

Measurement-Based Deterministic Imaginary Time Evolution

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We introduce a method to perform imaginary time evolution in a controllable quantum system using measurements and conditional unitary operations. By performing a sequence of weak measurements based on the desired Hamiltonian constructed by a Suzuki-Trotter decomposition, an evolution approximating imaginary time evolution can be realized. The randomness due to measurement is corrected using conditional unitary operations, making the evolution deterministic. Both the measurements required for the algorithm and the conditional unitary operations can be constructed efficiently. We show that the algorithm converges only below a specified energy threshold and the complexity is estimated for some specific problem instances.

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Introduction.—Imaginary time evolution is an important and enduring concept in several areas of quantum physics, despite not being directly a physical process [1]. In imaginary time evolution (ITE) of a quantum system with Hamiltonian H , time t is replaced by imaginary time $t \rightarrow -i\tau$, such that the evolution operator is $e^{-H\tau}$ [2,3]. As such, for long evolution times, the state approaches the ground state of the Hamiltonian [4,5]. ITE can be directly applied as a numerical procedure on classical computers to obtain low-energy states [6–9]. It is also central in making a formal connection between a d -spatial dimensional quantum field theory and a $d + 1$ -dimensional classical statistical mechanics system, through the Wick rotation [10–12]. A variety of classical simulation methods take advantage of this connection, such as quantum Monte Carlo and its variants [13–17].

As a numerical procedure on a classical computer, ITE requires exponential resources that scale with the size of the Hilbert space. If there was a way of implementing ITE on a quantum computer efficiently, this could potentially be an extremely powerful tool. A direct implementation of the ITE operator $e^{-H\tau}$, assuming elementary ITE gates, would have a complexity that scales polynomially with the number of subsystems, e.g., qubits. In comparison to the same calculation performed on a classical computer, this

would give an exponential speedup. In ITE, convergence to a high fidelity state takes a timescale of the inverse energy gap. In a quantum simulation scenario, one is often interested in obtaining low-energy eigenstates of various systems, applicable to condensed matter physics, high-energy physics, and quantum chemistry [18–27]. More generally, it may also be used as a general optimization tool, where a cost function is minimized [28]. Applied to the context of solving the generalized Ising model, a problem that can be mapped to any optimization problem in the complexity class NP in polynomial time, the approach could be used to optimize problems in a variety of contexts such as logistics, financial applications, artificial intelligence, pharmaceutical development, and material development [28–32]. Another application of ITE is as a state preparation protocol. For applications such as quantum metrology [33–35] and alternative models of quantum computation [36–38], resource states need to be generated, which are sometimes difficult to produce. By engineering a suitable Hamiltonian where the desired state is the ground state, ITE can be used to generate and stabilize the state [39–42].

Several methods have been proposed to perform ITE in a controllable quantum system. In variational imaginary time evolution (VITE) [6], McArdle, Yuan, and co-workers introduced a hybrid quantum-classical approach to achieve

ITE. Here, the Schrödinger equation is first solved in imaginary time on a classical computer to determine the parameters of a trial state, then this is used as the approximation of the quantum state for the quantum circuit. This method has been used to simulate the spectra of a Hamiltonian [43], perform generalized time evolution [44], and to solve quantum many-body problems [45]. Motta, Chan, and co-workers proposed the quantum imaginary time evolution (QITE) method [46], where nonunitary time evolution is approximated by a unitary operator which contains the variation of the quantum systems [47–51]. This method has been applied to the study of quantum simulation [52], nuclear energy level computation [47], and quantum chemistry [48]. In another approach, Williams proposed a probabilistic approach to nonunitary quantum computing [53]. For example, in probabilistic imaginary time evolution (PITE) [54], an L qubit nonunitary gate simulation can be probabilistically obtained by designing an $L + 1$ qubit system and measuring the ancilla qubit [55]. When measuring the ancilla qubit, the L -qubit state will collapse into the desired state with a certain probability. PITE exploits Grover’s algorithm [56] to enhance the probability of getting the desired state while maintaining a high fidelity. PITE is suggested to be applicable to quantum chemistry problems [57]. The above ITE methods can be applied to various quantum algorithms. It has been shown that VITE can be applied to variational quantum algorithms for Boltzmann machine learning [58], while QITE can be applied to the quantum Lanczos algorithm [46,59] and variational quantum algorithms for Hamiltonian diagonalization [60].

In this Letter, we propose a general method of performing ITE in a controllable quantum system. Our method relies upon performing measurements that mimic the ITE operator for small times. By performing repeated measurements on the system using these measurement operators, combined with a unitary correction step that acts conditionally on the measurement outcomes, this allows for a way to drive the state towards the lowest energy state of the given Hamiltonian. Much like quantum feed forward approaches such as in quantum teleportation, this converts the stochastic evolution into a deterministic one, such that the desired state is obtained with unit probability for sufficiently long evolution times [61–63]. The basic idea of the approach is to perform a weak measurement in the energy eigenbasis of a given Hamiltonian. During the slow collapse of the state, if the energy estimate is higher than a given threshold, then a conditional unitary is applied to disturb the system. This is repeated until the energy is sufficiently low, after which full collapse to the ground state occurs. Similar approaches were used for quantum state preparation [64] using weak measurements [65,66]. Our approach differs from related works such as Refs. [54], where the desired outcome is obtained by postselection. It also differs from approaches such as in Refs. [6,46] since

the use of measurements involves an explicitly nonunitary step. As such, no precomputation needs to be performed to determine the evolution path.

Weak energy measurements.—We start by describing the general approach to performing ITE, then illustrate our approach with several examples. Our aim will be to perform ITE of an arbitrary Hamiltonian H , such that we obtain the ground state

$$e^{-H\tau}|\psi_0\rangle \xrightarrow{\tau \rightarrow \infty} |E_0\rangle, \quad (1)$$

where $|\psi_0\rangle$ is an arbitrary initial state and $|E_0\rangle$ is the ground state of H . We start by constructing measurement operators that take a similar form to the exponentiated Hamiltonian (1). This can be achieved by performing a weak measurement of the Hamiltonian, with measurement operators

$$\begin{aligned} M_0 &= \langle 0|_a e^{-i\epsilon H \otimes Y} |+\rangle_a = \frac{1}{\sqrt{2}} (\cos \epsilon H - \sin \epsilon H) \\ &= \frac{1}{\sqrt{2}} \sum_n (\cos \epsilon E_n - \sin \epsilon E_n) |E_n\rangle \langle E_n| \approx \frac{e^{-\epsilon H}}{\sqrt{2}} \end{aligned} \quad (2)$$

$$\begin{aligned} M_1 &= \langle 1|_a e^{-i\epsilon H \otimes Y} |+\rangle_a = \frac{1}{\sqrt{2}} (\cos \epsilon H + \sin \epsilon H) \\ &= \frac{1}{\sqrt{2}} \sum_n (\cos \epsilon E_n + \sin \epsilon E_n) |E_n\rangle \langle E_n| \approx \frac{e^{\epsilon H}}{\sqrt{2}}, \end{aligned} \quad (3)$$

where Pauli spin operators are denoted X, Y, Z , and the approximation is valid for $\|\epsilon H\| \ll 1$. The Hamiltonian is taken to have a suitable energy offset and ϵ is chosen such that the energy spectrum fits in the region $-\pi/4 \leq \epsilon E_n \leq \pi/4$. This measurement can be realized by preparing an ancilla qubit in the state $|+\rangle_a = (|0\rangle_a + |1\rangle_a)/\sqrt{2}$ and performing an interaction with Hamiltonian $H \otimes Y$, and measuring the ancilla in the Z basis. The measurement operators satisfy $M_0^\dagger M_0 + M_1^\dagger M_1 = I$, where I is the identity matrix. In the case that the interaction $H \otimes Y$ is not directly accessible due to the Hamiltonian being composed of a sum of terms $H = \sum_{j=1}^N H^{(j)}$, a Suzuki-Trotter decomposition [67,68] of $e^{-i\epsilon H \otimes Y}$ to suitable order is instead performed (see Supplemental Material [73]). This has the effect of changing the precise form of (3), but is still an approximation to the imaginary time exponentiated Hamiltonian.

We wish to perform the ITE to amplify the ground state as in (1). If it were possible to apply M_0 only, this would achieve a similar evolution to (1) since $\cos \epsilon E_n - \sin \epsilon E_n$ is monotonically decreases in the domain $-\pi/4 \leq \epsilon E_n \leq \pi/4$, such that $M_0^k |\psi_0\rangle \xrightarrow{k \rightarrow \infty} |E_0\rangle$. However, since the two outcomes $\{M_0, M_1\}$ occur randomly according to quantum measurement probabilities, such a sequence is typically a rare occurrence. Let us analyze a particular measurement sequence where there are k_0 counts of M_0 and k_1 counts of

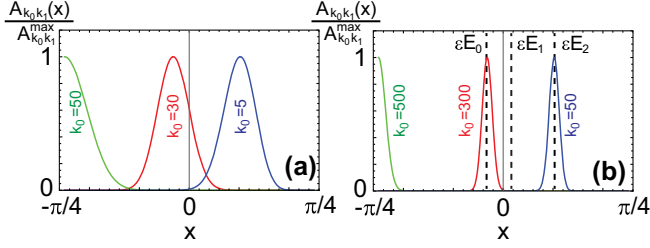


FIG. 1. The amplitude modulation function $A_{k_0 k_1}(x)$ as defined in (5). The functions (solid lines) are normalized to their peak values, defined by $A_{k_0 k_1}^{\max} = A_{k_0 k_1}(x_{k_0 k_1}^{\max})$. The total number of measurements is fixed to (a) $k_0 + k_1 = 50$ and (b) $k_0 + k_1 = 500$ and the value of k_0 is as marked. Dashed vertical lines are values of the energy eigenstates multiplied by ϵ .

M_1 . Since $[M_0, M_1] = 0$, the order of the outcomes does not matter and this measurement sequence can be written

$$M_0^{k_0} M_1^{k_1} |\psi_0\rangle = \sum_n A_{k_0 k_1}(\epsilon E_n) \langle E_n | \psi_0 \rangle |E_n\rangle \quad (4)$$

where we defined the amplitude function

$$A_{k_0 k_1}(x) = \frac{1}{\sqrt{2^{k_0 + k_1}}} (\cos x - \sin x)^{k_0} (\cos x + \sin x)^{k_1} \\ = \cos^{k_0}(x + \pi/4) \sin^{k_1}(x + \pi/4). \quad (5)$$

In Fig. 1(a) we show a plot of the function A . We see that for $-\pi/4 \leq x \leq \pi/4$ and a large number of measurements it has a Gaussian form [69], where the peak value occurs at

$$x_{k_0 k_1}^{\max} = \epsilon E_{k_0 k_1}^{\max} = \frac{1}{2} \arcsin\left(\frac{k_1 - k_0}{k_0 + k_1}\right) \quad (6)$$

and the width is $\sigma \approx 1/\sqrt{2(k_0 + k_1)}$. Here, $E_{k_0 k_1}^{\max}$ is the peak value in terms of energy. As the number of measurements are increased, the Gaussians become increasingly well defined [Fig. 1(b)]. In the limit of a large number of measurements, a collapse on the energy basis occurs.

In order to increase the amplitude of the ground state in (4), we require that the Gaussian is peaked with an outcome with $x_{k_0 k_1}^{\max} < \epsilon(E_0 + E_1)/2$ [see Fig. 1(b)]. This will create an amplitude gain of the ground state over all the remaining states, since the peak of the Gaussian is closer to ϵE_0 than any other eigenvalue, and the tail of the Gaussian on the higher energy side will suppress all higher energy states. So our strategy will then be to control the position of the Gaussian such that it lies in the desired energy range.

The algorithm.—To this end, we turn to an adaptive strategy, where a unitary operation is applied conditioned on the measurement outcomes. Our basic strategy will be to continually monitor the location of the Gaussian using the expression (6). If the location of the Gaussian corresponds to a sufficiently low energy state, then no unitary is applied.

If the Gaussian is located at a value that is of a higher energy than a chosen energy threshold E_{th} , then a corrective unitary is applied. Concretely, we iteratively perform

$$|\psi_{t+1}\rangle = \frac{U_{k_0^{(t+1)} k_1^{(t+1)}} M_n |\psi_t\rangle}{\sqrt{\langle \psi_t | M_n^\dagger M_n | \psi_t \rangle}} \quad (7)$$

where $n \in \{0, 1\}$ labels the $(t+1)$ th measurement outcome, with

$$U_{k_0 k_1} = \begin{cases} I & \text{if } x_{k_0 k_1}^{\max} < \epsilon E_{\text{th}} \\ U_C & \text{otherwise} \end{cases}, \quad (8)$$

and

$$k_m^{(t+1)} = \begin{cases} k_m^{(t)} + \delta_{mn} & \text{if } x_{(k_0^{(t)} + \delta_{0n})(k_1^{(t)} + \delta_{1n})}^{\max} < \epsilon E_{\text{th}} \\ 0 & \text{otherwise} \end{cases} \quad (9)$$

are the cumulative measurement outcomes starting with $k_m^{(0)} = 0$. In words, this counts the number of M_0 , M_1 measurements, respectively, until it is found that the energy estimate is above the threshold, at which point the counts are reset to zero. To ensure convergence of the sequence to the ground state, we demand a nonzero transition amplitude between all energy eigenstates $|\langle E_n | U_C | E_m \rangle| > 0$, $\forall n, m$. For $E_0 < E_{\text{th}} < E_1$, this ensures that only the ground state is the unique fixed point of the evolution (see Supplemental Material [73]). The requirement $|\langle E_n | U_C | E_m \rangle| > 0$ is not usually very difficult to satisfy since it merely requires off-diagonal matrix elements in the energy basis, which occurs for a large number of matrices. Practically, one may choose a random unitary matrix based on readily available gates. In this way, the wave function for the ground state does not need to be known for the procedure. We note that if there is some knowledge of the eigenstates $|E_n\rangle$, then more sophisticated strategies beyond the above requirement and (8) can be used to construct U_C . For instance, rotations targeting the ground state based on the energy estimate $E_{k_0 k_1}^{\max}$ could be implemented.

Example 1: One qubit.—We start with the simplest example of a single qubit with Hamiltonian $H = Z$. In Figs. 2(a) and 2(b) we show the evolution of the states on the Bloch sphere for the measurements M_0, M_1 . We see that M_0 has the effect of driving all states towards the south pole of the Bloch sphere, while M_1 drives all states to the north pole, following longitudinal lines. This is consistent with the imaginary time operator $e^{\pm \epsilon Z}$, as given in (2) and (3). In Fig. 2(c), we show the fidelity $F = |\langle \psi_t | E_0 \rangle|^2$ for three different measurement sequences. Because of the randomness of quantum measurements, each sequence gives a different trajectory, but all cases converge to the ground state $|E_0\rangle = |1\rangle$. Averaging over many random trajectories yields a smooth exponential curve approaching the target

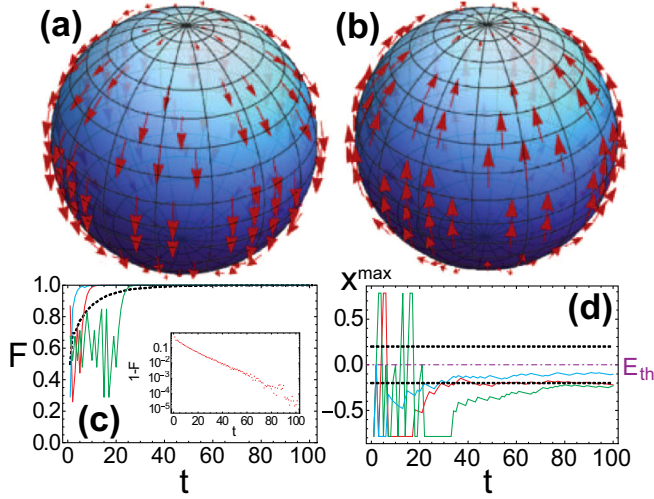


FIG. 2. (a),(b) Vector map on the Bloch sphere for the change induced by the operators M_0 and M_1 , respectively, where $M_n = [I \cos \epsilon - (-1)^n Z \sin \epsilon] / \sqrt{2}$. (c) Fidelity of the state with respect to ground state $|E_0\rangle = |1\rangle$ for the Hamiltonian $H = Z$ after t rounds of measurement and correction under (7) for three random initial states (solid lines) and $\epsilon = 0.2$. We take $U_C = X$ and $E_{\text{th}} = 0$. Dashed line shows the averaged fidelity of 1000 evolutions starting from the initial state $|+\rangle$. Inset shows a semilog plot of $1 - F$ with t . (d) The peak position $x_{k_0 k_1}^{\text{max}}$ as defined in (6) of the function A (solid lines). Dashed lines show the energy eigenstates ϵE_n and the dashed dotted line E_{th} . For the measurements in (c) and (d), the outcomes are chosen randomly according to Born probabilities.

state. A semilog plot [Fig. 2(c) inset] verifies the exponential evolution, consistent with ITE. In fact, for this case it can be shown exactly that any trajectory is equivalent to applying a power of M_0 which approaches the ground state (see Supplemental Material [73]). In Fig. 2(d) we plot the peak position of the A function for the same three trajectories as in Fig. 2(c). We see that there are broadly two regimes, where there is a random movement of the peak position, followed by a region of stability, where the Gaussian approaches the ground state energy. In the initial random evolution, when $x_{k_0 k_1}^{\text{max}} > \epsilon E_{\text{th}}$, several spin flips induced by U_C occur, until the random movement stabilizes to the correct energy range. After the correct peak position is established, the fidelity quickly evolves towards the ground state.

Example 2: Transverse-field Ising model.—We next show an example of the transverse-field Ising model with the Hamiltonian $H^{(1)} = \lambda \sum_{n=1}^L X_n$, $H^{(2)} = \sum_{n=1}^{L-1} Z_n Z_{n+1}$, $H = H^{(1)} + H^{(2)}$. Here, L is the number of qubits in the chain, and we take $E_{\text{th}} = (E_0 + E_1)/2$. We assume that each of the terms in the Hamiltonian must be implemented separately to construct the measurement operators. We perform a second order Suzuki-Trotter expansion with $M_n = \langle n|_a e^{-i\epsilon H^{(1)} \otimes Y/2} e^{-i\epsilon H^{(2)} \otimes Y} e^{-i\epsilon H^{(1)} \otimes Y/2} |+\rangle_a$ (see Supplemental Material [73]). The conditional operator is chosen to be a random local unitary

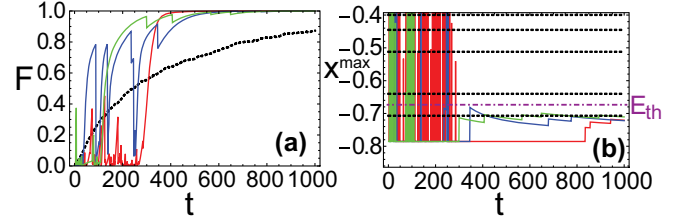


FIG. 3. (a) The fidelity of the state with respect to the ground state of the $L = 5$ site transverse Ising model with $\lambda = 1$ and $\epsilon = 0.12$ after t rounds of measurement and correction under (7) for three random initial states (solid lines). Dashed lines show the averaged fidelity of 1000 evolutions. (b) The peak position $x_{k_0 k_1}^{\text{max}}$ as defined in (6) of the function A (solid lines). Dashed lines show the energy eigenstates ϵE_n and the dashed dotted line E_{th} .

$U_C = \otimes_{n=1}^L e^{2\pi i(\phi_n^x X_n + \phi_n^y Y_n + \phi_n^z Z_n)}$, where $\phi_n^\alpha \in [0, 1]$. We show the fidelity of the procedure with respect to the target state in Fig. 3(a). Again we see two stages, where there is a random evolution of the fidelity, followed by a smoother time evolution once the peak of Gaussian amplitude function is in the correct range. For longer chains we observe a longer period of random evolution before the correct energy range is established, after which the system quickly converges to the ground state.

Complexity estimate.—We now briefly discuss the complexity of the proposed algorithm. First, the measurements M_n can be typically performed efficiently for a given Hamiltonian using a Suzuki-Trotter decomposition (see Supplemental Material [73]). Because of the flexibility of the choice of the operator U_C , this can also typically be implemented efficiently. The complexity of the algorithm then results from the number of measurements that need to be made in total. Based on the behavior observed in Figs. 2 and 3, we model the initial part of the measurement sequence as a stochastic process, where the algorithm repeats until the criterion $x_{k_0 k_1}^{\text{max}} < \epsilon E_{\text{th}}$ is satisfied (see Supplemental Material [73]). The number of required measurements until this occurs can be estimated by evaluating the probability of obtaining a sequence with k consecutive M_0 outcomes together with the average failed sequence length. Although it is not easy to obtain a simple expression for the general case complexity, for two particular cases, assuming an initial state with equal superposition, it is possible to estimate the typical number of measurements before convergence. These are Hamiltonians with (i) a uniform density of states and (ii) a completely degenerate spectrum of excited states (see Supplemental Material [73]). For (i), we obtain a scaling as $O[1/(\epsilon \Delta)^2]$, where $\Delta = E_1 - E_0$ is the gap. We note that there is an implicit dependence upon system dimension in this relation, due to the requirement that $-\pi/4 \leq \epsilon E_n \leq \pi/4$. For example, for an exponential number of states, $\epsilon \Delta$ is exponentially vanishing and the final scaling increases exponentially for unstructured problems. For (ii), we find that the scaling is $O(D)$, where D is the system dimension.

Conclusions.—We have proposed a method of performing deterministic ITE, using measurements and conditional unitary operations. Because of the use of quantum measurements, the evolution is stochastic within Hilbert space on a shot-to-shot basis. Averaging over trajectories reveals an exponential evolution that is consistent with ITE. The approach is generic, one does not need to know the ground state before executing the algorithm, and the measurement operators can be constructed with a Suzuki-Trotter decomposition so that it is compatible with gate based quantum computing. The measurement operators and unitary operators can be constructed efficiently, but the number of measurements that need to be performed before convergence depends upon the nature of the Hamiltonian and the initial state. The algorithm is guaranteed to only converge if the energy of the state is lower than E_{th} .

The algorithm that we present here can be considered a generalization of several related works which use the same basic framework. For example in Ref. [70] a similar method was proposed to generate supersinglet states, and also maximally entangled states of atomic ensembles in Ref. [71]. A four-qubit linear graph state was also deterministically generated using the method in Ref. [72]. We have found that the algorithm converges to the ground state for every problem Hamiltonian that we have given it. In our algorithm, we chose a relatively simple strategy for the adaptive unitary operator (8) where the state is rotated if the measurement outcomes do not fall in the targeted range. Since $E_{k_0, k_1}^{\text{max}}$ is an energy estimate of the state, more complex strategies to rotate the state to the ground state could be made. Another potential improvement is to choose a judicious initial state to improve the convergence of the scheme.

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