and approximate the non-unitary propagator with qubitization [21]. However, the overheads of implementing so-called block-encodings preclude flexible near-term experiments. In other words, constructing efficient circuits for QITE remains an open problem.

In this work, we offer a resolution to this problem by drawing on the observation that ITE is a solution to well-studied differential equations known as *double-bracket flows (DBF)* [60–77]. DBFs are appealing for quantum computation because their solutions arise from unitaries, a feature recently exploited for quantum circuit synthesis by means of double-bracket quantum algorithms (DBQA) [30, 51, 52]. DBFs come with local optimality proofs in that they implement gradient flows [61, 63, 65, 75, 76] and these are known to converge exponentially fast to their fixed points [78]. Accordingly,

	Fluctuation-Refrigeration Relation	Fidelity
ITE	$\partial_\tau E(\tau) = -2V(\tau)$ [Eq. (3)]	$1 - \mathcal{O}(e^{-2\tau\Delta})$ [Eq. (57)]
DB-QITE	$E_{k+1} \leq E_k - 2s_k V_k + \mathcal{O}(s_k^2)$ [Proposition 1]	$1 - \mathcal{O}(q^k)$ [Theorem 2]

TABLE I. **Energy reduction guarantees for DB-QITE**. It is known that the ITE can lower the energy $E(\tau)$ by an amount proportional to the energy fluctuation $V(\tau)$. We call this a fluctuation-refrigeration relation. ITE is also guaranteed to improve the fidelity to the ground-state exponentially in the imaginary-time τ. Similarly to ITE, DB-QITE agrees with the amount of energy reduction $E_{k+1} - E_k$ up to corrections of order $\mathcal{O}(s_k^2)$, and improve the fidelity exponentially fast in the time of algorithm iterations k.

DBQAs have recently been shown to provide a compilation procedure which is able to significantly improve on circuits optimized by brute-force [51]. Here we introduce an algorithm, that we call DB-QITE, that implements steps of gradient flows *coherently* on a quantum computer [30], without resorting to classical computations, heuristic hybrid quantum-classical variational methods, or block encodings. Instead, the DBQA approach produces recursive quantum circuits which at every step approximates the DBF of ITE, as sketched in Fig. 1.

Crucially, DB-QITE inherits the cooling properties of ITE, as summarized in Table I. Namely, we provide rigorous guarantees that DB-QITE systematically lowers the energy of a state and increases its fidelity with the ground-state. As we will see, DB-QITE has a similar cooling rate as ITE, with the rate larger for quantum states with high energy fluctuations. Moreover, a single step of DB-QITE is guaranteed to increase the fidelity with the ground-state by an amount proportional to the initial fidelity with the ground-state and the spectral gap of the target Hamiltonian. Furthermore, as our bounds hold for any input state (in contrast to Ref. [79]) this argument can be applied iteratively to show that the DB-QITE unitaries yield states which converge exponentially fast in the number of iterations to the ground-state. Given the recursive structure of these additional iterations the circuit depths required to implement DB-QITE grow exponentially with each additional step but can be controlled by keeping the number of iterations moderate.

Thus DB-QITE provides a means to systematically reduce the energy of an approximate ground-state. We expect our algorithm to be used both as a standalone ground-state preparation method in the early fault-tolerant era, as well as in conjunction with more established [20–22, 32–34] and heuristic approaches [36–39, 53, 54] to ground-state preparation.

Fluctuation-refrigeration relation of ITE.—ITE defined in Eq. (1) satisfies [57]

$$\partial_\tau |\Psi(\tau)\rangle = -(\hat{H} - E(\tau))|\Psi(\tau)\rangle \qquad (2)$$

with the energy $E(\tau) = \langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle$. Under such evolutions, the state is guaranteed to converge to the ground-state of

the Hamiltonian in the limit of $\tau \to \infty$ as long as the initial state $|\Psi_0\rangle$ has some non-zero overlap to the ground-state [57]. This fact has driven the exploration of how to implement ITE on classical [80] and quantum computers [34, 36–41]. From Eq. (2), a direct computation (see Supplemental Materials II B) gives

$$\partial_\tau E(\tau) = -2V(\tau), \qquad (3)$$

where $V(\tau) = \langle\Psi(\tau)|(\hat{H} - E(\tau))^2|\Psi(\tau)\rangle$ is the energy fluctuation (the operator variance of the Hamiltonian). It follows that higher energy fluctuations in the state lead to a faster energy decrease. We call this a *fluctuation-refrigeration relation*, and will show that an analogous relation holds for the quantum circuits that we will propose to approximate ITE.

ITE is a solution of DBF—. We next observe that ITE Eq. (2) can be rewritten as

$$\partial_\tau |\Psi(\tau)\rangle = [\Psi(\tau), \hat{H}]|\Psi(\tau)\rangle, \qquad (4)$$

where $\Psi(\tau) = |\Psi(\tau)\rangle\langle\Psi(\tau)|$ is the density matrix of the ITE state and $[A, B] = AB - BA$ is the commutator [81]. In terms of the density matrix $\Psi(\tau)$, we get

$$\frac{\partial\Psi(\tau)}{\partial\tau} = \left[[\Psi(\tau), \hat{H}], \Psi(\tau)\right]. \qquad (5)$$

This equation is exactly in the form of a well-studied Brockett's DBF [76]. We include a brief discussion of Eq. (5) in relation to the unitary manifolds, the relevant cost functions and a review of Riemannian gradient flows in End Matter. Given Eq. (5), these results from DBF theory now apply to QITE and in essence signify its local optimality.

QITE from ITE DBF.— The difficulty of implementing ITE on quantum computers lies in the non-unitarity of the propagator in Eq. (1) and its state-dependence in Eq. (2). The challenge of circuit synthesis for QITE is to find a unitary Q_τ such that

$$|\Psi(\tau)\rangle \approx Q_\tau |\Psi_0\rangle. \qquad (6)$$

This transition from non-unitary propagation in the ITE of Eq. (1) to unitary implementation in Eq. (6) is termed QITE. Intuitively, we have from Eq. (4) that for short durations s,

$$|\Psi(s)\rangle \approx e^{s[\Psi(0), \hat{H}]}|\Psi_0\rangle. \qquad (7)$$

Thus, writing ITE as a DBF directly results in a proposal for QITE, at least for short durations. It is not straightforward to rigorously quantify the approximation in Eq. (7), see Prop. 1 of [30]. Nevertheless, we show in Prop. 11 of App. III B that the energy decrease of this dynamics agrees with Eq. (3) up to corrections of order $\mathcal{O}(s^2)$.

Motivated by this, we initialize a recursion by the initial state $|\sigma_0\rangle = |\Psi_0\rangle$ and define

$$|\sigma_{k+1}\rangle = e^{s_k[\sigma_k, \hat{H}]}|\sigma_k\rangle. \qquad (8)$$

Here, we denote the time step size in the $(k + 1)$-th step as s_k and $\sigma_k = |\sigma_k\rangle\langle\sigma_k|$. Rigorous results from Refs. [61, 65, 75,

76] apply to Eq. (8) and prove convergence to the ground-state as $k \to \infty$. The recursion in Eq. (8) provides an explicit recipe for QITE unitaries in Eq. (6). However, further circuit synthesis is needed as $e^{s_k[\sigma_k, \hat{H}]}$ is challenging to execute directly on a quantum computer.

DB-QITE circuit synthesis— Here we show that QITE unitaries can be compiled to a quantum circuit using the group commutator iterations first introduced in Ref. [30]. In the context of QITE we define the group commutator of any density matrix Ω as

$$G_s(\Omega) = e^{i\sqrt{s}\hat{H}} e^{i\sqrt{s}\Omega} e^{-i\sqrt{s}\hat{H}} e^{-i\sqrt{s}\Omega}. \tag{9}$$

The Supplemental Materials of Ref. [30] provides a quantitative proof that

$$G_s(\Omega) = e^{s[\Omega, \hat{H}]} + \mathcal{O}(s^{3/2}), \tag{10}$$

see Refs. [82–84] for further context. In order to formulate the circuit synthesis for DB-QITE we first notice that the application of $G_s(\omega)$ to $|\Omega\rangle$ results in

$$e^{-i\sqrt{s}} G_s(\Omega)|\Omega\rangle = e^{i\sqrt{s}\hat{H}} e^{i\sqrt{s}\Omega} e^{-i\sqrt{s}\hat{H}} |\Omega\rangle. \tag{11}$$

This allows us to arrive at the following DB-QITE states

$$|\omega_{k+1}\rangle = e^{i\sqrt{s_k}\hat{H}} e^{i\sqrt{s_k}\omega_k} e^{-i\sqrt{s_k}\hat{H}} |\omega_k\rangle. \tag{12}$$

Finally, let U_k denote the circuit to prepare $|\omega_k\rangle$ from a trivial reference state $|0\rangle$, i.e., $|\omega_k\rangle = U_k|0\rangle$. We can now use unitarity to simplify $e^{i\sqrt{s}\omega_k} = U_k e^{i\sqrt{s}|0\rangle\langle 0|} U_k^\dagger$ and arrive at a recursive formula for DB-QITE circuit synthesis:

$$U_{k+1} = e^{i\sqrt{s_k}\hat{H}} U_k e^{i\sqrt{s_k}|0\rangle\langle 0|} U_k^\dagger e^{-i\sqrt{s_k}\hat{H}} U_k. \tag{13}$$

For $k = 1$ this expression involves U_0 which can be any unitary which when applied to $|0\rangle$ yields an approximation $|\omega_0\rangle := U_0|0\rangle$ to the ground-state $|\lambda_0\rangle$ of the input Hamiltonian $\hat{H}$, and subsequent steps of DB-QITE continue to leverage on U_0 implicitly. Thus DB-QITE is formulated by the recursive circuit synthesis shown in Fig. 1. In End Matter we elaborate on the compilation costs of the Hamiltonian simulation and partial reflection primitives using known results.

Fluctuation-refrigeration relation for DB-QITE.— Similarly to standard ITE, we here show that the approximation to ITE implemented via DB-QITE obeys a fluctuation-refrigeration relation where the energy reduction in every step is bounded by the energy fluctuations.

Theorem 1. *Fluctuation-refrigeration relation. The average energy $E_k := \langle \omega_k | \hat{H} | \omega_k \rangle$ of the states $|\omega_k\rangle := U_k|0\rangle$, where U_k is defined recursively in Eq. (13), are bounded as*

$$E_{k+1} \leq E_k - 2s_k V_k + \mathcal{O}(s_k^2) \tag{14}$$

where $V_k := \langle \omega_k | \hat{H}^2 | \omega_k \rangle - E_k^2$ is the variance of the energy in state $|\omega_k\rangle$.

We prove this statement in Theorem 15, Sec. IV A of the Supplemental Materials. This shows that in every step of DB-QITE cooling rate matches the cooling rate of continuous ITE up to $\mathcal{O}(s_k^2)$. Moreover, we give sufficient conditions on s_k such that the higher order terms $\mathcal{O}(s_k^2)$ do not overhaul the first order cooling.

The energy reduction of DB-QITE quantified in Eq. (14) is warranted by non-negativity of the energy variances $V_k > 0$. However, Eq. (14) does not yet exclude the possibility of converging to an excited energy eigenstate. Next, we will show that such scenarios do not occur.

Guaranteed ground-state fidelity increase via DB-QITE.— We now proceed to show that each step of DB-QITE is guaranteed to increase the fidelity with the true ground-state. Concretely, as proven in Supplemental Materials Sec. IV, the following theorem holds.

Theorem 2. *ground-state fidelity increase guarantee. Suppose that DB-QITE is initialized with some non-zero initial ground-state overlap F_0. Let $\hat{H}$ be a Hamiltonian with a unique ground-state $|\lambda_0\rangle$, spectral gap Δ and spectral radius $\|\hat{H}\| \geq 1$. Let U_0 be an arbitrary unitary and set*

$$s = \frac{\Delta}{12\|\hat{H}\|^3}. \tag{15}$$

The states $|\omega_k\rangle := U_k|0\rangle$, where U_k is defined recursively in Eq. (13), satisfy

$$F_{k+1} := |\langle \lambda_0 | \omega_{k+1}\rangle|^2 \geq F_k \left(1 + \frac{(1 - F_k)\Delta^2}{12\|\hat{H}\|^3}\right) \geq 1 - q^k \tag{16}$$

where $q = 1 - sF_0\Delta$.

This result shows that DB-QITE systematically synthesizes circuits that improve on previous circuits to prepare a better approximation to the ground-state. In particular, the first step is guaranteed to increase the fidelity with the ground-state by $F_0(1 - F_0)\Delta^2/12\|\hat{H}\|^3$ where F_0 is the fidelity of the initial guess state $U_0|0\rangle$ and Δ is the spectral gap. Moreover, subsequent iterations are guaranteed to further increase the fidelity to the ground-state. Thus we see that repeated iterations of DB-QITE inherently avoid converging to excited states (as could be consistent with Theorem 1) but rather transitions through many states with small energy fluctuations V_k to converge to the ground-state. Hence DB-QITE provides a means of systematically preparing states with increased fidelity with the ground-state.

Scaling of DB-QITE.—Theorem 1 and Theorem 2 entail that DB-QITE can be implemented to systematically reduce the energy and increase the ground-state fidelity of a given trial state. As one would expect, the resources required become more demanding with system size, but for a gapped local Hamiltonian the improvement from a single step of DB-QITE only degrades polynomially with system size L. Namely, it is clear from the formal statement of Theorem 1 (i.e., Theorem 15 of the Supplemental Materials) that a polynomially decreasing s

suffices to ensure the inequality in Eq. (14) holds strictly and so for constant fluctuations V_k the energy only reduces polynomially. Similarly, if $\Delta \in \Theta(1)$ and $\|\hat{H}\| \in \Theta(L)$ then the fidelity gain for a constant initial fidelity is only reduced by a polynomial factor. Moreover, the circuit depth required to implement a single iteration of DB-QITE only increases polynomially with system size (inline with the standard scaling of reflections and Hamiltonian simulation) and thus our circuit scalings for a single iteration of DB-QITE are favorable. In the End Matter we further discuss the scaling for consecutive iterations of DB-QITE which are less favorable due to DB-QITE's recursive structure but can plausibly be improved by using larger step sizes.

Comparison with prior work— The most closely related work to our proposal is Ref. [79]. There they proposed circuit synthesis strategy which provides an energy gain decided by energy fluctuations, similarly to Eq. (14). As is explained above, the appearance of energy fluctuations in both Ref. [79] and Eq. (14) can be understood as the result of attaining the cooling rate of steepest-descent flows. However, the results in Ref. [79] improves the energy only of product states and hence can only be applied to a single iteration with a relatively poor initial approximation. In contrast, Theorem 1 and Theorem 2 apply to any state. Thus we not only achieve increased energy reductions for similarly short depth circuits as Ref. [79], but also allow the energy of arbitrary initial states to be reduced and further open up the potential of apply our algorithm iteratively. In this sense, the fact that our algorithm can be applied iteratively should be viewed as a bonus despite the overheads associated with its recursive form.

Ref. [50] also exploits the technique of Riemannian optimization algorithms to derive a method for optimizing quantum circuits. Their proposal aims to approximate Eq. (8) using a different implementation. In particular, their implementation, which is targeted towards noisy intermediate scale devices, is variationally learned from measurements and so does not enjoy rigorous guarantees and could be prohibitively expensive. More generally, there exist numerous algorithms for ground-state preparation that are targeted towards fault tolerant hardware [20–34] - we leave an extensive comparison with these methods for future work.

Discussion— There is widespread interest in the quantum community in methods for ground-state preparation, not just for many-body physics problems but also more generally for machine learning and combinatorial optimization tasks. Variational strategies in particular have gathered much attention [53, 85]. However, the early optimism for these heuristic methods has been tempered in recent years by a growing awareness of the challenge of scaling them to modest problem sizes [58, 86–89]. At the heart of the matter is the fact that unstructured search methods in exponentially large spaces face a curse of dimensionality that necessitates exponential precision [59]. Our approach here sidesteps such issues by taking a thermodynamically inspired approach whereby a quantum computer can coherently evaluate steepest-descent directions and gain energy reduction even while operating in exponential spaces.

Namely, the fact that imaginary-time evolution (ITE) is a solution to double-bracket flows implies that ITE is an optimal gradient descent method in the sense of being a steepest-descent flow. The local optimality of DBFs has previously been investigated in the context of circuit compilation [50] and has motivated tangent-space methods crucial for tensor network simulations [90–95]. However, these studies involved classical processing at its core. Here we took the radically different approach of implementing double-bracket flows *coherently* on the quantum computer [30], rather than resorting to classical computations or heuristic hybrid quantum-classical variational methods.

Concretely, our work answers the question of how to synthesize quantum circuits for imaginary-time evolution. That is, how to systematically find unitaries Q_τ that implement ITE without employing heuristic hybrid quantum-classical variational methods. In particular, using the link between DBF and ITE we formulated DB-QITE, a double-bracket quantum algorithm for quantum imaginary-time evolution using the group-commutator Eq. (9). Our resulting algorithm, defined iteratively in Eq. (13), involves forward and backward evolutions under the target Hamiltonian interspersed with refection operations and the initial state preparation unitaries. These ingredients are similar to bang-bang protocols for quantum control [96–98]. However, while this quantum control paradigm is usually restricted to small systems, DB-QITE can be viewed as a quantum many-body echo protocol. As imaginary-time evolution is a fundamental primitive in diverse areas, our circuit synthesis strategy can have implications for fields other than quantum computing which also employ ITE, e.g. path-integral optimization used to study holographic complexity in AdS/CFT correspondence [99, 100].

We have shown that DB-QITE inherits the guarantees of ITE for ground-state preparation. In particular, Theorem (2) establishes that states prepared via DB-QITE are guaranteed to converge exponentially in the number of iteration towards the ground-state and Eq. (14) shows that DB-QITE has, to first order, the same cooling rate as QITE. Both properties are ramifications of QITE's rooting in gradient flow theory [61, 65, 75, 76, 78]. That the cooling rate of QITE is, similarly to ITE, determined by the energy fluctuations in the initial state is in line with the physical intuition that fast control of a system needs coherence in the energy basis [101, 102]. This suggests the possibility to derive quantum speed limits for cooling with a measurable metric that involves energy fluctuations.

Theorem 2 shows that DB-QITE is guaranteed to converge to the ground-state. Concretely, each step of DB-QITE is guaranteed to increase the fidelity of any trial state with the ground-state. For iterative applications of DB-QITE the increased fidelity comes with the trade off of increasing circuit depths. Namely, while the individual operations are simple—both Hamiltonian simulation [103–107] and reflections [108] have known efficient compilation schemes — the amount to queries to these two subroutines grows exponentially with the number of DBQA steps. Nonetheless, each of these steps leads to guaranteed improvements and thus if restricted to a modest number of iterations DB-QITE provides a means to systemati-

cally reduce the energy of a state with a reasonably short depth circuits.

We believe that future refinements of DB-QITE can reduce the circuit depths of ITE inspired algorithms. Concretely, in End Matter we discuss how quantum dynamic programming can reduce depths of DB-QITE. This is done at the cost of extending the circuit width but it can be used to perform a few additional DBQA steps that otherwise would exceed available circuit depths. Alternatively, one could investigate hybrid quantum-classical variational approaches where DB-QITE is used as an initial ansatz but the step sizes s_k are left as free variables to be optimized [30, 51, 52, 109]. Such a hybrid approach is likely to perform better than our general analytical bounds, and could even provide a means of learning approximate ground-states for subsequent refinement via the vanilla

DB-QITE proposed here or other algorithms intended to improve ground-states [20–34].

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End Matter

Geometry of ITE DBF. — We show that the ITE dynamics in Eq. (5) represents the minimization of a cost function using its steepest gradient on the Riemannian manifold. To this end, we first show the fundamentals of DBFs and then elaborate on the property of ITE in terms of DBFs.

In general, DBFs are matrix-valued ordinary differential equations which have been shown to realize diagonalization, QR decompositions, sorting and other tasks [63, 67, 68, 76]. Brockett first introduced the flow equation by studying the minimization of the least square of two matrices with the steepest descent techniques. Let $\mathcal{M}(A) = \{UAU^\dagger \text{ s.t. } U^{-1} = U^\dagger\}$ be the set of all matrices generated by evolving a Hermitian operator A under a unitary U. Consider the loss $\mathcal{L}_{A,B}(U) = -\frac{1}{2}\|UAU^\dagger - B\|_{\text{HS}}^2$ where B is also Hermitian. Then, the Riemannian gradient evaluated at $P = UAU^\dagger$ for the loss function $\mathcal{L}_B(P) = -\frac{1}{2}\|P - B\|_{\text{HS}}^2$ is given by [50, 76]

$$\text{grad}_P \mathcal{L}_B(P) = [[P, B], P]. \tag{17}$$

We note that the the derivation relies on two conditions of Riemannian geometry, namely, the tangency condition and the compatibility condition, see Refs. [50, 76] for a derivation.

This indicates that the the right-hand side of Eq. (17) is indeed the steepest descent direction of the cost function on the Riemannian manifold $\mathcal{M}(A)$. As the steepest-descent flow is the set of points $A(\ell) \in \mathcal{M}(A)$ which satisfy

$$\partial A(t)/\partial t = \text{grad}_{A(t)} \mathcal{L}_B(A(t)), \tag{18}$$

we arrive at the flow equation

$$\partial A(t)/\partial t = [[A(t), B], A(t)], \tag{19}$$

which is exactly the DBF.

In case of the ground-state preparation task, we obtain the ITE in Eq. (5) by setting $A = \Psi(\tau) = |\Psi(\tau)\rangle\langle\Psi(\tau)|$ and $B = \hat{H}$. Namely, the ITE realizes the minimization of the cost function

$$\mathcal{L}_{\hat{H}}(\Psi(\tau)) = -\frac{1}{2}\|\Psi(\tau) - \hat{H}\|_{\text{HS}}, \tag{20}$$

using its steepest descent direction on the Riemannian manifold. Eq. (20) can be simplified to

$$\mathcal{L}_{\hat{H}}(\Psi(\tau)) = E(\tau) - \frac{1}{2}(1 + \|\hat{H}\|_{\text{HS}}^2). \tag{21}$$

As the second term is independent of τ, we can clearly verify that the cost function considered in this task is equivalent to the minimization of the energy, i.e., the preparation of the ground-state. Combining this observation with Eq. (19) we obtain Eq. 5. That is, we see that DBFs provide a solution to ITE, as claimed. We remark that the ITE and Brockett's DBF have been extensively studied in slightly different fields, but their link has not been pointed out to the best of our knowledge.

We also demonstrate some properties of QITE that can be inferred through the lens of DBF. For instance, the convergence to the ground-state can be checked by utilizing the properties of the DBF flow. The solution of the DBF in Eq. (19) is known to converge to the equilibria point that is characterized by $[A(\infty), B] = 0$; that is, $A(\infty)$ shares the same eigenbasis with B. Also, the DBF has the isospectral property, meaning any solution of the DBF has the same set of eigenvalues. In case of the setting in Eq. (20), as the initial state $\Psi(0)$ is pure (i.e., a rank-one matrix) and the cost function in Eq. (21) indicates the energy minimization, the solution always converges to only one non-trivial eigenstate, i.e., the ground-state.

One can also derive the energy-fluctuation refrigeration relation for ITE in Eq. (3) directly from the link with DBFs. Concretely, by taking the derivative of Eq. (1), we can see that the energy of ITE is driven by the energy fluctuation. As for the DBF, the derivative of the cost function in Eq. (20) reads

$$\partial\mathcal{L}_{\hat{H}}(\Psi(\tau))/\partial\tau = -\|[\Psi(\tau), \hat{H}]\|_{\text{HS}} \tag{22}$$

and further calculation reveals that

$$\|[\Psi(\tau), \hat{H}]\|_{\text{HS}} = 2V(\tau). \tag{23}$$

This indicates that the energy dynamics of both cases are the same. See II B of Supplemental Materials for more discussion.

Circuit depths for iterative applications of DB-QITE.— Theorem 2 ensures that the fidelity with the ground-state converges exponentially with the number of DBQA *steps* k. However, the depth of circuit (i.e., the number of queries to the Hamiltonian simulation, to reflections around the reference state or to initial state preparation circuit) also scales exponentially in k. Specifically, Eq. (13) reveals that k steps of DB-QITE require $\mathcal{O}(3^k)$ subroutine queries to Hamiltonian simulation or partial reflections around the reference state.

The reflection unitary is a multi-qubit controlled parameterized phase gate, assuming the quantum state is the tensor-product zero state; we see it by writing $e^{i\sqrt{t}|0\rangle\langle0|} = I + (e^{i\sqrt{t}} - 1)|0\rangle\langle0|$ with matrix representation

$$e^{i\sqrt{t}|0\rangle\langle0|} = \begin{bmatrix} e^{i\sqrt{t}} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \tag{24}$$

This means that the first qubit is the target to which the operation $diag(e^{i\sqrt{t}}, 1)$ is applied, and the remaining $L - 1$ qubits are the control qubits. Multi-qubit controlled gates can be implemented efficiently without qubit overheads [110]. Indeed

Theorem 1 of Ref. [108] proves that any multi-qubit controlled unitary gate with $m \geq 6$ controls is realizable by $12L - 32$ CNOT gates with depth $8L - 8$, $16L - 48$ T gates with depth $8L - 6$ and $8L - 32$ Hadamard gates with depth $4L - 11$. This suggests that the gate complexity is linear in the number of qubits which is similar to efficient Hamiltonian simulation compiling [103–107].

Given the exponential query complexity in k, the DB-QITE analyzed in Theorem 2 amplifies the initial fidelity F_0 to a prescribed final fidelity F_{th} in depth

$$\mathcal{O}(L) \times O\left(\left(\frac{1 - F_0}{1 - F_{\text{th}}}\right)^{24\|\hat{H}\|^3/(F_0\Delta^2)}\right), \qquad (25)$$

where we multiplied the depth upper bound of the subroutines $\mathcal{O}(L)$ by the exponential query complexity, see Sec. IV for derivation. Thus, the depth scales exponentially with the inverse spectral gap Δ and with the inverse of the initial ground-state fidelity F_0. The base of the exponential scaling is the ratio of the initial and final infidelity. The last factor in the exponent is the inverse dependence on the step duration given in Eq. (15). For local Hamiltonians this step duration is polynomially decreasing in the number of qubits L implying that the runtime grows exponentially with L^3. Thus, the DB-QITE scheduling involved in the rigorous analysis allows for only a small number of steps k so that circuit depths are modest.

There are strong indications that this runtime analysis is unnecessarily pessimistic. In order to prove the Theorem we needed to use bounds that facilitated multiplicative rather than additive relations between the infidelities of consecutive DB-QITE states. This is rather intricate and the bounds can be expected to not be tight. More specifically, Eq. (15) arises from taking a coarse lower bound $E_k \geq \Delta(1 - F_k)$ which relates the energy to the fidelity F_k. This lower bound is saturated if the k'th DB-QITE state $|\omega_k\rangle$ is supported only on the the ground-state $|\lambda_0\rangle$ and the first excited state $|\lambda_1\rangle$. For such superposition of the two unknown lowest eigenstates, we can replace the Hamiltonian in our analysis by $\hat{H}_{\text{eff}} = \Delta|\lambda_1\rangle\langle\lambda_1|$. If $\hat{H}$ is gapped then the scheduling Eq. (15) would be independent of the system size and the runtime would be system-size independent.

In turn, when the bound is not saturated then knowledge of E_k (which is a basic measurement for monitoring any ground-state preparation quantum algorithm) would allow to choose a longer step duration and hence gain a larger energy decrease [30, 52]. For an unconstrained step duration s_k in Eq. (12) an intermediate relation in the proof states

$$F_{k+1} = F_k + 2E_k s_k + \mathcal{O}(s_k^2). \qquad (26)$$

The magnitude of the higher-order terms determines the maximal step duration s_k. Rather than taking worst case estimates as we had to do in the proof, the higher-order terms can be estimated from simple measurements of the energy E_k as a function of s_k in Eq. (12), see Ref. [52] for numerical examples. In the proof, we upper bound the higher-order terms by the norm of the Hamiltonian but this is very likely a big over-estimate. Indeed, those upper bounds are saturated when $|\omega_k\rangle$ is a superposition of the lowest and highest eigestates, which is highly

unlikely. Indeed, there is strong numerical evidence that in practice rather long steps can be used [30, 34, 51, 52, 109]. This makes it plausible that DB-QITE can be scheduled to gain much more fidelity in every step than is guaranteed by the worst-case lower bound (16) which implies a much shorter circuit depth in those cases.

Quantum dynamic programming.— Let us comment how to reduce the circuit depth by extending its width. Any state $|\psi\rangle = U_\psi|0\rangle$ can be improved into a state with lowered energy by setting $|\psi'\rangle = U^{(\psi)}|\psi\rangle$ where

$$U^{(\psi)} = e^{i\sqrt{\tau}\hat{H}}e^{i\sqrt{\tau}|\psi\rangle\langle\psi|}e^{-i\sqrt{\tau}\hat{H}}. \qquad (27)$$

Thus in each step, DB-QITE depends on the input state's density matrix in a non-trivial way and so it is a quantum recursion. Recently, quantum dynamic programming has been proposed [111] which similarly to ordinary dynamic programming leverages memoization to reduce the runtime of recursions. In this case it suffices to combine density matrix exponentiation for the reflector $e^{i\sqrt{\tau}|\psi\rangle\langle\psi|}$ with regular Hamiltonian simulation. See [20, 21] for discussion how to perform QITE using qubitization.

Another way of implementing the reflection operator is to straightforwardly use the density matrix exponentiation of $|0\rangle\langle0|$. Here, the cost scalings of the circuit depth and the number of copies of quantum states are respectively $\mathcal{O}(n\theta^2/\epsilon)$ and $\mathcal{O}(\theta^2/\epsilon)$ for implementing $e^{-i\theta\rho}$ [112, 113]. While the precise realization could be costly, performing density-matrix exponentiation also seems feasible because the $|0\rangle$ is known and so each time a copy is needed it can be prepared through a reset operation [114].

We stress that $U^{(\psi)}$ can be implemented obliviously to the circuit that prepares $|\psi\rangle$. Thus, DB-QITE implemented through dynamic programming could be viewed a *distillation* protocol of states with lowered energy. The inverse of the number of quantum states needed to implement one step of density matrix exponentiation is a lower bound to the rate of approximate distillation. If we want the distillation to have an increased gain we can perform more steps but with the trade-off that the rate will decay exponentially.

Supplemental Material for "Double-bracket quantum algorithms for quantum imaginary-time evolution"

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Contents

I. Common terminology and techniques

In this section, we make a comprehensive list of common terminology used throughout the rest of the appendix.

1. The *Hilbert-Schmidt norm* (or *Frobenius norm*) of an operator A acting on a Hilbert space $\mathcal{H}$ is defined as:

$$\|A - B\|_{\mathrm{HS}} = \sqrt{\mathrm{Tr}((A - B)^\dagger (A - B))}. \tag{28}$$

2. The *operator norm* $\|\hat{X}\|$ is defined as the smallest number such that for all normalized vectors, $\|\hat{X}\psi\| \leq \|\hat{X}\|$ holds:

$$\|\hat{X}\| = \sup_{\|\psi\|=1} \|\hat{X}\psi\|. \tag{29}$$

When the operator $\hat{X}$ is Hermitian on a finite-dimensional inner product space, its operator norm is equal to the maximum absolute value of its eigenvalues. Any norm satisfies the *triangle inequality* $\|x + y\| \leq \|x\| + \|y\|$.

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3. The Taylor series expansion of a function $f(x)$ around x_0, truncated at the n-th term, is

$$f(x) = f(x_0) + f^{(1)}(x_0)(x - x_0) + \cdots + \frac{f^{(n-1)}(x_0)}{(n-1)!}(x - x_0)^{n-1} + \frac{1}{n!}(x - x_0)^n f^{(n)}(\xi) . \tag{30}$$

where $f^{(n+1)}(t)$ is the $(n+1)$-th derivative of f and $\xi \in [x_0, x]$.

4. For two pure quantum states $|\psi\rangle$ and $|\Omega\rangle$, the fidelity is defined as $F(|\psi\rangle, |\Omega\rangle) = |\langle\psi|\Omega\rangle|^2$. To analyze fidelity convergence in QITE, it is useful to derive bounds on the expected energy and energy variance in terms of the ground-state infidelity, $\epsilon = 1 - F$ and the spectrum of eigenenergies $\{\lambda_j\}_j$.

Lemma 3. *Let $|\Omega\rangle$ be any pure state. Denote Hamiltonian as $\hat{H} = \sum_{j=0}^{d-1} \lambda_j |\lambda_j\rangle\langle\lambda_j|$ where we assume that the eigenvalues of $\hat{H}$ are ordered increasingly and we set $\lambda_0 = 0$. Suppose that the ground-state fidelity is given by $F = 1 - \epsilon$, then we have*

$$E_k \geq \lambda_1 \epsilon , \quad \text{and} \quad V_k \leq \lambda_{d-1}^2 \epsilon , \tag{31}$$

where $E_k = \langle\Omega|\hat{H}^2|\Omega\rangle$ is the expected energy and $V_k = \langle\Omega|\hat{H}^2|\Omega\rangle - E_k^2$ is the energy variance.

Proof. Let's define the probability to occupy the i-th eigenstate $|\lambda_i\rangle$ as p_i. As the ground-state fidelity is given by $F = 1 - \epsilon$, the state has probability $p_0 = 1 - \epsilon$ to occupy the ground-state. Since $\lambda_0 = 0$ by assumption, we obtain

$$E_k = \sum_{i=1}^{d-1} \lambda_i p_i \geq \lambda_1 \sum_{i=1}^{d-1} p_i = \lambda_1 \epsilon , \quad \text{and} \quad V_k \leq \sum_{i=1}^{d-1} \lambda_i^2 p_i \leq \|\hat{H}\|^2 \sum_{i=1}^{d-1} p_i = \|\hat{H}\|^2 \epsilon_k . \tag{32}$$

$\square$

	Sec. (II): ITE	Sec. (III): QITE DBI	Sec. (IV): DB-QITE
Initial state	$|\Psi_0\rangle$	$|\sigma_0\rangle = |\Psi_0\rangle$	$|\omega_0\rangle = |\Psi_0\rangle$
Evolution time step	Continuous duration τ	Discrete duration s_k	Discrete duration s_k
Evolved states	$|\Psi(\tau)\rangle$, see Eq. (33)	$|\sigma_k\rangle$, see Eq. (60)	$|\omega_k\rangle$, see Eq. (121)
Expected energy	$E(\tau) = \langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle$	$\overline{E}_k = \langle\sigma_k|\hat{H}|\sigma_k\rangle$	$E_k = \langle\omega_k|\hat{H}|\omega_k\rangle$
Energy variance	$V(\tau) = \langle\Psi(\tau)|\hat{H}^2|\Psi(\tau)\rangle - E(\tau)^2$	$\overline{V}_k = \langle\sigma_k|\hat{H}^2|\sigma_k\rangle - \overline{E}_k^2$	$V_k = \langle\omega_k|\hat{H}^2|\omega_k\rangle - E_k^2$
Fluctuation-refrigeration relation	$\partial_\tau E(\tau) = -2V(\tau)$	$\overline{\overline{E}}_{k+1} \leq \overline{\overline{E}}_k - 2s_k\overline{V}_k + \mathcal{O}(s_k^2)$	$\overline{E}_{k+1} \leq \overline{E}_k - 2s_k V_k + \mathcal{O}(s_k^2)$
Time step conditions for $E_{k+1} - E_k \leq -s_k V_k$	N.A.	$s_k \leq \dfrac{\overline{V}_k}{4\|\hat{H}\|\langle\sigma_k|\hat{H}^2|\sigma_k\rangle}$ (Proposition 11)	$s_k \leq \dfrac{4V_k}{5\epsilon_k\|\hat{H}\|^4}$ (Theorem 15)
ground-state fidelity	$F(|\Psi(\tau)\rangle, |\lambda_0\rangle) = |\langle\lambda_0|\Psi(\tau)\rangle|^2$	$F_k = |\langle\lambda_0|\sigma_k\rangle|^2 = 1 - \epsilon_k$	$F_k = |\langle\lambda_0|\omega_k\rangle|^2 = 1 - \epsilon_k$
ground-state fidelity convergence	$F(|\Psi(\tau)\rangle, |\lambda_0\rangle) \geq 1 - \delta_H$	$F_k \geq 1 - q^k$ with $q = 1 - sF_0\lambda_1$	$F_k \geq 1 - q^k$ with $q = 1 - sF_0\Delta$
Time step conditions for the above fidelity convergence	$\tau_H = \log\left[O\left(\dfrac{L}{\delta_H|\langle\lambda_0|\Psi_0\rangle|^2)}\right)\right]$ (Sec. II D)	$s = \dfrac{\lambda_1 F_0}{4\|\hat{H}\|^2}$ (Theorem 12)	$s = \dfrac{\Delta}{12\|\hat{H}\|^3}$ (Theorem (2) of main text and Sec. IV B)

TABLE II. The summary of notations for imaginary-time evolution (ITE), quantum imaginary-time evolution with double-bracket flows (QITE DBI), and with the explicit compilation using techniques in double-bracket quantum algorithms (DB-QITE), for ease of reference. For all sections of the supplemental materials, we define the Hamiltonian as $\hat{H} = \sum_{j=1}^{d-1} \lambda_j |\lambda_j\rangle\langle\lambda_j|$ where d is the dimension of the Hamiltonian. We also denote the spectral gap as $\Delta = \lambda_1 - \lambda_0$ where λ_1 and λ_0 represent the first excited and ground-state energy respectively. We also define $\|\hat{H}\|$ as the operator norm of the Hamiltonian. Finally, we assume that the initial state has some non-zero ground-state overlap $F_0 > 0$.

II. Key properties of imaginary-time evolution (ITE)

This is a section that outlines all the key properties of ITE which are relevant for the scope of our work. We begin with the key observation in Section II A that the state defined via ITE is a solution to the double-bracket flow equation. This leads to the decrease in average energy of the ITE state with respect to time, indicating convergence towards the ground-state. In Section II B, we derive a fluctuation-refrigeration relation which shows that states with higher energy fluctuations have a higher cooling rate. We next provide a digression in Section II C discussing convergence of thermal states to ground-states. We then carry over the techniques used in this section, to present in Section II D an exponential convergence of the ITE state's fidelity to the ground-state. This means that implementation of ITE DBF Eq. (34) as a double-bracket quantum algorithm [30] will converge to the ground-state too.

A. Proof that imaginary-time evolution is a solution to a double-bracket flow

Recall the definition for $\tau > 0$, and an initial pure state vector $|\Psi_0\rangle$ we set

$$|\Psi(\tau)\rangle = \frac{e^{-\tau\hat{H}}|\Psi_0\rangle}{\|e^{-\tau\hat{H}}|\Psi_0\rangle\|} \, , \tag{33}$$

where $\||\psi\rangle\| = \sqrt{\langle\psi|\psi\rangle}$ for any vector $|\psi\rangle$. Next, we prove a key connection between ITE and DBFs.

Proposition 4 (ITE is a solution to a DBF). *The ITE pure state $\hat{\Psi}(\tau) = |\Psi(\tau)\rangle\langle\Psi(\tau)|$ is a unique solution to Brockett's double-bracket flow equation, i.e.*

$$\frac{\partial\Psi(\tau)}{\partial\tau} = \left[[\Psi(\tau),\hat{H}],\Psi(\tau)\right] \, . \tag{34}$$

We refer to Eq. (34) as ITE DBF.

Proof. First, observe that the ITE map Eq. (1) is smooth as a function of τ. Second, ITE preserves the state vector normalisation so there must exist a unitary U_τ that implements it. Smoothness implies that there is a unique unitary U_τ such that $|\Psi(\tau)\rangle = U_\tau|\Psi_0\rangle$. We begin the proof by denoting the normalization factor of ITE as

$$N(\tau) = \|e^{-\tau\hat{H}}|\Psi_0\rangle\| = \sqrt{\langle\Psi_0|e^{-2\tau\hat{H}}|\Psi_0\rangle},$$

and evaluating its derivative to be

$$\partial_\tau\left(N(\tau)\right) = \frac{-\langle\Psi_0|\hat{H}e^{-2\tau\hat{H}}|\Psi_0\rangle}{N(\tau)} \, . \tag{35}$$

Thus the change of the ITE state vector as a function of τ is [57]

$$\partial_\tau|\Psi(\tau)\rangle = \partial_\tau\left(\frac{e^{-\tau\hat{H}}|\Psi_0\rangle}{N(\tau)}\right) = \frac{-\hat{H}e^{-\tau\hat{H}}|\Psi_0\rangle}{N(\tau)} + \frac{e^{-\tau\hat{H}}|\Psi_0\rangle \cdot (-\partial_\tau N(\tau))}{N(\tau)^2} \tag{36}$$

$$= -\hat{H}|\Psi(\tau)\rangle + \frac{\langle\Psi_0|\hat{H}e^{-2\tau\hat{H}}|\Psi_0\rangle}{N(\tau)^2}|\Psi(\tau)\rangle \tag{37}$$

$$= -\hat{H}|\Psi(\tau)\rangle + \langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle|\Psi(\tau)\rangle \, . \tag{38}$$

As a remark, this is of the form of a nonlinear Schrödinger equation. On the other hand, we note that the ITE density matrix also satisfies $\Psi(\tau) = |\Psi(\tau)\rangle\langle\Psi(\tau)| \equiv U_\tau\Psi_0 U_\tau^\dagger$ satisfies

$$[\Psi(\tau),\hat{H}]|\Psi(\tau)\rangle = |\Psi(\tau)\rangle\langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle - \hat{H}|\Psi(\tau)\rangle\langle\Psi(\tau)|\Psi(\tau)\rangle = -\hat{H}|\Psi(\tau)\rangle + E(\tau)|\Psi(\tau)\rangle \, . \tag{39}$$

Thus, from Eq. (38) we have $\partial_\tau|\Psi(\tau)\rangle = [\Psi(\tau),\hat{H}]|\Psi(\tau)\rangle$. To complete the proof we set $\mathcal{W} = i[\Psi(\tau),\hat{H}]$ and obtain Eq. (5) as the von Neumann evolution equation of the ITE density matrix.

$\square$

Remark. *Note that Eq. (5) is a Brockett DBF, see discussion in End Matter. Let us discuss the physical meaning of this ITE state. First, the expected energy of $\Psi(\tau)$ will keep decreasing until it reaches some fixed point Ψ_∞. Clearly, the condition for a fixed point is $[\Psi_\infty, \hat{H}] = 0$, i.e. both of them are diagoanalizable in the energy basis. Thus, they can be expressed as*

$$\hat{H} = \sum_{j=1}^{d-1} \lambda_j |\lambda_j\rangle\langle\lambda_j| \quad and \quad |\Psi(\infty)\rangle = \sum_{j=0}^{d-1} c_j |\lambda_j\rangle\langle\lambda_j| . \tag{40}$$

Without loss of generality, we assume that the eigenvalues of $\hat{H}$ are ordered increasingly, i.e. $\lambda_n \leq \lambda_{n+1}$. Note that $\Psi(\tau)$ is a pure state, and any unitary conjugation preserves rank. Additionally, since Ψ_∞ is diagonalizable in the energy basis, this means that it is an energy eigenstate. This means that for values of $\tau > 0$, the ITE state converges to the ground-state $\Psi_\infty = |\lambda_0\rangle\langle\lambda_0|$. On the other hand, if $\tau < 0$, then the ITE state converges to $\Psi_\infty = |\lambda_{d-1}\rangle\langle\lambda_{d-1}|$ which is the highest energy state of $\hat{H}$.

B. Fluctuation-refrigeration relation for the ITE cooling rate

In this section, our aim is to derive a *fluctuation-refrigeration relation* for DBF, which shows that states with high energy fluctuation will converge to the ground-state more quickly by ITE procedure. We have seen that in the continuous-time DBF formalism, the average energy in the ITE state vector should decrease when τ increases as it converges to the ground-state, i.e.

$$E(\tau) := \langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle \tag{41}$$

is a decreasing function of τ. We show that the decrease rate is dictated by the energy variance $V(\tau) := \langle\Psi(\tau)|\hat{H}^2|\Psi(\tau)\rangle - E(\tau)^2$.

Proposition 5 (ITE Fluctuation-refrigeration relation)**.** *The derivative of average energy with respect to inverse temperature, $\partial_\tau E(\tau)$, is given by*

$$\partial_\tau E(\tau) = -2V(\tau) . \tag{42}$$

Proof. We may evaluate the derivative directly using Eq. (38) and the Leibniz chain rule,

$$\partial_\tau E(\tau) = \langle\Psi(\tau)|(E(\tau) - \hat{H})\hat{H}|\Psi(\tau)\rangle + \langle\Psi(\tau)|\hat{H}(E(\tau) - \hat{H})|\Psi(\tau)\rangle . \tag{43}$$

Combining the two terms give $\partial_\tau E(\tau) = -2\langle\Psi(\tau)|\hat{H}^2|\Psi(\tau)\rangle + 2E(\tau)\langle\Psi(\tau)|\hat{H}|\Psi(\tau)\rangle = -2V(\tau)$. □

Remark. *To understand the limits of the relation let us look at asymptotic upper bounds. We will find that they can be attained for 'hot' states, where energy fluctuations scale in the system size. On the other hand, for states close to eigenstates energy fluctuations vanish. For a general quantum system, the energy fluctuation is upper bounded by*

$$V(\tau) \leq \langle\Psi(\tau)|\hat{H}^2|\Psi(\tau)\rangle \leq \|\hat{H}\|^2 . \tag{44}$$

A stronger bound is obtained for local Hamiltonians, e.g. if they involve I terms $\hat{H} = \sum_{i=1}^I \hat{H}_i$ where each $\|\hat{H}_i\| \leq \mathcal{O}(1)$ has norm independent of system size. In this case, for a system containing L qubits,

$$E(\tau) \leq \mathcal{O}(L), \qquad V(\tau) \leq \mathcal{O}(L^2) . \tag{45}$$

For example for the transverse field Ising model $\hat{H}_{TFIM} = \sum_{i=1}^{L-1}(Z_i Z_{i+1} + X_i)$ we can set $\hat{H}_i = Z_i Z_{i+1} + X_i$ where Z_i and X_i act on qubit i and we have $\|\hat{H}_i\| = 2$. For $|\Psi_0\rangle = |+\rangle^{\otimes L}$ we have $E(0) = L - 1$ and $V(0) = L - 1$ because $(Z_i Z_{i+1})^2 = 1$ and contribute to the energy fluctuation.

C. Digression: Exponential convergence of thermal states to ground-states in 1-norm

We will next recall a result by Hastings [115] who showed that thermal states of gapped Hamiltonians converge exponentially fast to the ground-state if it is unique and the density of eigenstates above the gap is polynomial. This is a digression because in our work we are dealing with pure states rather than thermal states which are generically mixed. However, the discussion is instructive because the same assumption and same mathematical idea will allow us to show an analogous result for ITE.

More specifically, in Ref. [115], Hastings identified a condition on the density of states which suffices to obtain the scaling of the inverse temperature of a thermal state such that it approximates the unique ground-state of a gapped system. More specifically,

let $\hat{H}$ be a Hamiltonian with eigenvalues $\{\lambda_j\}$ and we have labeled by $j = 0, 1, \ldots, \dim(\hat{H}) - 1$, again ordering the eigenvalues increasingly such that $\lambda_j \leq \lambda_{j+1}$. Furthermore, let us set the ground-state energy as $\lambda_0 = 0$. We can define a simple counting function that captures the density of energy eigenstates. In particular, given the spectral gap $\Delta = \lambda_1 - \lambda_0$, let us define a series of intervals $\mathcal{M}_m := [m\Delta, (m+1)\Delta)$. The function $\rho_m(\hat{H}) = \big|\{\lambda_j \in \mathcal{M}_m\}\big|$, for $m = 0, 1, 2, \ldots$ therefore counts the number of eigenvalues in each interval $\mathcal{M}_m$. With this definition, Hastings' polynomial density of states condition is expressed as

$$\rho_m(\hat{H}) \leq (c_H L)^m / m! \tag{46}$$

for $c_H = O(1)$, L being the number of qubits. In other words, we assume that the distribution of eigenenergies is sparse near the ground-state for any gapped Hamiltonian. This allows to bound for any inverse temperature β the partition function

$$Z_\beta = \sum_{j=0}^{\dim(\hat{H})-1} e^{-\beta\lambda_j} \leq e^{-\beta\lambda_0}\left[\sum_{m=0}^{\infty} \rho_m(\hat{H})e^{-\beta\Delta m}\right] \leq e^{-\beta\lambda_0}\sum_{m=0}^{\infty} \frac{(e^{-\beta\Delta}c_H L)^m}{m!} \tag{47}$$

$$= e^{-\beta\lambda_0}\exp(e^{-\beta\Delta E}c_H L) \tag{48}$$

where in the first inequality, we use the fact that for all $\lambda_j \in \mathcal{M}_m$, we have that $\lambda_j \geq m\Delta$ and therefore $e^{-\beta E} \leq e^{-\beta\Delta m}$. To illustrate this further, if $\rho_0 = |\lambda_0\rangle\langle\lambda_0|$ is the ground-state projector and $\rho^{(\beta)} = \exp(-\beta\hat{H})/Z_\beta$ is the thermal state (as opposed to ITE state it is generically mixed and not pure), then

$$\|\rho^{(\beta)} - \rho_0\| \leq 2\sum_{m=1}^{\infty} \rho_m(\hat{H})e^{-\beta\Delta E m} \leq 2\left[\exp(e^{-\beta\Delta E}c_H L) - 1\right]. \tag{49}$$

Thus, if we set

$$\beta_H = \frac{1}{\Delta}\left[\log\left(\frac{c_H L}{\log(1 + \varepsilon/2)}\right)\right], \tag{50}$$

then $\|\rho^{(\beta_H)} - \rho_0\| \leq \varepsilon$. To understand this more intuitively we use $\log(1 + \varepsilon/2) \geq \varepsilon/4$ which implies $\beta_H \leq \frac{1}{\Delta}\log(\mathcal{O}(L\epsilon^{-1}))$. This means that thermal states of gapped Hamiltonians converge to the respective ground-states in inverse temperature scaling logarithmically in the system size and the desired approximation precision.

D. Exponential convergence of fidelity to the ground-state through ITE

In the previous section, we studied the exponential convergence of thermal states to the ground-state, under Hasting's condition on the system Hamiltonian. However, the central interest of this work revolves around ITE states. While such states are pure as opposed to generically mixed thermal states, both involve an imaginary-time exponential of the Hamiltonian and a normalization. This is a key feature that allows for similar fidelity convergence behavior on the ITE state, to the ground-state.

To see this explicitly, we apply a similar consideration to the ground-state fidelity of the ITE which we define as

$$F(|\Psi(\tau)\rangle, |\lambda_0\rangle) = |\langle\lambda_0|\Psi(\tau)\rangle|^2 = \frac{e^{-2\tau\lambda_0}|\langle\lambda_0|\Psi_0\rangle|^2}{\left\|e^{-\tau\hat{H}}|\Psi_0\rangle\right\|^2}, \tag{51}$$

where one should recall that $|\Psi_0\rangle$ is the initial state of ITE, see Eq. (33). A lower bound for Eq. (51) can be obtained by upper bounding the ITE normalization

$$\|e^{-\tau\hat{H}}|\Psi_0\rangle\|^2 = \langle\Psi_0|e^{-2\tau\hat{H}}|\Psi_0\rangle = \sum_{j=0}^{d} |\langle\lambda_j|\Psi_0\rangle|^2 e^{-2\tau\lambda_j} \tag{52}$$

$$= |\langle\lambda_0|\Psi_0\rangle|^2 e^{-2\tau\lambda_0} + \sum_{j=1}^{d} |\langle\lambda_j|\Psi_0\rangle|^2 e^{-2\tau\lambda_j} \tag{53}$$

$$\leq e^{-2\tau\lambda_0}\left[|\langle\lambda_0|\Psi_0\rangle|^2 + \sum_{m=1}^{\infty} e^{-2\tau m\Delta}\sum_{j:\lambda_j \in \mathcal{M}_m} |\langle\lambda_j|\Psi_0\rangle|^2\right] \tag{54}$$

$$\leq e^{-2\tau\lambda_0}\left[|\langle\lambda_0|\Psi_0\rangle|^2 + \sum_{m=1}^{\infty} \rho_m(\hat{H})e^{-2\tau m\Delta}\right] \tag{55}$$

$$\leq e^{-2\tau\lambda_0}\left(|\langle\lambda_0|\Psi_0\rangle|^2 + \exp\left(e^{-2\tau\Delta}c_H L\right) - 1\right). \tag{56}$$

In Eq. (55) we use a very loose upper bound $|\langle\lambda_j|\Psi_0\rangle\rangle| \leq 1$ to insert the density of states $\rho_m(\hat{H})$, and in the last line we invoked Hastings' condition. Finally, we proceed to upper bound $F(\Psi_0, \lambda_0)$ in Eq. (51):

$$F(|\Psi(\tau)\rangle, |\lambda_0\rangle) \geq \frac{|\langle\lambda_0|\Psi_0\rangle|^2}{|\langle\lambda_0|\Psi_0\rangle|^2 + \exp\left(e^{-2\tau\Delta}c_H L\right) - 1} \geq \frac{1}{1 + \delta_H} \geq 1 - \delta_H, \tag{57}$$

where we have set $\delta_H = \dfrac{\exp\left(e^{-2\tau\Delta}c_H L\right) - 1}{|\langle\lambda_0|\Psi_0\rangle|^2}$. Inverting this relation we find that it suffices for imaginary-time evolution to have the duration given by

$$\tau_H = \frac{1}{2\Delta} \log\left(\frac{c_H L}{\log(1 + \delta_H|\langle\lambda_0|\Psi_0\rangle|^2)}\right). \tag{58}$$

In Eq. (57) we defined $\delta_H > 0$ as the desired ground-state infidelity for ITE initialized with a non-zero ground-state overlap $F(|\Psi_0\rangle, |\lambda_0\rangle) = |\langle\lambda_0|\Psi_0\rangle|^2 \neq 0$. If $\hat{H}$ has a unique gapped ground-state and it satisfies Hastings' density of states condition in Eq. (46), then the scaling

$$\tau_H = \log(O(L\delta_H^{-1}|\langle\lambda_0|\Psi_0\rangle|^{-2})) \tag{59}$$

in Eq. (58) suffices for ITE to achieve the desired high fidelity.

III.   Double-bracket iteration (DBI) approach to QITE

In the previous section, we established that QITE is a DBF. Importantly, we were able to show two key performance indicators of QITE: the cooling rate as a function of energy variance, and the fact that under Hastings' assumption, one may obtain an exponential convergence for the fidelity of the QITE state to target ground-state. Nevertheless, for both numerical and compilation purposes, it will be necessary to demonstrate these properties for *discretizations* of the DBF method. We begin by a considering the discretization which we referred to as *double-bracket iteration* (DBI) though previous works used the name Lie bracket recursions [76].

For the computational purposes of this appendix, we introduce the following notation: denote $|\sigma_0\rangle$ as the initial state fed into a discretized DBI computation, and $\{|\sigma_k\rangle\}_k$ as the sequence of states that solve the QITE DBI, which takes on a recursive form:

$$|\sigma_{k+1}\rangle = e^{s_k[\sigma_k, \hat{H}]}|\sigma_k\rangle. \tag{60}$$

In the above, we have denoted the time step size in the $(k + 1)$-th DBI iteration as s_k. Furthermore, to simplify the notation we use the density matrix representation $\sigma_k = |\sigma_k\rangle\langle\sigma_k|$. The quantities of interest, as in Section II B, are given by the average and variance of energy after k-th DBI iteration:

$$\overline{E}_k = \langle\sigma_k|\hat{H}|\sigma_k\rangle, \quad \text{and} \quad \overline{V}_k = \langle\sigma_k|\hat{H}^2|\sigma_k\rangle - \langle\sigma_k|\hat{H}^2|\sigma_k\rangle^2. \tag{61}$$

A.   Useful lemmas for proving fluctuation-refrigeration relation and fidelity convergence of QITE DBI

1. We will use the following lemma in Sec. III B.

Lemma 6. *Let $\hat{W} = -\hat{W}^\dagger$ and $\hat{H} = \hat{H}^\dagger$. Then*

$$\partial_s^n \left(e^{-s\hat{W}} \hat{H} e^{s\hat{W}} \right) = e^{s\hat{W}}[(\hat{W})^n, \hat{H}]e^{-s\hat{W}} \,, \tag{62}$$

where $n \in \mathbb{N}$ indicates the order of the derivative and we define the notation for nested commutators

$$[(X)^n, Y] = \left[X, [(X)^{n-1}, Y] \right] \quad with \quad [(X)^0, Y] = Y \,, \tag{63}$$

Proof. We prove it by mathematical induction. For the base case $n = 1$, we have

$$\partial_s \left(e^{s\hat{W}} \hat{H} e^{-s\hat{W}} \right) = e^{s\hat{W}} \hat{W} \hat{H} e^{-s\hat{W}} - e^{s\hat{W}} \hat{H} \hat{W} e^{-s\hat{W}} = e^{s\hat{W}}[\hat{W}, \hat{H}]e^{-s\hat{W}} \tag{64}$$

Next, we assume that for some integer $n \geq 1$:

$$\partial_s^n \left(e^{s\hat{W}} \hat{H} e^{-s\hat{W}} \right) = e^{s\hat{W}}[(\hat{W})^n, \hat{H}]e^{-s\hat{W}} \tag{65}$$

The $(n+1)$-th derivative is then given by

$$\partial_s^{n+1} \left(e^{s\hat{W}} \hat{H} e^{-s\hat{W}} \right) = \partial_s \left(e^{s\hat{W}}[(\hat{W})^n, \hat{H}]e^{-s\hat{W}} \right) \tag{66}$$

$$= e^{s\hat{W}} \hat{W}[(\hat{W})^n, \hat{H}]e^{-s\hat{W}} - e^{s\hat{W}}[(\hat{W})^n, \hat{H}]\hat{W} e^{-s\hat{W}} \tag{67}$$

$$= e^{s\hat{W}}[\hat{W}, [(\hat{W})^n, \hat{H}]]e^{-s\hat{W}}. \tag{68}$$

Using the definition of the nested commutator, we have $[\hat{W}, [(\hat{W})^n, \hat{H}]] = [(\hat{W})^{n+1}, \hat{H}]$, and thus we obtain

$$\partial_s^{n+1} \left(e^{s\hat{W}} \hat{H} e^{-s\hat{W}} \right) = e^{s\hat{W}}[(\hat{W})^{n+1}, \hat{H}]e^{-s\hat{W}}. \tag{69}$$

By induction, the formula holds for all $n \geq 1$. $\qquad\square$

2. Let us consider the state $|\psi\rangle = \hat{H}|\phi\rangle/\|\hat{H}|\phi\rangle\|$. We will use it as follows.

   Lemma 7 (Second moment bound). *Let $\hat{A} = \hat{A}^\dagger$, then we have $\langle\phi|\hat{H}\hat{A}\hat{H}|\phi\rangle \leq \langle\phi|\hat{H}^2|\phi\rangle\|\hat{A}\|$.*

   Proof. By definition

   $$\langle\phi|\hat{H}\hat{A}\hat{H}|\phi\rangle = \langle\phi|\hat{H}^2|\phi\rangle\langle\psi|\hat{A}|\psi\rangle \tag{70}$$

   and we use the variational definition of the operator norm. $\qquad\square$

3. Usually, operator norms should be used to bound the proximity of unitaries. However, while in general $\|[\hat{H}, \Omega]\| \leq 2\|\hat{H}\|\,\|\Omega\|$ is the standard bound, we can get a much stronger bound as follows.

   Lemma 8 (Bracket perturbation). *Let $\hat{H} = \hat{H}^\dagger$ and $\Omega = |\Omega\rangle\langle\Omega|$ then $\|1 - e^{[\hat{H},\Omega]}\| \leq 2\sqrt{V(\Omega)}$.*

   Proof. Following Bhatia [116] or using Eq. (115) of Ref. [30] one can prove

   $$\|1 - e^{[\hat{H},\Omega]}\| \leq \|[\hat{H}, \Omega]\| \,, \tag{71}$$

   which holds for any unitarily invariant norm, in particular the operator norm. By using $\|[\hat{H}, \Omega]\| \leq \|[\hat{H}, \Omega]\|_{\mathrm{HS}}$ and Lemma 9 we obtain the result. $\qquad\square$

   Note, that normally upper bounding the operator norm by the Hilbert-Schmidt norm gives exponentially loose bounds. This is not the case here.

4. For QITE, we are often interested in the commutator of the state and the system Hamiltonian. In the case of pure states, we may show that its Hilbert Schmidt norm is related to thermodynamic properties of the state, in particular energy variance.

Lemma 9 (Bracket-variance duality). *For any Hamiltonian $\hat{H} = \hat{H}^\dagger$ and pure state $\Omega = |\Omega\rangle\langle\Omega|$,*

$$\left\|[\hat{H}, \Omega]\right\|_{\mathrm{HS}}^2 = 2V(\Omega) = 2\langle\Omega|\hat{H}^2|\Omega\rangle - 2\Omega|\hat{H}|\Omega\rangle^2 . \tag{72}$$

Proof. Using the definition of Hilbert-Schmidt norm, we have

$$\left\|[\hat{H}, \Omega]\right\|_{\mathrm{HS}}^2 = -\mathrm{Tr}\Big((\hat{H}\Omega - \Omega\hat{H})(\hat{H}\Omega - \Omega\hat{H})\Big) = -\mathrm{Tr}(\hat{H}\Omega\hat{H}\Omega - \Omega\hat{H}^2\Omega - \hat{H}\Omega\hat{H} + \Omega\hat{H}\Omega\hat{H}) . \tag{73}$$

We evaluate the trace in a basis that includes $|\Omega\rangle$ and obtain the result by collecting repeated terms. $\square$

5. The error term in the linear approximation of the QITE DBI is bounded above by the product of the step size and the energy fluctuations raised to the second power.

Lemma 10. *Let $\hat{H}$ be a Hamiltonian and a density matrix Ω corresponding to a pure state. For any real parameter $r \in \mathbb{R}$ the error associated with the linear approximation of the QITE DBR*

$$\mathcal{R}_r := e^{-r[\hat{H}, \Omega]} - \mathbb{1} + r[\hat{H}, \Omega] \tag{74}$$

satisfies $\|\mathcal{R}_r\|_{\mathrm{HS}} \leq r^2 \overline{V}_k$.
Proof. Using Taylor's theorem we have

$$\mathcal{R}_r = \mathcal{R}_0 + \int_0^r dx \, \partial_x \mathcal{R}_x = \int_0^r dx \, [\hat{H}, \Omega]\left(1 - e^{-x[\hat{H}, \Omega]}\right) , \tag{75}$$

where we use the fact that $\mathcal{R}_0 = 0$. Taking the Hilbert-Schmidt norm for the last expression becomes

$$\|\mathcal{R}_r\|_{\mathrm{HS}} = \left\|\int_0^r dx \, [\hat{H}, \Omega]\left(1 - e^{-x[\hat{H}, \Omega]}\right)\right\|_{\mathrm{HS}} \leq \left\|[\hat{H}, \Omega]\right\|_{\mathrm{HS}} \times \left\|\int_0^r dx \, 1 - e^{-x[\hat{H}, \Omega]}\right\|_{\mathrm{HS}} . \tag{76}$$

Set $[H, \Omega] \to x[H, \Omega]$ in Lemma. 8, we have

$$\left\|1 - e^{-x[H, \Omega]}\right\|_{\mathrm{HS}} \leq x \|[H, \Omega]\|_{\mathrm{HS}} . \tag{77}$$

Thus, it simplifies to

$$\|\mathcal{R}_r\|_{\mathrm{HS}} \leq \left\|[H, \Omega]\right\|_{\mathrm{HS}}^2 \times \left\|\int_0^r dx \, x\right\|_{\mathrm{HS}} = \frac{r^2}{2}\left\|[H, \Omega]\right\|_{\mathrm{HS}}^2 . \tag{78}$$

Using Lemma. 9, we then obtain $\|\mathcal{R}_r\|_{\mathrm{HS}} \leq r^2 \overline{V}_k$. $\square$

B. Proof of fluctuation-refrigeration relation for QITE DBI and its cooling rate

In this section, we derive the cooling rate of QITE state by using DBI implementation.

Proposition 11 (QITE-DBI Fluctuation-refrigeration relation). *Let $\{|\sigma_k\rangle\}_k$ be a sequence of states that solve the QITE-DBI relation in Eq. (12). The first-order cooling rate of QITE DBI equals that of QITE*

$$\overline{E}_{k+1} - \overline{E}_k \leq -2s_k\overline{V}_k + \mathcal{O}(s_k^2) . \tag{79}$$

If each time step is chosen such that $s_k \leq \dfrac{\overline{V}_k}{4\|\hat{H}\|\langle\sigma_k|\hat{H}^2|\sigma_k\rangle}$, then the DBI cooling rate is lower bounded as

$$\overline{E}_{k+1} - \overline{E}_k \leq -s_k\overline{V}_k , \tag{80}$$

where the average energies $\overline{E}_k$ and variances $\overline{V}_k$ are defined in Eq. (61).

Proof. Let us begin by defining the average energy of the k-th DBI state as a function of the time step s,

$$\overline{E}_k(s) = \langle\sigma_k|e^{-s[\sigma_k, \hat{H}]}\hat{H}e^{s[\sigma_k, \hat{H}]}|\sigma_k\rangle . \tag{81}$$

Note that the derivative of $\overline{E}_k(s)$ when evaluated at $s = 0$ gives $\partial_s \overline{E}_k(0) = -2\overline{V}_k$, exactly as in Proposition. 5. The difference in factor 2 here is that we need to provide a lower bound to the cooling rate for a finite double-bracket rotation duration $s \neq 0$.

By using a Taylor expansion on Eq. (81), we find

$$\overline{E}_k(s_k) = \overline{E}_k + s_k \partial_s \overline{E}_k(s)_{|s=0} + \frac{1}{2} s_k^2 \partial_s^2 \overline{E}_k(s)_{|s=\xi_k} , \tag{82}$$

where $\xi_k \in [0, s_k]$ is the point of the Lagrange remainder (point 6, Sec. I). Next, recall that $\overline{E}_k(s_k)$ is simply equal to $\overline{E}_{k+1}$ by definition, hence

$$\overline{E}_{k+1} - \overline{E}_k = s_k \partial_s \overline{E}_k(s)_{|s=0} + \frac{1}{2} s_k^2 \partial_s^2 \overline{E}_k(s)_{|s=\xi_k} . \tag{83}$$

To simplify the notation, it is convenient to use the following shorthands

$$\hat{W}_k = [\sigma_k, \hat{H}], \qquad \hat{H}_k(s) = e^{-s\hat{W}_k} \hat{H} e^{s\hat{W}_k} . \tag{84}$$

Note that $e^{-s\hat{W}_k}$ is unitary, and hence $\|\hat{H}_k(s)\| = \|\hat{H}\|$. The 1st order derivative of average energy is then given by $\partial_s \overline{E}_k(s) = \langle \sigma_k | [\hat{H}_k(s), \hat{W}_k] | \sigma_k \rangle$. Expanding this yields for $s = 0$

$$\partial_s \overline{E}_k(s)\big|_{s=0} = \langle \sigma_k | (\hat{H}\sigma_k\hat{H} - \hat{H}^2\sigma_k - \sigma_k\hat{H}^2 + \hat{H}\sigma_k\hat{H}) | \sigma_k \rangle \tag{85}$$

$$= -2\langle \sigma_k | \hat{H}^2 | \sigma_k \rangle + 2\overline{E}_k^2 = -2\overline{V}_k \leq 0 . \tag{86}$$

For the 2nd order derivative, we use a double-nested commutator Eq. (62) and by explicit computation

$$\partial_s^2 \overline{E}_k(s) = \langle \sigma_k | [[\hat{H}_k(s), \hat{W}_k], \hat{W}_k] | \sigma_k \rangle \tag{87}$$

$$= \langle \sigma_k | \hat{H}_k(s) \hat{W}_k^2 | \sigma_k \rangle + \langle \sigma_k | \hat{W}_k^2 \hat{H}_k(s) | \sigma_k \rangle - 2\langle \sigma_k | \hat{W}_k \hat{H}_k(s) \hat{W}_k | \sigma_k \rangle , \tag{88}$$

where we commuted $\hat{W}_k$'s with its exponentials. Next, we will use

$$\hat{W}_k^2 | \sigma_k \rangle = (\sigma_k \hat{H} \sigma_k \hat{H} - \sigma_k \hat{H}^2) | \sigma_k \rangle \tag{89}$$

to expand the DBI brackets. This gives us

$$\partial_s^2 \overline{E}_k(s) = \langle \sigma_k | \hat{H}_k(s) \sigma_k \hat{H} \sigma_k \hat{H} | \sigma_k \rangle - \langle \sigma_k | \hat{H}_k(s) \sigma_k \hat{H}^2 | \sigma_k \rangle + \langle \sigma_k | \hat{H} \sigma_k \hat{H} \sigma_k \hat{H}_k(s) | \sigma_k \rangle - \langle \sigma_k | \hat{H}^2 \sigma_k \hat{H}_k(s) | \sigma_k \rangle$$
$$- 2\langle \sigma_k | \hat{H} \hat{H}_k(s) \sigma_k \hat{H} | \sigma_k \rangle + 2\langle \sigma_k | \hat{H} \hat{H}_k(s) \hat{H} | \sigma_k \rangle + 2\langle \sigma_k | \hat{H} \sigma_k \hat{H}_k(s) \sigma_k \hat{H} | \sigma_k \rangle - 2\langle \sigma_k | \hat{H} \sigma_k \hat{H}_k(s) \hat{H} | \sigma_k \rangle \tag{90}$$

$$= -2\overline{V}_k \overline{E}_k(s) + 2\langle \sigma_k | \hat{H} \hat{H}_k(s) \hat{H} | \sigma_k \rangle + 2\overline{E}_k^2 \overline{E}_k(s) - 4\overline{E}_k \mathrm{Re}(\langle \sigma_k | \hat{H} \hat{H}_k(s) | \sigma_k \rangle) . \tag{91}$$

The first term is negative so reduces the energy of the state (to 2nd order). The second term can be bound using Lemma 7 as

$$|\langle \sigma_k | \hat{H} \hat{H}_k(s) \hat{H} | \sigma_k \rangle| \leq \langle \sigma_k | \hat{H}^2 | \sigma_k \rangle \|\hat{H}_k(s)\| \leq \langle \sigma_k | \hat{H}^2 | \sigma_k \rangle \|\hat{H}\| . \tag{92}$$

To bound the last term in Eq. (91), we have

$$|\mathrm{Re}(\langle \sigma_k | \hat{H} \hat{H}_k(s) | \sigma_k \rangle)| \leq |\langle \hat{H} | \sigma_k \rangle, \hat{H}_k(s) | \sigma_k \rangle\rangle| \leq \sqrt{\langle \sigma_k | \hat{H}^2 | \sigma_k \rangle} \sqrt{\langle \sigma_k | \hat{H}_k(s)^2 | \sigma_k \rangle} \tag{93}$$

$$\leq \sqrt{\langle \sigma_k | \hat{H}^2 | \sigma_k \rangle} \|\hat{H}\| , \tag{94}$$

where we used Cauchy-Schwarz in the second inequality. Therefore, we have

$$\partial_s^2 \overline{E}_k(s) \leq -2\overline{V}_k \overline{E}_k(s) + 2\overline{E}_k^2 \|\hat{H}\| + 4\overline{E}_k \sqrt{\langle \sigma_k | \hat{H}^2 | \sigma_k \rangle} \|\hat{H}\| + 2\langle \sigma_k | \hat{H}^2 | \sigma_k \rangle \|\hat{H}\| \leq 8\langle \sigma_k | \hat{H}^2 | \sigma_k \rangle \|\hat{H}\|. \tag{95}$$

As a remark, from the end of Eq. (95) we can obtain a weaker bound by using the sub-multiplicativity of the operator norm, i.e. we have $\partial_s^2 \overline{E}_k(s) \leq 8\|\hat{H}\|^3$. Finally, we have

$$\overline{E}_{k+1} - \overline{E}_k \leq -2s_k \overline{V}_k + 4s_k^2 \langle \sigma_k | \hat{H}^2 | \sigma_k \rangle \|\hat{H}\| , \tag{96}$$

so as we place the constraint that $-s_k \overline{V}_k + 4s_k^2 \langle \sigma_k | \hat{H}^2 | \sigma_k \rangle \|\hat{H}\| \leq 0$, this leads to $\overline{E}_{k+1} - \overline{E}_k \leq -s_k \overline{V}_k$. Evaluating the constraint as an upper bound on s_k, we obtain $s_k \leq \dfrac{\overline{V}_k}{4\|\hat{H}\| \langle \sigma_k | \hat{H}^2 | \sigma_k \rangle}$. $\qquad\square$

Remark. *Scrutinizing Eq. (91) around $s = 0$ allows us to further see the significance of higher moments of energy distribution, for the purposes of QITE. In particular, using Eq. (91), we have*

$$\partial_s^2 \overline{E}_k(s)\big|_{s=0} = -2\overline{V}_k \overline{E}_k + 2\langle\sigma_k|\hat{H}^3|\sigma_k\rangle + 2\overline{E}_k^2 \overline{E}_k - 4\overline{E}_k \langle\sigma_k|\hat{H}^2|\sigma_k\rangle \tag{97}$$

$$= 2\left(\langle\sigma_k|\hat{H}^3|\sigma_k\rangle - \overline{V}_k \overline{E}_k + \overline{E}_k^3 - 2\overline{E}_k(\overline{V}_k + \overline{E}_k^2)\right) \tag{98}$$

$$= 2\left(\langle\sigma_k|\,\hat{H}^3|\sigma_k\rangle - 3\overline{E}_k \overline{V}_k - \overline{E}_k^3\right) = 2\langle\sigma_k|(\hat{H} - \overline{E}_k)^3|\sigma_k\rangle, \tag{99}$$

because one can verify that

$$\langle\sigma_k|(\hat{H} - \overline{E}_k)^3|\sigma_k\rangle = \langle\sigma_k|\hat{H}^3|\sigma_k\rangle - 3\langle\sigma_k|\hat{H}^2 \overline{E}_k|\sigma_k\rangle + 3\langle\sigma_k|\hat{H}\overline{E}_k^2|\sigma_k\rangle - \langle\sigma_k|\overline{E}_k|\sigma_k\rangle^3 \tag{100}$$

$$= \langle\sigma_k|\,\hat{H}^3|\sigma_k\rangle - 3\overline{E}_k \overline{V}_k - \overline{E}_k^3. \tag{101}$$

Combining Eq. (86) and Eq. (99), the Taylor expansion of the expected energy is given by

$$\overline{E}_k(s) = \overline{E}_k - 2s\langle\sigma_k|(\hat{H} - \overline{E}_k)^2|\sigma_k\rangle + s^2\langle\sigma_k|(\hat{H} - \overline{E}_k)^3|\sigma_k\rangle + \mathcal{O}(s^3). \tag{102}$$

This means that whenever skewness is negative, then one can analytically justify longer double-bracket rotation durations – the second order term would then enhance cooling process for the state.

C. Exponential fidelity convergence of QITE DBI

In this section, we first establish a lemma regarding the Hilbert-Schmidt norm of the commutator between the Hamiltonian H and the DBI state σ_k.

Theorem 12 (Exponential fidelity convergence for QITE DBI). *Let $\hat{H} = \sum_{j=0}^{d-1} \lambda_j |\lambda_j\rangle\langle\lambda_j|$ be a Hamiltonian where $d = dim(\hat{H})$, $\{|\lambda_i\rangle\}$ is the set of increasingly ordered eigenstates, and $|\lambda_0\rangle$ denotes the ground-state. Let $|\sigma_0\rangle$ be an initial state with non-zero overlap to the ground-state $F_0 = |\langle\lambda_0|\sigma_0\rangle|^2$. Consider QITE DBI with*

$$|\sigma_{k+1}\rangle = e^{s_0[|\sigma_k\rangle\langle\sigma_k|,\hat{H}]}|\sigma_k\rangle, \tag{103}$$

where $s_0 = \lambda_1 F_0 / 4\lambda_{d-1}^2$ is the same in all steps. The fidelity forth the k-th DBI step defined by $F_k = |\langle\lambda_0|\sigma_k\rangle|^2$ satisfies

$$F_k \geq 1 - q^k, \quad where \quad q = 1 - \left(\frac{1}{2}\frac{\lambda_1}{\lambda_{d-1}}F_0\right)^2 = 1 - \left(\frac{1}{2}\frac{\lambda_1}{\|\hat{H}\|}F_0\right)^2. \tag{104}$$

This implies that the runtime of QITE DBI is at least exponential in the number of recursion steps. The rate is set by a quantity related to the condition number of the Hamiltonian which also appears in classical algorithms. For a non-singular matrix A the condition number is defined as $\kappa(A) = \|A^{-1}\| \|A\|$. In our problem, we have affine invariance $\hat{H} \mapsto \hat{H} + \alpha\mathbb{I}$ which does not change the ground-state state vector $|\lambda_0\rangle$ or the dynamics of the Hamiltonian. Thus, for us more meaningful is the definition of the condition number as

$$\kappa_0(\hat{H}) = \lambda_{d-1}/\lambda_1. \tag{105}$$

In classical numerical analysis we have $\kappa(A) \geq 1$ and whenever $\kappa(A)$ is large then A is considered badly conditioned. Using this notation allows us to write

$$q = 1 - \left(\frac{1}{2}\frac{F_0}{\kappa_0(\hat{H})}\right)^2. \tag{106}$$

If $\kappa_0(\hat{H})$ is large, which for local Hamiltonians corresponds to a small spectral gap, then the QITE DBI converges more slowly.

Proof. Observe that DBIs are invariant under affine shifts of the Hamiltonian, in particular we have $[\hat{H} - \lambda_0\mathbb{I}, \sigma_k] = [\hat{H}, \sigma_k]$ which means that $\hat{H}' = \hat{H} - \lambda_0\mathbb{I}$ with vanishing ground-state energy $\hat{H}'|\lambda_0\rangle = 0$ has the same DBI unitaries. Thus, without loss of generality, we assume the ground-state to be zero, i.e. $\lambda_0 = 0$.

Next, the ground-state fidelity after each round of QITE DBI iteration is given by

$$F_{k+1} = |\langle\lambda_0|\sigma_{k+1}\rangle|^2 = \left|\langle\lambda_0|\sigma_k\rangle - s_0\langle\lambda_0|[\hat{H},\sigma_k]|\sigma_k\rangle + \langle\lambda_0|R|\sigma_k\rangle\right|^2 \tag{107}$$

$$= \left|\langle\lambda_0|\sigma_k\rangle(1 + s_0\langle\sigma_k|\hat{H}|\sigma_k\rangle) - s_0\langle\lambda_0|\hat{H}|\sigma_k\rangle + \langle\lambda_0|R|\sigma_k\rangle\right|^2 \tag{108}$$

$$= \left|\langle\lambda_0|\sigma_k\rangle(1 + s_0\overline{E}_k) + \langle\lambda_0|R|\sigma_k\rangle\right|^2, \tag{109}$$

where R denotes the error term of the linear approximation to the QITE DBI. Since we set $\lambda_0 = 0$, the term $s_0\langle\lambda_0|\hat{H}|\sigma_k\rangle$ vanishes. Furthermore, note that $|\langle\lambda_0|\sigma_k\rangle|^2 = F_k$. Hence we have

$$F_{k+1} = F_k(1 + s_0\overline{E}_k)^2 + 2(1 + s_0\overline{E}_k)\mathrm{Re}\left(\langle\lambda_0|\sigma_k\rangle\langle\sigma_k|R^\dagger|\lambda_0\rangle\right) + |\langle\lambda_0|R|\sigma_k\rangle|^2. \tag{110}$$

Next, note that $0 \leq |\langle\lambda_0|R|\sigma_k\rangle|^2 \leq \|R\|_{\mathrm{HS}} = \|R^\dagger\|_{\mathrm{HS}} \leq s_0^2 V_k$ by Lemma. 10. Thus, Eq. (110) becomes

$$F_{k+1} \geq F_k(1 + s_0\overline{E}_k)^2 - 2s_0^2\overline{V}_k\left(1 + s_0\overline{E}_k\right)\sqrt{F_k}, \tag{111}$$

where we dropped the third term in Eq. (110), and use the bound $\langle\sigma_k|R^\dagger|\lambda_0\rangle \geq -\|R^\dagger\|_{\mathrm{HS}} \geq -s_0^2\overline{V}_k$.

Using the definition of the infidelity $F_k = 1 - \epsilon_k$, we can rewrite it as

$$1 - \epsilon_{k+1} \geq (1 - \epsilon_k)(1 + s_0\overline{E}_k)^2 - 2s_0^2\overline{V}_k\left(1 + s_0\overline{E}_k\right)\sqrt{1 - \epsilon_k} \tag{112}$$

$$\epsilon_{k+1} \leq 1 - (1 - \epsilon_k)(1 + s_0\overline{E}_k)^2 + 2s_0^2\overline{V}_k\left(1 + s_0\overline{E}_k\right)\sqrt{1 - \epsilon_k} \tag{113}$$

$$\leq \epsilon_k - 2s_0\overline{E}_k(1 - \epsilon_k) - s_0^2\overline{E}_k^2(1 - \epsilon_k) + 2s_0^2 k\overline{V}_k\left(1 + s_0\overline{E}_k\right)\sqrt{1 - \epsilon_k} \tag{114}$$

$$\leq \epsilon_k - 2s_0\overline{E}_k(1 - \epsilon_k) + 2s_0^2\overline{V}_k\left(1 + s_0\overline{E}_k\right)\sqrt{1 - \epsilon_k}. \tag{115}$$

Next, note that according to the assumed form s_0 in the theorem statement, and the fact that $\overline{E}_k \leq \|H\| = \lambda_{d-1}$, we have that $s_0\overline{E}_k \leq \frac{1}{4}\frac{\lambda_1}{\lambda_{d-1}^2}F_0\lambda_{d-1} \leq 1$, so we can simplify the above bound by relaxing it further:

$$\epsilon_{k+1} \leq \epsilon_k - 2s_0\overline{E}_k(1 - \epsilon_k) + 4s_0^2\overline{V}_k\sqrt{1 - \epsilon_k} \leq \epsilon_k - 2s_0\overline{E}_kF_0 + 4s_0^2\overline{V}_k. \tag{116}$$

Our goal is to suppress the second-order term by utilizing half of the first-order infidelity reduction. To do so, the condition $4s_0^2\overline{V}_k \leq s_0\overline{E}_kF_0$ must be satisfied, which is equivalent to $s_0 \leq \overline{E}_kF_0/(4\overline{V}_k)$. Next, From Lemma. 3, we have

$$\overline{E}_k \geq \lambda_1\epsilon_k, \quad \text{and} \quad \overline{V}_k \leq \lambda_{d-1}^2\epsilon_k. \tag{117}$$

Using these two bounds, we can verify that indeed,

$$s_0 = \frac{1}{4}\frac{\lambda_1}{\lambda_d^2}F_0 \leq \frac{\overline{E}_k}{4\overline{V}_k}F_0. \tag{118}$$

Since the condition $s_0 \leq \overline{E}_kF_0/(4\overline{V}_k)$ holds, Eq. (116) can be directly upper-bounded by $\epsilon_{k+1} \leq \epsilon_k - s_0\overline{E}_kF_0$. Finally, using the definition of s_0, we have that the error reduces to

$$\epsilon_{k+1} \leq \epsilon_k - \frac{1}{4}\frac{\lambda_1^2}{\lambda_d^2}F_0^2\epsilon_k = \left(1 - \left(\frac{1}{2}\frac{\lambda_1}{\lambda_{d-1}}F_0\right)^2\right)\epsilon_k. \tag{119}$$

$$\square$$

IV. Double-Bracket Quantum Imaginary-Time Evolution (DB-QITE)

In Sec. II and Sec. III, we consider the QITE realization via the continuous DBF and discrete DBI method. Here, we aim to employ the discrete group commutator iteration (GCI) to approximate DBI. As demonstrated in Lemma. (9) from [30], we can approximate DBI steps by group-commutators with an error term of magnitude $\mathcal{O}(s_k^{3/2})$, i.e. we have

$$\left\| e^{i\sqrt{s_k}\hat{H}}e^{i\sqrt{s_k}\omega_k}e^{-i\sqrt{s_k}\hat{H}}e^{-i\sqrt{s_k}\omega_k} - e^{s_k[\omega_k,\hat{H}]} \right\| \le s_k^{3/2}\left(\|[\hat{H},[\hat{H},\omega_k]]\| + \|[\omega_k,[\omega_k,\hat{H}]]\| \right), \tag{120}$$

where $\|.\|$ represents the operator norm, and k denotes the number of iteration in both DBI and GCI. Next, observe that $e^{-i\sqrt{s_k}\omega_k}|\omega_k\rangle = e^{-i\sqrt{s_k}}|\omega_k\rangle$ which motivates the definition of the *reduced group-commutator iteration (DB-QITE)*:

$$|\omega_{k+1}\rangle = e^{i\sqrt{s_k}\hat{H}}e^{i\sqrt{s_k}\omega_k}e^{-i\sqrt{s_k}\hat{H}}|\omega_k\rangle. \tag{121}$$

This is essentially Eq. (12) in the main text, but in general one can optimize the individual step sizes s_k in each round. Lastly, we denote the expected energy and variance after the k-th round of DB-QITE as

$$E_k = \langle\omega_k|\hat{H}|\omega_k\rangle \qquad \text{and} \qquad V_k = \langle\omega_k|\hat{H}^2|\omega_k\rangle - \langle\omega_k|\hat{H}^2|\omega_k\rangle^2. \tag{122}$$

Intuitively due to Eq. (120), one expects a qualitatively similar behavior between DB-QITE and DBF/DBI. We derive quantitative bounds in the next sections, to compare their explicit differences.

Before proving the main results in this section, i.e. analytical guarantees for energy loss and fidelity improvement in DB-QITE implementation, let's first present two key lemmas that will be handy in the proof.

Lemma 13. *Suppose that the DB-QITE state $|\omega_k\rangle$ is a pure state, then we have the following equivalent representation for the next DB-QITE state $|\omega_{k+1}\rangle$:*

$$|\omega_{k+1}\rangle = e^{i\sqrt{s_k}\hat{H}}e^{i\sqrt{s_k}\omega_k}e^{-i\sqrt{s_k}\hat{H}}|\omega_k\rangle \iff |\omega_{k+1}\rangle = \left(1 - (1-e^{i\sqrt{s_k}})\phi(-\sqrt{s_k})e^{i\sqrt{s_k}\hat{H}}\right)|\omega_k\rangle, \tag{123}$$

where we define the characteristic function as

$$\phi(t) := \langle\omega_k|e^{it\hat{H}}|\omega_k\rangle. \tag{124}$$

Proof. Since we consider a pure state $\omega_k = |\omega_k\rangle\langle\omega_k|$, we obtain the following identity

$$e^{i\sqrt{s_k}\omega_k} = \mathbb{1} - (1-e^{i\sqrt{s_k}})\omega_k. \tag{125}$$

Therefore, the DB-QITE recursion can be simplified to

$$|\omega_{k+1}\rangle = e^{i\sqrt{s_k}\hat{H}}\left(\mathbb{1} - (1-e^{i\sqrt{s_k}})\omega_k\right)e^{-i\sqrt{s_k}\hat{H}}|\omega_k\rangle \tag{126}$$

$$= |\omega_k\rangle - (1-e^{i\sqrt{s_k}})e^{i\sqrt{s_k}\hat{H}}|\omega_k\rangle\langle\omega_k|e^{-i\sqrt{s_k}\hat{H}}|\omega_k\rangle \tag{127}$$

$$= \left(1 - (1-e^{i\sqrt{s_k}})\phi(-\sqrt{s_k})e^{i\sqrt{s_k}\hat{H}}\right)|\omega_k\rangle, \tag{128}$$

where we use the density matrix representation in the second line and the definition of the characteristic function in the last line. $\square$

Lemma 14. *Denote the characteristic function as $\phi(t) := \langle\omega_k|e^{it\hat{H}}|\omega_k\rangle$. Then the n-th power of $\phi(t)$ can be upper-bounded by*

$$|\phi^{(n)}(\xi)| \le \|\hat{H}^n\|, \tag{129}$$

where $\xi \in [0,t]$. Moreover, suppose one knows the ground-state infidelity $\epsilon_k = 1 - F_k$ at k-th QITA DBQA iteration, then we can obtain a tighter bound for $|\phi^{(n)}(\xi)|$, i.e.

$$|\phi^{(n)}(\xi)| \le \epsilon_k\|\hat{H}^n\|. \tag{130}$$

Proof. Directly evaluating the n-th order derivative of $\phi(t)$ gives

$$\phi^{(n)}(\xi) = i^n \langle \omega_k | e^{i\xi\hat{H}} \hat{H}^n | \omega_k \rangle \,. \tag{131}$$

As the operator norm is equal to the largest eigenvalue, we obtain the bound

$$|\phi^{(n)}(\xi)| = |\langle \omega_k | e^{i\xi\hat{H}} \hat{H}^n | \omega_k \rangle| \le \|e^{i\xi\hat{H}} \hat{H}^n\| = \|\hat{H}^n\| \,, \tag{132}$$

where we use the unitary invariant property of the operator norm in the last equality and neglect the factor i^n as it is of norm 1. Thus, the first part of this lemma has been proven.

Next, to prove the second part, we denote $\Pi_0, \Pi_\perp$ as the ground-state projector and its complement (i.e. $\Pi_0 + \Pi_\perp = \mathbb{1}$), then $F_k = \langle \omega_k | \Pi_0 | \omega_k \rangle$ and $\epsilon_k = \langle \omega_k | \Pi_\perp | \omega_k \rangle$. Therefore, we obtain

$$|\phi^{(n)}(\xi)| = |\langle \omega_k | e^{i\xi\hat{H}} \hat{H}^n | \omega_k \rangle| \le |\langle \omega_k | \Pi_0 e^{-i\xi\hat{H}} H^n | \omega_k \rangle + \langle \omega_k | \Pi_\perp e^{-i\xi\hat{H}} H^n | \omega_k \rangle| \tag{133}$$

$$= |\langle \omega_k | \Pi_\perp e^{-i\xi\hat{H}} H^n | \omega_k \rangle| \le \epsilon_k \|\hat{H}^n\| \,, \tag{134}$$

where in the last inequality, one may expand the projector and use the fact that $\hat{H}^n e^{-\xi\hat{H}} |\lambda_j\rangle = \lambda_j^n e^{-i\xi\lambda_j} |\lambda_j\rangle \ge \lambda_{d-1} e^{-i\xi\lambda_j}$ (recall that λ_{d-1} is the largest energy eigenvalue). $\qquad\square$

A. Fluctuation-refrigeration relation of DB-QITE

Theorem 15. *DB-QITE satisfies the fluctuation-refrigeration up to correction terms,*

$$E_{k+1} \le E_k - 2s_k V_k + \mathcal{O}(s_k^2) \,. \tag{135}$$

In particular, if the step sizes are chosen such that $s_k \le 4V_k \cdot \left[5\epsilon_k \|\hat{H}\|^4\right]^{-1}$, then $E_{k+1} \le E_k - s_k V_k$.

Proof. We start from RHS of Eq. (123), i.e.

$$|\omega_{k+1}\rangle = \left(1 - (1 - e^{i\sqrt{s_k}})\phi(-\sqrt{s_k})e^{i\sqrt{s_k}\hat{H}}\right)|\omega_k\rangle \,, \tag{136}$$

where we employ the same notation for the characteristic function defined in Eq. (124), i.e.

$$\phi(t) := \langle \omega_k | e^{it\hat{H}} | \omega_k \rangle \,. \tag{137}$$

To simplify calculational notation, we drop the square root and index from step sizes, i.e. $\sqrt{s_k} \to t$ for the moment. Moreover, we define $c = (1 - e^{-it})\phi(-t)$ and hence we have

$$|\omega_{k+1}\rangle = (1 - ce^{it\hat{H}})|\omega_k\rangle \,. \tag{138}$$

To derive the cooling rate, we calculate

$$E_{k+1} = \langle \omega_{k+1} | \hat{H} | \omega_{k+1} \rangle = \langle \omega_k | \left[1 - c^* e^{-it\hat{H}}\right] \cdot \hat{H} \cdot \left[1 - ce^{it\hat{H}}\right] | \omega_k \rangle \tag{139}$$

$$= E_k + |c|^2 E_k - 2\text{Re}\left(\langle \omega_k | ce^{itH} \hat{H} | \omega_k \rangle\right) \,, \tag{140}$$

where we have already made use of the fact that $\hat{H}$ commutes with $e^{-it\hat{H}}$. To achieve Eq. (135), we need to derive upper bounds from Eq. (140), which we do for the individual terms:

1. The second term on the R.H.S. of Eq. (140) can be upper bounded by the fact that

$$|c|^2 = |(1 - e^{-it})\phi(-t)|^2 \le |(1 - e^{-it})|^2 \cdot |\phi(-t)|^2 \le t^2, \tag{141}$$

since $(1 - e^{-it})(1 - e^{-it}) = 2(1 - \cos(t)) \le t^2$, and $|\phi(-t)| \le \|e^{-it\hat{H}}\| \le 1$.

2. The third term in Eq. (140) can be rewritten as

$$f(t) := -2\text{Re}\left(c\langle\omega_k|e^{it\hat{H}}\hat{H}|\omega_k\rangle\right) = -2\text{Re}\left((1-e^{-it})\cdot\langle\omega_k|e^{-it\hat{H}}|\omega_k\rangle\cdot\langle\omega_k|e^{it\hat{H}}\hat{H}|\omega_k\rangle\right) \tag{142}$$

$$= -2\text{Im}\left[(1-e^{it})\phi(-t)\phi^{(1)}(t)\right], \tag{143}$$

since the first derivative of $\phi(t)$ with respect to t is given by $\phi^{(1)}(t) = i\langle\omega_k|e^{it\hat{H}}\hat{H}|\omega_k\rangle$. Our grand goal is to upper bound this term. At this point, let us note that $f(t)$ is an even function with $f(0) = 0$. We may then omit odd derivatives of it, and write the following Taylor expansion,

$$f(t) = \frac{f^{(2)}(0)}{2}t^2 + \frac{f^{(4)}(\xi)}{24}t^4. \tag{144}$$

To access the higher derivatives of $f(t)$, we start by defining

$$h(t) := \phi(-t)\phi^{(1)}(t), \tag{145}$$

and write derivatives of $f(t)$ as

$$f^{(2)}(t) = -2\text{Im}\left[e^{it}h(t) - 2ie^{it}h^{(1)}(t) + (1-e^{it})h^{(2)}(t)\right], \tag{146}$$

$$f^{(4)}(t) = -2\text{Im}\left[-e^{it}h(t) + 4ie^{it}h^{(1)}(t) + 6e^{it}h^{(2)}(t) - 4ie^{it}h^{(3)}(t) + (1-e^{it})h^{(4)}(t)\right]. \tag{147}$$

i) Evaluating $f^{(2)}(0)$ in Eq. (146)

The first term is easy; we have explicitly derived $f^{(2)}(t)$ in Eq. (146), and we need the expression for $h(t)$ as detailed in Eq. (145) and (137). In particular, one can verify that $h(0) = iE_k$ and $h^{(1)}(0) = -V_k$. Therefore, we have

$$f^{(2)}(0) = -2\text{Im}\left[h(0) - 2ih^{(1)}(0)\right] = -2E_k - 4V_k. \tag{148}$$

At this point, it is good to note that by combining Eqns. (141) and Eq. (148) into the equation for cooling, i.e. Eq. (140),

$$E_{k+1} \le E_k - 2V_kt^2 + \frac{f^{(4)}(\xi)}{24}t^4 = \le E_k - V_kt^2 - V_kt^2 + \frac{f^{(4)}(\xi)}{24}t^4, \tag{149}$$

which will give us the desired fluctuation-refrigeration relation $E_{k+1} \le E_k - V_kt^2$ if we can choose t such that

$$-V_kt^2 + \frac{f^{(4)}(\xi)}{24}t^4 \le 0 \qquad \implies \qquad t^2 \le \frac{24V_k}{f^{(4)}(\xi)}. \tag{150}$$

In other words, our next step is to formulate an upper bound $f^{(4)}(\xi) \le X$, such that by choosing $t^2 \le \frac{24V_k}{X}$, we complete the proof.

ii) Upper bounding $f^{(4)}(0)$ in Eq. (147)

We proceed to carefully bound each individual term contained in $f^{(4)}(t)$, since

$$f^{(4)}(t) = -2\text{Im}\left[-e^{it}h(t) + 4ie^{it}h^{(1)}(t) + 6e^{it}h^{(2)}(t) - 4ie^{it}h^{(3)}(t) + (1-e^{it})h^{(4)}(t)\right] \tag{151}$$

$$\le 2\left[|h(t)| + 4\left|h^{(1)}(t)\right| + 6\left|h^{(2)}(t)\right| + 4\left|h^{(3)}(t)\right| + \left|(1-e^{-it})h^{(4)}\right|\right], \tag{152}$$

where note that most e^{it} terms are omitted since its norm is bounded by 1. Recall that $h(t)$ is defined in Eq. (145) in terms of derivatives of $\phi(t)$, and so $h^{(n)}(t)$ needs to be explicitly derived as functions containing derivatives of $\phi(t)$ via chain rule. To bound the term $h^{(n)}(t)$, we first recall the bound of $|\phi^{(n)}(\xi)|$ from Eq. (129) in Lemma. 14, i.e.

$$|\phi^{(n)}(\xi)| \le \|\hat{H}^n\|, \tag{153}$$

where $\xi \in [0, t]$.

Furthermore, let us assume that $\|\hat{H}\| \geq 1$ so that $\|\hat{H}^n\| \geq \|\hat{H}^{n-1}\|$. We summarize the bounds below:

$$|h(t)| \leq E_k \leq \|\hat{H}\| \leq \|\hat{H}^4\| \, , \tag{154}$$

$$|h^{(1)}(t)| \leq V_k \leq 4\|\hat{H}^2\| \leq \|\hat{H}^4\| \, , \tag{155}$$

$$|h^{(2)}(t)| \leq |\langle\omega_k|\hat{H}^3|\omega_k\rangle - E_k\langle\omega_k|\hat{H}^2|\omega_k\rangle| \leq \|\hat{H}^3\| \leq \|\hat{H}^4\| \, , \tag{156}$$

$$|h^{(3)}(t)| \leq |\langle\omega_k|H^4|\omega_k\rangle - \langle\omega_k|H^3|\omega_k\rangle E_k - 3\langle\omega_k|H^3|\omega_k\rangle E_k + 3\langle\omega_k|H^2|\omega_k\rangle^2| \leq 4\|\hat{H}^4\| \, . \tag{157}$$

The final term requires an additional assumption that $t\|\hat{H}\| \leq 1$. With this,

$$|(1 - e^{it})h^{(4)}(t)| \leq t|-3\langle\omega_k|H^4|\omega_k\rangle E_k + 2\langle\omega_k|H^3|\omega_k\rangle\langle\omega_k|H^2|\omega_k\rangle + \langle\omega_k|H^5|\omega_k\rangle|. \tag{158}$$

$$\leq t\langle\omega_k|H^5|\omega_k\rangle + 2t\max\{\langle\omega_k|H^4|\omega_k\rangle E_k, \langle\omega_k|H^3|\omega_k\rangle\langle\omega_k|H^2|\omega_k\rangle\} \tag{159}$$

$$\leq 3t\|\hat{H}^5\| \leq 3\|\hat{H}^4\|. \tag{160}$$

Putting Eqn. (154)-(160) back into Eq. (152), we obtain

$$f^{(4)}(\xi) \leq 30\epsilon_k\|\hat{H}\|^4 \, . \tag{161}$$

Plugging Eq. (161) into the choice of t as detailed after Eq. (150) concludes the proof of the theorem (recall that $t = \sqrt{s_k}$).

□

B. Exponential fidelity convergence of DB-QITE: Proof of Theorem 2

Before we begin, recall that $|\lambda_0\rangle$ denotes the ground-state. In this section, we set the reference point $\lambda_0 = 0$, i.e. the ground-state is of zero energy. Consequently, the spectral gap is given by $\Delta = \lambda_1 - \lambda_0 = \lambda_1$. With this assumption, we now present the proof of Theorem. 2 of main text.

Theorem 2. *ground-state fidelity increase guarantee. Suppose that DB-QITE is initialized with some non-zero initial ground-state overlap F_0. Let $\hat{H}$ be a Hamiltonian with a unique ground-state $|\lambda_0\rangle$, spectral gap Δ and spectral radius $\|\hat{H}\| \geq 1$. Let U_0 be an arbitrary unitary and set*

$$s = \frac{\Delta}{12\|\hat{H}\|^3} \, . \tag{162}$$

The states $|\omega_k\rangle := U_k|0\rangle$, where U_k is defined in main text, i.e.

$$U_{k+1} = e^{i\sqrt{s_k}\hat{H}}U_k e^{i\sqrt{s_k}|0\rangle\langle0|}U_k^\dagger e^{-i\sqrt{s_k}\hat{H}}U_k \ , \tag{163}$$

has the ground-state fidelity lower-bounded by

$$F_k := |\langle\lambda_0|\omega_k\rangle|^2 \geq 1 - q^k \tag{164}$$

where $q = 1 - sF_0\Delta$.

Proof. From RHS of Eq. (123), the DB-QITE recursion is given by

$$|\omega_{k+1}\rangle = \left(1 - (1 - e^{i\sqrt{s_k}})\phi(-\sqrt{s_k})e^{i\sqrt{s_k}\hat{H}}\right)|\omega_k\rangle \, , \tag{165}$$

where we use the same notation again for the characteristic function (similar to Theorem. 15), i.e.

$$\phi(t) := \langle\omega_k|e^{it\hat{H}}|\omega_k\rangle \, . \tag{166}$$

For all subsequent calculations in this proof, we define $t = \sqrt{s_k}$ to simplify the notation. Our ultimate goal is to show that the fidelity between the ground-state and the k-th DBQA state (F_k) can be lower-bounded by

$$F_k \geq 1 - q^k \, , \tag{167}$$

where q is a real parameter such that $0 < q < 1$. To do so, we define the ground-state infidelity $\epsilon_k := 1 - F_k$ and we will derive a recursive inequality relating ϵ_k and ϵ_{k+1}.

First, let us define the overlap between the ground-state and the k-th DBQA state as $\langle \lambda_0 | \omega_k \rangle$, which is related to the fidelity F_k by $F_k = |\langle \lambda_0 | \omega_k \rangle|^2$. Using Eq. (165), the overlap at $(k+1)$-th and k-th DBQA recursion is related by

$$\langle \lambda_0 | \omega_{k+1} \rangle = \langle \lambda_0 | \omega_k \rangle - (1 - e^{it})\phi(-t)\langle \lambda_0 | e^{it\hat{H}} | \omega_k \rangle \tag{168}$$

$$= \left(1 - (1 - e^{it})\phi(-t)\right) \langle \lambda_0 | \omega_k \rangle , \tag{169}$$

where we use the expression $\langle \lambda_0 | e^{it\hat{H}} = \langle \lambda_0 | e^{it\lambda_0}$ and the assumption $\lambda_0 = 0$ in the last line. Using Eq. (169), the ground-state fidelities F_{k+1} and F_k is related by

$$F_{k+1} = |\langle \lambda_0 | \omega_{k+1} \rangle|^2 = |g(t)|^2 F_k , \tag{170}$$

where we define $g(t) = 1 - (1 - e^{it})\phi(-t)$. Using the definition of the infidelities, the ground-state infidelities ϵ_k and ϵ_{k+1} is related by

$$\epsilon_{k+1} = 1 - |g(t)|^2(1 - \epsilon_k) = \epsilon_k - p(t)(1 - \epsilon_k) . \tag{171}$$

where we also define $p(t) = |g(t)|^2 - 1$ for simplicity. Now, the remaining task is to show that $p(t) \geq c\epsilon_k$ for some positive constant c. We start by applying Taylor's theorem (see Sec. I), i.e.

$$p(t) = p(0) + tp^{(1)}(0) + \frac{t^2}{2}p^{(2)}(0) + \frac{t^3}{6}p^{(3)}(0) + \frac{t^4}{24}p^{(4)}(\xi) , \tag{172}$$

where $\xi \in [0, t]$. Notice that $p(t)$ is an even function with $p(0) = 0$ as

$$p(-t) = |g(-t)|^2 - 1 = |g(t)^*|^2 - 1 = |g(t)|^2 - 1 = p(t) , \tag{173}$$

Hence, all odd order derivatives of $f(t)$ vanish, i.e. $p^{(2n+1)}(0) = 0$ for any non-negative integer n. Therefore, the Taylor series reduces to

$$p(t) = \frac{t^2}{2}p^{(2)}(0) + \frac{t^4}{24}p^{(4)}(\xi) . \tag{174}$$

1. Directly evaluating $p^{(2)}(t)$ yields

$$p^{(2)}(t) = 2\mathrm{Re}[g^*(t)g^{(2)}(t)] + 2|g^{(1)}(t)|^2 , \tag{175}$$

To determine the expression of the term $p^{(2)}(0)$, we explicitly compute the derivatives of $g(t)$ up to second order. The results are given by

$$g^{(1)}(t) = ie^{it}\phi(-t) + (1 - e^{it})\phi^{(1)}(-t) , \tag{176}$$

$$g^{(2)}(t) = -e^{it}\phi(-t) - 2ie^{it}\phi^{(1)}(-t) - (1 - e^{it})\phi^{(2)}(-t) . \tag{177}$$

Thus, we obtain

$$p^{(2)}(0) = 2\mathrm{Re}[g^*(0)g^{(2)}(0)] + 2|g^{(1)}(0)|^2 \tag{178}$$

$$= 2\mathrm{Re}[1 \cdot (-1 + 2E_k)] + 2|i|^2 \quad = 4E_k . \tag{179}$$

where we use the relation $g^{(1)}(0) = i$, $\phi(0) = 1$ and $\phi^{(1)}(0) = iE_k$.

2. Here, we will derive an lower bound for the term $p^{(4)}(\xi)$.

First, recall that $p(t) = g(t)g^*(t) - 1$ and hence its n-th order derivative is given by

$$p^{(n)}(t) = \sum_{\substack{n_a, n_b = 1, \\ n_a + n_b = n}}^{n} g^{(n_a)}(t)g^{*(n_b)}(t) , \tag{180}$$

where the constraint $n_a + n_b = n$ arises from the Leibniz rule. We can collect identical terms and rewrite it as

$$p^{(n)}(t) = \sum_{r=0}^{n} \binom{n}{r} g^{(r)}(t) g^{*(n-r)}(t) \,, \tag{181}$$

where we introduce the factor $\binom{n}{r}$ to account for combinatorial degeneracy. In particular, for $n = 4$, we have

$$p^{(4)}(t) = g(t)g^{*(4)}(t) + 4g^{(1)}(t)g^{*(3)}(t) + 6g^{(2)}(t)g^{*(2)}(t) + 4g^{(3)}(t)g^{*(1)}(t) + g^{(4)}(t)g^{*}(t) \,. \tag{182}$$

To obtain the lower bound for $p^{(4)}(\xi)$, we first derive an upper bound for $|g^{(r)}(\xi)|$ with arbitrary non-negative integer r.

(a) In this part, we will determine the upper bound for $|g(\xi)|$.
Recall that $g(t) = 1 - (1 - e^{it})\phi(-t)$ and we define $a(t) = -(1 - e^{it})$ for notational simplicity. For the factor $a(\xi)$, it gives

$$|a(\xi)| = |1 - e^{i\xi}| = \sqrt{(1 - \cos\xi)^2 + \sin^2\xi} = \sqrt{2 - 2\cos\xi} = \sqrt{4\sin^2\frac{\xi}{2}} \leq 2\left|\sin\frac{\xi}{2}\right| \leq \xi \,, \tag{183}$$

where we use the trigonometric identities $\cos\xi = 1 - 2\sin^2\frac{\xi}{2}$ in the last equality and we use the relation $|\sin\frac{\xi}{2}| \leq \frac{\xi}{2}$ in the last inequality. Thus, we have

$$|g(\xi)| \leq 1 + |a(\xi)||\phi(-\xi)| \leq 1 + \xi \leq 2 \,, \tag{184}$$

where we use the triangle inequality in the first inequality and we use the bound $|\phi(-\xi)| \leq 1$. Note that $\xi \leq t \leq 1$ by assumption.

(b) Next, we compute the upper bound for $|g^{(r)}(\xi)|$. For r-th order derivatives of $g(t)$, we have

$$|g^{(r)}(\xi)| = \left|\sum_{m=0}^{r} \binom{r}{m} a^{(m)}(\xi)\phi^{(r-m)}(-\xi)\right| \leq \sum_{m=0}^{r} \binom{r}{m} \left|a^{(m)}(\xi)\right| \left|\phi^{(r-m)}(-\xi)\right| \,, \tag{185}$$

where we use a similar procedure from Eq. (181) to deal with the combinatorial degeneracy. We then split the sum into $m = 0$ case and $m \neq 0$ cases to evaluate the upper bound, i.e. it becomes

$$|g^{(r)}(\xi)| \leq |a(\xi)||\phi^{(r)}(-\xi)| + \sum_{m=1}^{r} \binom{r}{m} |a^{(m)}(\xi)||\phi^{(r-m)}(-\xi)| \tag{186}$$

$$\leq \xi\epsilon_k\|\hat{H}\|^r + \sum_{m=1}^{r} \binom{r}{m} \epsilon_k\|\hat{H}\|^{r-m} \,. \tag{187}$$

For the first term, we use the bound $|a(\xi)| \leq \xi$ (Eq. (183)) and Eq. (130). Similarly, for the second term, we use the bound $|a^{(m)}(\xi)| \leq 1$ and Eq. (130). Furthermore, let us assume that $1 \leq \|\hat{H}\|$ which leads to $\|\hat{H}^r\| \geq \|\hat{H}^{r-1}\|$. Thus, it simplifies to

$$|g^{(r)}(\xi)| \leq \epsilon_k\|\hat{H}\|^{r-1} + \sum_{m=1}^{r} \binom{r}{m} \epsilon_k\|\hat{H}\|^{r-1} = \epsilon_k\|\hat{H}\|^{r-1}\left(1 + \sum_{m=1}^{r} \binom{r}{m}\right) \tag{188}$$

$$= 2^r \epsilon_k\|\hat{H}\|^{r-1} \,. \tag{189}$$

where we assume that $\xi\|\hat{H}\| \leq 1$ in the first inequality and we employ binomial identity in the last inequality.

Finally, observe that Eq. (182) can be upper-bounded by

$$|p^{(4)}(\xi)| \leq 2|g(\xi)| \times |g^{(4)}(\xi)| + 8|g^{(1)}(\xi)| \times |g^{(3)}(\xi)| + 6|g^{(2)}(\xi)|^2 \,, \tag{190}$$

where we use the fact that $|g^{(r)}(\xi)| = |g^{*(r)}(\xi)|$. Using Eq. (184) and Eq. (189), it becomes

$$|p^{(4)}(\xi)| \leq 64\epsilon_k\|\hat{H}\|^3 + 128\epsilon_k^2\|\hat{H}\|^2 + 96\epsilon_k^2\|\hat{H}\|^2 \tag{191}$$

$$\leq 64\epsilon_k\|\hat{H}\|^3 + 128\epsilon_k\|\hat{H}\|^3 + 96\epsilon_k\|\hat{H}\|^3 = 288\epsilon_k\|\hat{H}\|^3 \,, \tag{192}$$

where we use the bounds $\epsilon_k^2 \leq \epsilon_k$ and $\|\hat{H}\|^2 \leq \|\hat{H}\|^3$ in the last line. Finally, the lower bound for $p^{(4)}(\xi)$ is given by

$$|p^{(4)}(\xi)| \leq 288\epsilon_k\|\hat{H}\|^3 \implies p^{(4)}(\xi) \geq -288\epsilon_k\|\hat{H}\|^3 \,. \tag{193}$$

Combining Eq. (174), Eq. (179) and Eq. (193) yields

$$p(t) \geq 2t^2 E_k - 12t^4 \epsilon_k \|\hat{H}\|^3 \tag{194}$$

$$\geq 2t^2 \Delta \epsilon_k - 12t^4 \epsilon_k \|\hat{H}\|^3 , \tag{195}$$

where we use the bound $E_k \geq \lambda_1 \epsilon_k = \Delta \epsilon_k$ as shown in Lemma. 3. As stated in Theorem. 2, we set $t^2 = s = \dfrac{\Delta}{12\|\hat{H}\|^3}$ as a constant for all k-th DB-QITE recursions. Thus, $p(t)$ can be lower-bounded by

$$p(t) \geq 2\epsilon_k \left(\frac{\Delta^2}{12\|\hat{H}\|^3} - \frac{6\Delta^2}{144\|\hat{H}\|^3} \right) = \frac{\Delta^2 \epsilon_k}{12\|\hat{H}\|^3} . \tag{196}$$

Substituting it into Eq. (171) yields

$$\epsilon_{k+1} \leq \epsilon_k - (1 - \epsilon_k)\frac{\Delta^2 \epsilon_k}{12\|\hat{H}\|^3} = \left(1 - \frac{\Delta^2 F_k}{12\|\hat{H}\|^3} \right) \epsilon_k \leq \left(1 - \frac{\Delta^2 F_0}{12\|\hat{H}\|^3} \right) \epsilon_k = q\epsilon_k , \tag{197}$$

where $q = 1 - sF_0\Delta$ as mentioned in Theorem. 2. Ultimately, the ground-state fidelity is given by

$$\epsilon_k \leq q^k \epsilon_0 \implies F_k \geq 1 - q^k F_0 \geq 1 - q^k \tag{198}$$

where we used that $\epsilon_0 = 1 - F_0 \leq 1$.

$\square$

C.   Runtime consideration

We remark that Eq. (174) implies the relation $F_{k+1} = F_k + 2E_k s + \mathcal{O}(s^2)$ stated as Eq. (26) above. Next, we provide a calculation of the depth in DB-QITE in the weaker setting of choosing s via Eq. (15), so independent of encountered energy E_k or energy variance V_k.

Corollary 3. *For L qubits, DB-QITE amplifies initial fidelity F_0 to desired fidelity F_{th} in circuit depth*

$$\mathcal{O} \left(L \left(\frac{1 - F_0}{1 - F_{th}} \right)^{2/(sF_0\Delta)} \right) . \tag{199}$$

where $s = \dfrac{\Delta}{12\|\hat{H}\|^3}$ as defined in Theorem. 2.

Proof. We use Eq. (198) to find k such that

$$\epsilon_k \leq q^k \epsilon_0 \leq \epsilon_{\text{th}} := 1 - F_{\text{th}} . \tag{200}$$

By taking the logarithm on both sides we have

$$k \geq \log(\epsilon_{\text{th}}/\epsilon_0)/\log(q) . \tag{201}$$

Finally, we insert the lower bound to the query complexity estimate

$$\mathcal{O}(3^k) = \mathcal{O}\left((\epsilon_{\text{th}}/\epsilon_0)^{\log(3)/\log(q)} \right) \tag{202}$$

$$= \mathcal{O}\left((\epsilon_{\text{th}}/\epsilon_0)^{\log(3)/\log(1 - sF_0\Delta)} \right) \tag{203}$$

$$= \mathcal{O}\left((\epsilon_0/\epsilon_{\text{th}})^{\log(3)/(sF_0\Delta)} \right) , \tag{204}$$

where we use the identity $a^{\log_x(b)} = b^{\log_x(a)}$ in the first line and $\log(1 - x) \approx -x$ in the last line. We bound the depth of each subroutine query as $\mathcal{O}(L)$ (i.e. dominated by reflections [108] as opposed to Hamiltonian simulations which can be done in $\mathcal{O}(1)$ time) so the overall depth is as stated. $\square$