

Exact Equivalence between Quantum Adiabatic Algorithm and Quantum Circuit Algorithm *

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We present a rigorous proof that quantum circuit algorithm can be transformed into quantum adiabatic algorithm with the exact same time complexity. This means that from a quantum circuit algorithm of L gates we can construct a quantum adiabatic algorithm with time complexity of $O(L)$. Additionally, our construction shows that one may exponentially speed up some quantum adiabatic algorithms by properly choosing an evolution path.

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Quantum algorithms have two paradigms, quantum circuit algorithm^[1] and quantum adiabatic algorithm.^[2] The latter works by adiabatically evolving in the ground state of a system with Hamiltonian

$$H(s) = (1-s)H_B + sH_P, \quad (1)$$

where s increases with time slowly from 0 to 1. The beginning Hamiltonian H_B has a ground state which is easy to construct and the problem Hamiltonian H_P has a ground state that encodes the solutions of the problem. According to the quantum adiabatic theorem,^[2,3] the speed of the algorithm is limited by the minimum energy gap between the ground state and the first excited state during the evolution of $H(s)$. When $H(s)$ has an exponentially small minimum gap, the algorithm is inefficient.

These two kinds of quantum algorithms are shown to be *polynomially* equivalent to each other in terms of time complexity.^[4,5] Here we present a rigorous proof that any quantum circuit algorithm can be converted into a quantum adiabatic algorithm with the *same* time complexity. As it has been shown that a quantum adiabatic algorithm can be converted into a quantum circuit algorithm with the same time complexity,^[5] our result means that quantum circuit algorithm and quantum adiabatic algorithm are exactly equivalent to each other.

Consider a quantum circuit algorithm that has n qubits and L universal quantum gates,

$$|\alpha_0\rangle \xrightarrow{U_1} |\alpha_1\rangle \cdots |\alpha_{\ell-1}\rangle \xrightarrow{U_\ell} |\alpha_\ell\rangle \cdots |\alpha_{L-1}\rangle \xrightarrow{U_L} |\alpha_L\rangle, \quad (2)$$

where U_ℓ represents the ℓ th quantum gate operation, $|\alpha_\ell\rangle = U_\ell |\alpha_{\ell-1}\rangle$. Usually, $|\alpha_0\rangle = |00 \cdots 0\rangle$. Our aim is to construct a corresponding quantum adiabatic algorithm that has the same time complexity. For this purpose, we introduce additional L clock qubits and focus on a special type of clock states $|\ell\rangle^c = |1^\ell 0^{L-\ell}\rangle^c$, which denotes that the first ℓ qubits are ones and the

rest are zeros.^[4,6] Corresponding to the ℓ th gate operation, we define an operator

$$\mathcal{O}_\ell = \frac{\eta}{2} I \otimes |\ell-1\rangle^c \langle \ell-1|^c - \frac{1}{2} U_\ell \otimes |\ell\rangle^c \langle \ell-1|^c - \frac{1}{2} U_\ell^\dagger \otimes |\ell-1\rangle^c \langle \ell|^c + \frac{1}{2\eta} I \otimes |\ell\rangle^c \langle \ell|^c, \quad (3)$$

where $\eta \geq 1$. This operator with $\eta = 1$ was introduced in Refs. [4,6]. We construct the beginning and problem Hamiltonians

$$H_B = I \otimes \sum_{l=1}^L |\ell\rangle^c \langle \ell|^c; \quad (4)$$

$$H_P = \sum_{\ell=1}^L \mathcal{O}_\ell. \quad (5)$$

The ground state of H_P with $\eta > 1$ is

$$|\psi^\eta\rangle = \sqrt{\frac{\eta^2 - 1}{\eta^{2L+2} - 1}} \sum_{\ell=0}^L \eta^\ell |\gamma_\ell\rangle, \quad (6)$$

where $|\gamma_\ell\rangle = |\alpha_\ell\rangle \otimes |\ell\rangle^c$. The ground state energy is 0. According to the Gershgorin circle theorem, its first excited state has an energy larger than $\frac{1}{2}(\eta^{-1} + \eta) - 1$, which is finite and independent of the system size. If our algorithm is successful, that is, we manage to reach the ground state of H_P , the probability of finding the solution $|\gamma_L\rangle$ is $\frac{\eta^{2L+2} - \eta^{2L}}{\eta^{2L+2} - 1} \sim 1 - \eta^{-2}$, which can be made very close to one with large η .

The whole Hilbert space is of dimension 2^{n+L} . However, our adiabatic operation will stay in the subspace of dimension $L+1$ spanned by $|\gamma_\ell\rangle$, where H_B and H_P have the following matrix forms,

$$H_B = \begin{pmatrix} 0 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & 0 & \cdots & \vdots \\ \vdots & 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & \cdots & 0 & 1 \end{pmatrix}, \quad (7)$$

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$$H_P = \begin{pmatrix} \frac{\eta}{2} & -\frac{1}{2} & 0 & \cdots & \cdots & 0 \\ -\frac{1}{2} & \frac{\eta+\eta^{-1}}{2} & -\frac{1}{2} & 0 & \cdots & \vdots \\ 0 & -\frac{1}{2} & \frac{\eta+\eta^{-1}}{2} & -\frac{1}{2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \cdots & \ddots & -\frac{1}{2} & \frac{\eta+\eta^{-1}}{2} & -\frac{1}{2} \\ 0 & \cdots & \cdots & 0 & -\frac{1}{2} & \frac{1}{2\eta} \end{pmatrix}. \quad (8)$$

We can immediately construct a quantum adiabatic algorithm with the following Hamiltonian

$$H(s) = (1 - s)H_B + sH_P. \quad (9)$$

When $\eta = 1$, this is the algorithm studied in Ref. [4], which is polynomially slower than the corresponding quantum circuit algorithm. When $\eta > 1$, this algorithm is exponentially slow as we can show rigorously that $H(s)$ has an exponentially small energy gap $\sim \eta^{-L}$ at $s^* = 2/(\eta - \eta^{-1} + 2)$ (see Appendix A for details). We will show in the following how to avoid this small energy gap by introducing an intermediate Hamiltonian $H_I(t)$.

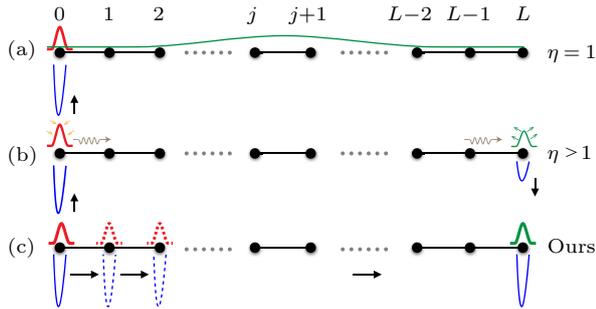


Fig. 1. Schematic representations of three different quantum adiabatic algorithms. Each site of the lattice represents a quantum state $|\gamma_j\rangle$. Initially, a quantum particle resides in a potential well at site 0. (a) Algorithm Eq. (9) with $\eta = 1$: the potential well at site 0 slowly disappears and the wave packet of the particle spreads over the whole lattice. (b) Algorithm Eq. (9) with $\eta > 1$: the potential well at site 0 is lifted up slowly while the other potential well is created at site L with increasing depth; during this process, the particle tunnels from site 0 to site L . (c) Our algorithm with an intermediate Hamiltonian: the potential well is moved adiabatically site by site while carrying the particle with it.

Before we present our adiabatic algorithm we first review the algorithm in Eq. (9) in an alternative perspective. As shown in Fig. 1, we can construct a one-dimensional lattice, where each site represents a quantum state $|\gamma_j\rangle$. H_B and H_P , as either diagonal or tridiagonal matrices (see Eqs. (7) and (8)), can be viewed as Hamiltonians defined on this lattice. H_B represents a potential well at site 0. The diagonal elements of H_P represent a potential that has two wells, one at site 0 and the other at site L while its off-diagonal elements gives rise to hopping between lattice sites. In this perspective, the adiabatically evolving Hamiltonian $H(s)$ in Eq. (9) is to move a particle initially residing in the potential well at site 0 to site L . When $\eta = 1$, al-

though H_P has two potential wells at sites 0 and L , they are too shallow to hold bound states. As a result, the end result of the adiabatic evolution is a wave packet spreading almost evenly over the whole lattice. One has to repeat the process about L times to find the particle at site L by measurement. This case is schematically shown in Fig. 1(a).

When $\eta > 1$, the potential well at site 0 becomes shallower while the potential well at site L gets deeper. The consequence is that H_P has a bound state localized at site L as described by Eq. (6). When s changes slowly, the potential well of $H(s)$ at site 0 becomes shallower and the potential well at site L becomes deeper. As the wells change their depths, the particle initially at site 0 will tunnel to site L . As H_P with $\eta > 1$ has only one bound state, one has to change s very slowly to keep the system in the ground state so that the particle will end up localized at site L . Physically, it is clear that this will become exponentially difficult as L increases. This is captured mathematically by the exponentially small gap at $s = s^*$. This case is shown in Fig. 1(b).

Our algorithm is to generate a scenario depicted in Fig. 1(c), where the potential well is moved slowly from site to site. We are able to find τ , the time spent moving the potential well from one site to the next, such that τ is independent of the system size L and at the same time τ is slow enough that the particle moves with the potential well. As a result, the time complexity of our algorithm is $O(L)$. The scenario shown in Fig. 1(c) reminds us of the quantum tweezer proposed in Ref. [7].

If the lattice in Fig. 1 were replaced by a continuous line, the scenario shown in Fig. 1(c) could be realized with the following Schrödinger equation

$$i \frac{\partial}{\partial t} \psi = -\frac{1}{2m} \frac{\partial^2}{\partial x^2} \psi + V(x - vt)\psi, \quad (10)$$

where $V(x - vt)$ is a moving Gaussian potential well proportional to $-\exp[-(x - vt)^2]$. With Galilean transformation, one can show that a particle initially in the ground state of $V(x)$ will remain in the ground state of $V(x - vt)$ at any time. That is, moving potential well $V(x - vt)$ will carry the particle with it. For a lattice, we only need to discretize the Hamiltonian in the above Schrödinger equation. We use $H_I(t)$ to denote the discretized Hamiltonian. Specifically, the matrix of $H_I(t)$ are tridiagonal with

$$(H_I)_{mm}(t) = \frac{1}{2\eta} + \frac{\eta}{2}[1 - e^{-(t/\tau - m)^2}], \quad (0 \leq m \leq L) \quad (11)$$

$$(H_I)_{m(m+1)}(t) = (H_I)_{(m+1)m}(t) = -\frac{1}{2}, \quad (0 \leq m \leq L - 1) \quad (12)$$

where τ is a parameter independent of L , and $v = 1/L\tau$. The detailed relation between $H_I(t)$ and the Schrödinger Eq. (10) is given in Appendix B.

Our algorithm is to use $H_I(t)$ as an intermediate Hamiltonian and to construct three adiabatically changing Hamiltonians

- (i) $H_1(s) = (1-s)H_B + sH_I(0)$ with s changing slowly from 0 to 1;
- (ii) $H_1(t)$ for $0 < t < L\tau$;
- (iii) $H_2(s) = (1-s)H_I(L\tau) + sH_P$ with s changing slowly from 0 to 1.

The algorithm works by preparing the system at state $|\gamma_0\rangle$ and evolving it according to the above Hamiltonians one by one.

We can show that the minimum gaps of $H_1(s)$ and $H_2(s)$ are finite and independent of the system size L (see Appendix A for detailed analysis). This means that the time spent with $H_1(s)$ and $H_2(s)$ is negligible when the system size L is large enough. This allows us to focus on the evolution with $H_1(t)$. The minimum gap of $H_I(t)$ is also finite and independent of the system size L . After the evolution with $H_1(s)$, the system will evolve into a state very close to the ground state $|\tilde{\gamma}_1\rangle$ of $H_I(0)$. Let us denote it as $|\psi_1\rangle = |\tilde{\gamma}_1\rangle + \delta$, where $|\delta| \ll 1$. If we evolve $|\psi_1\rangle$ with the continuous Schrödinger Eq. (10), with the Galilean transformation we can ensure that the system will stay very close to the ground state and the error δ will stay small. $H_I(t)$ is its discretized version. We show in Appendix B that during the evolution with $H_I(t)$ the error δ will also stay small. As the evolution time with $H_I(t)$ is $L\tau$, the time complexity of our algorithm is $O(L)$.

It is interesting to compare our algorithm with algorithm Eq. (9) (or equivalently, scenario (b) and scenario (c) in Fig. 1). Both the algorithms have the same beginning Hamiltonian and the problem Hamiltonian, and employ the adiabatic process. However, their time complexities are profoundly different: our algorithm is exponentially faster. The crucial difference is due to the additional Hamiltonian $H_I(t)$. Alternatively, we can say that we have chosen a different adiabatic evolution path. This shows that one may exponentially speed up a quantum adiabatic algorithm by carefully designing an evolution path.

There are infinitely many methods to construct intermediate Hamiltonians and, therefore, infinitely many ways to design an adiabatic evolution path from the beginning Hamiltonian and the problem Hamiltonian. The simplest evolution path as in Eq. (9) is likely not efficient. In our proof, the intermediate Hamiltonian $H_I(t)$ is introduced to effectively turn on the terms O_ℓ in H_P one by one. This turns out to be exponentially efficient than Eq. (9), where all the terms in H_P are turned on simultaneously. However, as there are now more switching on and off, one has to do it very smoothly to suppress the error that may occur during the switchings. It was pointed out in Ref. [3] that any discontinuity in the derivatives of a switching function may lead to errors. The use of the Gaussian function in our proof (or algorithm) is to suppress this

kind of error. In this perspective, our proof presents one possible effective way to design the adiabatic evolution path.

In summary, we have presented a method to transform a quantum circuit algorithm to quantum adiabatic algorithm without loss of efficiency. This means that in principle designing an efficient quantum algorithm is now entirely a physical endeavor. Furthermore, our method gives an analytical example to show that some quantum adiabatic algorithm can have an exponential speedup with a properly chosen evolution path.

Appendix A: Analytical results of energy gaps

In this Appendix we give detailed derivations of two mathematical results regarding minimum energy gaps used in the main article. We present these results in a self-contained manner so that they can be read without knowing anything in our main text.

We define three $N \times N$ ($N \gg 1$) matrices, \mathcal{B} , \mathcal{P} , and \mathcal{M} . The matrix \mathcal{B} is diagonal with $\mathcal{B}_{11} = 0$ and $\mathcal{B}_{mm} = 1$ ($2 \leq m \leq N$). The matrix \mathcal{P} is tridiagonal with

$$\begin{aligned} \mathcal{P}_{11} &= \eta/2, & \mathcal{P}_{mm} &= \frac{\eta + \eta^{-1}}{2}, & (2 \leq m \leq N-1) \\ \mathcal{P}_{NN} &= \frac{1}{2\eta}, & \mathcal{P}_{m(m+1)} &= \mathcal{P}_{(m+1)m} = -\frac{1}{2}, \\ & & & & (1 \leq m \leq N-1). \end{aligned} \quad (\text{A1})$$

And the matrix \mathcal{M} changes with time and is tridiagonal with

$$\begin{aligned} \mathcal{M}_{mm}(t) &= \frac{1}{2\eta} + \frac{\eta}{2}(1 - e^{-(t/\tau - m + 1)^2}), & (1 \leq m \leq N) \\ \mathcal{M}_{m(m+1)}(t) &= \mathcal{M}_{(m+1)m}(t) = -\frac{1}{2}, & (1 \leq m \leq N-1). \end{aligned} \quad (\text{A2})$$

We let $\mathcal{M}_0 = \mathcal{M}(0)$ and $\mathcal{M}_f = \mathcal{M}((N-1)\tau)$ for convenience.

1. Exponentially small energy gap

We consider Hamiltonian $\mathcal{H}_a(s) = (1-s)\mathcal{B} + s\mathcal{P}$ with $s \in [0, 1]$. We shall show that for $\eta \geq 4$ the gap between the lowest two eigenvalues of this Hamiltonian is exponentially small as $N \rightarrow \infty$ at

$$s^* = \frac{2}{\eta - \eta^{-1} + 2}. \quad (\text{A3})$$

At $s = s^*$, $\mathcal{H}_a(s^*)$ can be written as

$$\mathcal{H}_a(s^*) = s^* \begin{pmatrix} \frac{\eta}{2} & -\frac{1}{2} & 0 & \cdots & \cdots & 0 \\ -\frac{1}{2} & \eta & -\frac{1}{2} & 0 & \cdots & \vdots \\ 0 & -\frac{1}{2} & \eta & -\frac{1}{2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \cdots & \ddots & -\frac{1}{2} & \eta & -\frac{1}{2} \\ 0 & \cdots & \cdots & 0 & -\frac{1}{2} & \frac{\eta}{2} \end{pmatrix}. \quad (\text{A4})$$

Since s^* is a constant independent of N , we can just discuss the gap of $\mathcal{H}_a^* = \mathcal{H}_a(s^*)/s^*$. Assume that \mathcal{H}_a^* has an eigenvalue λ and an eigenvector $X = (x_1, x_2, \dots, x_N)^T$ that satisfy

$$\mathcal{H}_a^* X = \lambda X. \quad (\text{A5})$$

We write the above equation in its component form as

$$\begin{aligned} \frac{\eta}{2}x_1 - \frac{1}{2}x_2 &= \lambda x_1, \\ -\frac{1}{2}x_{k-1} + \eta x_k - \frac{1}{2}x_{k+1} &= \lambda x_k, \\ -\frac{1}{2}x_{N-1} + \frac{\eta}{2}x_N &= \lambda x_N, \end{aligned} \quad (\text{A6})$$

where $k = 2, \dots, N-1$. By introducing two additional variables x_0 and x_{N+1} , we can convert the above equations into the standard second-order difference equation

$$x_{k-1} - 2(\eta - \lambda)x_k + x_{k+1} = 0, \quad (\text{A7})$$

where $k = 1, 2, \dots, N$, and the boundary conditions are

$$x_0 = \eta x_1, \quad \eta x_N = x_{N+1}. \quad (\text{A8})$$

It has two types of solutions. Type I solution is given by

$$x_k = A \sin(k\alpha) + B \cos(k\alpha), \quad (\text{A9})$$

with $\lambda = \eta - \cos \alpha$. Type II solution is given by

$$x_k = A \sinh(k\alpha) + B \cosh(k\alpha), \quad (\text{A10})$$

with $\lambda = \eta - \cosh \alpha$. The two boundary conditions determine the value of α and λ . We are allowed to consider only the situation $\alpha > 0$.

For $\eta \geq 4$, type I eigenvalue $\lambda = \eta - \cos \alpha > (\eta + 1)/2$. However, according to the Gershgorin circle theorem, \mathcal{H}_a^* has and only has two eigenvalues smaller than $(\eta + 1)/2$. Therefore, the smallest two eigenvalues are of type II. For type II solution, the boundary conditions are

$$B = \eta(A \sinh \alpha + B \cosh \alpha), \quad (\text{A11})$$

and

$$\begin{aligned} \eta[A \sinh(N\alpha) + B \cosh(N\alpha)] \\ = A \sinh[(N + 1)\alpha] + B \cosh[(N + 1)\alpha]. \end{aligned} \quad (\text{A12})$$

After eliminating A and B we have

$$\frac{\eta \sinh \alpha}{1 - \eta \cosh \alpha} = \frac{\sinh[(N + 1)\alpha] - \eta \sinh \alpha}{\eta \cosh[N\alpha] - \cosh[(N + 1)\alpha]}, \quad (\text{A13})$$

which can be simplified to

$$\eta^2 \sinh[(N - 1)\alpha] - 2\eta \sinh[N\alpha] + \sinh[(N + 1)\alpha] = 0. \quad (\text{A14})$$

Let $z = e^\alpha$, we can rewrite the equation as follows:

$$z^2 - 2\eta z + \eta^2 - z^{-2(N-1)}(\eta - z^{-1})^2 = 0. \quad (\text{A15})$$

As $\alpha > 0$, we have $z > 1$. For convenience, we define

$$f(z) = z^2 - 2\eta z + \eta^2 - \Delta^2, \quad (\text{A16})$$

where $\Delta(z) = z^{-(N-1)}(\eta - z^{-1})$. Also note that in the following discussion we always have $N \gg 1$ and $\eta \geq 4$.

It is easy to find $f(1) = 0$, $f'(1) > 0$, $f(+\infty) > 0$, and $f(\eta) < 0$. Moreover, $f(z) = 0$ has at most 2 roots, for the \mathcal{H}_a^* has and only has 2 eigenvalues satisfying Eq. (A10). Thus there is one root z_1 in the interval $(1, \eta)$ and z_2 in $(\eta, +\infty)$. At the same time, we can make $\Delta(z)$ arbitrarily small by increasing N . This implies that we can focus on the behavior of $f(z)$ near $z = \eta$.

Consider the function $g(z) = z^2 - 2\eta z + \eta^2 - \delta^2$, where δ is a positive constant. It is clear that $g(z) = 0$ has two roots $z_\pm = \eta \pm \delta$. As we can find an N_0 so that $\Delta < \delta$ for all $N > N_0$ and arbitrarily small δ , the roots of $f(z)$, z_1 and z_2 , are within the interval $(\eta - \delta, \eta + \delta)$ for $N > N_0$. In other words, $|z_1 - z_2|$ is no more than 2δ . The energy gap $|\lambda_1 - \lambda_2|$ is bounded by the distance between z_1 and z_2 as

$$|\lambda_1 - \lambda_2| = \frac{1}{2}|z_1 - z_2 + z_1^{-1} - z_2^{-1}| < \frac{1}{2}|z_1 - z_2|. \quad (\text{A17})$$

Thus we come into the conclusion: For $\eta \geq 4$, there exists an N_0 and for all $N > N_0$, the gap of \mathcal{H}_a^* is smaller than $O((\eta - \delta)^{-N})$, where $\delta > 0$ is an arbitrarily small constant.

2. The first finite gap

Here we consider the energy gap for

$$\mathcal{H}_b(s) = (1 - s)\mathcal{B} + s\mathcal{M}_0. \quad (\text{A18})$$

We present a simple proof that $\mathcal{H}_b(s)$ has finite energy gap for the situation $\eta \geq 5$. It is convenient to study the eigenvalue of

$$\tilde{\mathcal{H}}_b(s) = \mathcal{H}_b(s)/s = \frac{1-s}{s}(\mathcal{B} - I) + \mathcal{M}_0, \quad (\text{A19})$$

where I is the identity matrix.

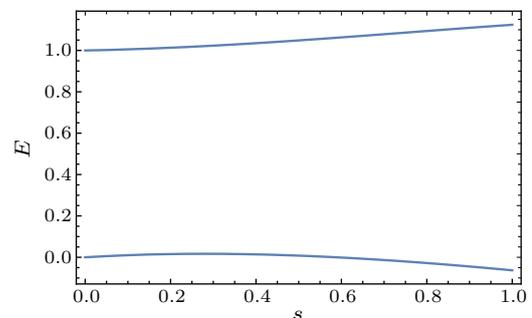


Fig. A1. The lowest two energy levels of (A18) at $\eta = 4$ and $N \rightarrow \infty$.

Using the Gershgorin circle theorem, we can easily check that $\tilde{\mathcal{H}}_b$ has an energy gap larger than $\eta(1 - 1/e)/2 - 3/2$, which is greater than 0 for $\eta \geq 5$. Therefore, for $1/\eta < s \leq 1$, $\mathcal{H}_b(s)$ has an energy gap

larger than $(1 - 1/e)/2 - 3/2\eta$. For $0 \leq s \leq 1/\eta$, we can continue applying the Gershgorin circle theorem to $\mathcal{H}_b(s)$ and find another gap lower bound $(3 - 1/e - 5/\eta)/2$. Thus $\mathcal{H}_b(s)$ has an N -independent gap between the smallest two eigenvalues.

For $\eta < 5$, the conclusion will also hold true if η is larger than a certain positive number. However, the proof is rather complicated. Here we just show the numerical results in Fig. A1 for the smallest two eigenvalues of (A18) at $\eta = 4$. In the discussion of the main text, η is an arbitrary number larger than one. Therefore, if one has some doubts about the results here for $\eta < 5$, one can safely choose $\eta \geq 5$.

3. The last finite gap

We consider the energy gap for

$$\mathcal{H}_c(s) = (1 - s)\mathcal{M}_f + s\mathcal{P}. \quad (\text{A20})$$

Note that (A20) can be written as

$$\mathcal{H}_c(s) - \mathcal{P} = (s - 1)[\mathcal{P} - \mathcal{M}_f]. \quad (\text{A21})$$

Let λ_1 and λ_2 be the two smallest eigenvalues of $\mathcal{H}_c(s)$, and κ_1 and κ_2 the two smallest eigenvalues of \mathcal{P} . From the main text, we have already known $\kappa_1 = 0$ and $\kappa_2 > \frac{1}{2}(\eta^{-1} + \eta) - 1$.

It can be easily checked that the maximum and minimum of the eigenvalues of $\mathcal{P} - \mathcal{M}(LT)$ are $\eta/2e$ and 0. With the Weyl's inequality, we have

$$\lambda_1 \leq (1 - s)\frac{\eta}{2e} < \frac{\eta}{2e} \quad (\text{A22})$$

and

$$\lambda_2 \geq \kappa_2. \quad (\text{A23})$$

This implies that the upper bound of λ_1 is $\eta/2e$ and the lower bound of λ_2 is $\frac{1}{2}(\eta^{-1} + \eta) - 1$, which gives

$$\lambda_2 - \lambda_1 > \frac{1}{2}\left(\frac{1}{\eta} + \eta\right) - 1 - \frac{\eta}{2e}. \quad (\text{A24})$$

This shows that the lowest energy gap of $\mathcal{H}_c(s)$ is finite and independent of N for $\eta \geq 4$. In Fig. A2 we show the numerical results for the smallest two eigenvalues of (A20) at $\eta = 4$.

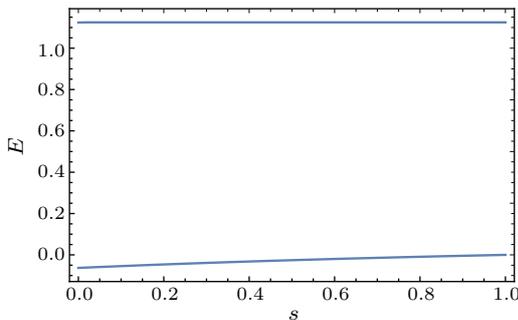


Fig. A2. The lowest two energy levels of (A20) for $\eta = 4$ and $N \rightarrow \infty$.

Appendix B: Error analysis for $H_I(t)$

In the main text, we considered two different but closely related quantum dynamics. One is given by

$$i\frac{d}{dt}U(t) = \mathcal{M}(t)U(t), \quad (\text{B1})$$

where $\mathcal{M}(t)$ is the matrix form of $H_I(t)$ in the subspace spanned by $|\gamma_\ell\rangle$ and

$$U(t) \equiv (u_0(t), u_1(t), \dots, u_L(t))^T. \quad (\text{B2})$$

Our goal is to prove that if $U(0)$ has a difference from the exact ground state $\tilde{\psi}(0)$ of $\mathcal{M}(0)$, the difference will not grow too much when t grows.

The other is given by

$$i\frac{\partial}{\partial t}\psi(x, t) = -\frac{1}{2m}\frac{\partial^2}{\partial x^2}\psi(x, t) + V(x - vt)\psi, \quad (\text{B3})$$

where $V(x - vt)$ is a moving Gaussian potential well and the wave function $\psi(x, t)$ is defined on the whole real axis. For this dynamical equation, by the argument of Galilean transformation, if $\psi(x, t)$ is initially the ground state for $V(x)$, $\psi(x, t)$ will stay in the ground state of $V(x - vt)$. We discretize Eq. (B3) as follows:

$$\frac{\partial^2}{\partial x^2}\psi(x, t) \rightarrow \frac{\psi(x - h, t) + \psi(x + h, t) - 2\psi(x, t)}{h^2}, \quad (\text{B4})$$

where $h = 1/L$. When the circuit gate number L is large, h will be a small interval of x . With such discretization, Eqs. (B3) and (B1) become identical to each other on the interval $x \in [0, 1]$ when we set

$$m = 1/h^2V(x - vt) = \frac{1}{2}\left(\eta + \frac{1}{\eta}\right) - 1 - \frac{\eta}{2}e^{-\left(\frac{x}{h} - \frac{t}{\tau}\right)^2}, \quad (\text{B5})$$

where $v = h/\tau$.

We are interested in how a small discrepancy between the initial states of Eqs. (B1) and (B3) will grow. Specifically, let us define the discrepancy

$$e_m(t) = \psi(mh, t) - u_m(t) \quad (\text{B6})$$

and let $E(t) = \{e_1(t), e_2(t), \dots\}^T$. We would like to know how large $E(t)$ can grow if initially $E(t)$ is small. It is straightforward to check that $E(t)$ satisfies

$$i\frac{\partial}{\partial t}E(t) = \mathcal{M}(t)E(t) + \psi^{(4)}(t)\frac{h^4}{24}, \quad (\text{B7})$$

with

$$\psi^{(4)}(t) \equiv \left(\frac{\partial^4\psi(h + \xi_1 h, t)}{\partial x^4}, \frac{\partial^4\psi(2h + \xi_2 h, t)}{\partial x^4}, \dots \right)^T, \quad (\text{B8})$$

where $\xi_m \in [0, 1)$ are constants appearing in the remainders of Taylor expansions.

We focus on the situation that $U(t)$ is initially close to the ground state $\psi(x, t)$. We can transform Eq. (B3) to an h -invariant form by rescaling $x = hs$, $v = hv_s$.

$$i\frac{\partial}{\partial t}\phi(s, t) = -\frac{1}{2}\frac{\partial^2}{\partial s^2}\phi(s, t) + \tilde{V}(s - v_s t)\phi(s, t), \quad (\text{B9})$$

where $\phi(s, t) = \psi(x = hs, t)$. The ground state can be written as

$$\phi(s, t) = \tilde{\phi}(s - v_s t) e^{i v_s s - i \frac{1}{2} v_s^2 t - i \varepsilon_0 t}, \quad (\text{B10})$$

where ε_0 is the energy of the ground state. We replace $\psi^{(4)}$ with $\tilde{\phi}^{(4)}$,

$$\psi^{(4)}(t) = h^4 e^{-i(\varepsilon_0 + \frac{1}{2} v_s^2) t} \tilde{\phi}^{(4)}(t), \quad (\text{B11})$$

where

$$\tilde{\phi}^{(4)}(t) \equiv \left(\dots, \frac{\partial^4 \tilde{\phi}(j + \xi_j - v_s t)}{\partial s^4} e^{i j v_s}, \dots \right)^T. \quad (\text{B12})$$

Then we get the ordinary differential equation (ODE) for the error $E(t)$ as follows:

$$i \frac{d}{dt} E(t) = \mathcal{M}(t) E(t) + \frac{1}{24} \tilde{\phi}^{(4)}(t) e^{-i(\varepsilon_0 + \frac{1}{2} v_s^2) t}. \quad (\text{B13})$$

The ODE can be directly solved as

$$\tilde{E}(t) = \int_0^{L\tau} \frac{1}{24} e^{i \int^t [\mathcal{M}(t') - (\varepsilon_0 + \frac{1}{2} v_s^2)] dt'} \phi^{(4)}(t) dt, \quad (\text{B14})$$

where

$$\tilde{E}(t) \equiv e^{i \int^t \mathcal{M}(t') dt'} E(t), \quad (\text{B15})$$

$\tau = 1/v_s$ is the evolution time for every step and L is the gate number. We notice that

$$\begin{aligned} |E(t)|^2 &= |\tilde{E}(t)|^2 \\ &= \left| \int_0^{L\tau} \frac{1}{24} e^{i \int^t [\mathcal{M}(t') - (\varepsilon_0 + \frac{1}{2} v_s^2)] dt'} \phi^{(4)}(t) dt \right|^2 \\ &\leq \frac{1}{576} \int_0^{L\tau} |\phi^{(4)}(t)|^2 dt, \end{aligned} \quad (\text{B16})$$

where $|\cdot|^2$ is the 2-norm of a vector. With

$$|\phi^{(4)}(t)|^2 = \sum_m \left(\frac{\partial^4 \tilde{\phi}(m + \xi_m - v_s t)}{\partial s^4} \right)^2 \quad (\text{B17})$$

$$\equiv \sum_m g_m(v_s t)^2, \quad (\text{B18})$$

we have

$$\begin{aligned} \int_0^{L\tau} |\phi^{(4)}(t')|^2 dt' &= \sum_m \int_0^{L\tau} g_m(v_s t')^2 dt' \\ &= \sum_{m=0}^L \tau \int_0^L g_m(t)^2 dt. \end{aligned} \quad (\text{B19})$$

It is evident that if $\int_{-\infty}^{\infty} |\partial^4 \tilde{\phi}(s)/\partial s^4|^2 ds$ converges, then all $\int_0^L g_m(t)^2 dt$ will converge. This is true because

$$\frac{\partial^2 \tilde{\phi}}{\partial s^2} = 2(\tilde{V}(s) - \varepsilon_0) \tilde{\phi}, \quad (\text{B20})$$

where

$$\tilde{V}(s) = \frac{1}{2} \left(\eta + \frac{1}{\eta} \right) - 1 - \frac{\eta}{2} e^{-s^2}, \quad (\text{B21})$$

and

$$\frac{\partial^4 \tilde{\phi}}{\partial s^4} = \left[4(\tilde{V}(s) - \varepsilon_0)^2 + 2 \frac{\partial^2 \tilde{V}(s)}{\partial s^2} \right] \tilde{\phi} + 4 \frac{\partial \tilde{V}(s)}{\partial s} \frac{\partial \tilde{\phi}}{\partial s}. \quad (\text{B22})$$

For a Gaussian potential $\tilde{V}(s)$, $4(\tilde{V}(s) - \varepsilon_0)^2 + 2 \frac{\partial^2 \tilde{V}(s)}{\partial s^2}$ has an upper bound, so the first term on the right-hand side (RHS) is square-integrable. Besides, when s is large, the ground state $\tilde{\phi}$ fades exponentially. With the Gaussian fades of $\partial \tilde{V}(s)/\partial s$, the second term on the RHS is also square-integrable. So $\partial^4 \tilde{\phi}/\partial s^4$ is square-integrable. Therefore, all $\int_0^L g_m(t)^2 dt$ will converge into a constant which is independent of the gate number L . Thus the error $|E(t)|^2$ is at most $O(L)$. Note that $U(t)$ is a discrete approximation of $\psi(x, t)$. As a result, it is normalized to

$$|U(t)|^2 = \sum_{m=0}^L |u_m(t)|^2 = L + 1, \quad (\text{B23})$$

the state of our quantum algorithm is $\tilde{U} = U/\sqrt{L+1}$. So, what matters is the relative error $|E(t)|^2/|U(t)|^2$. This quantity will not grow with gate number L .

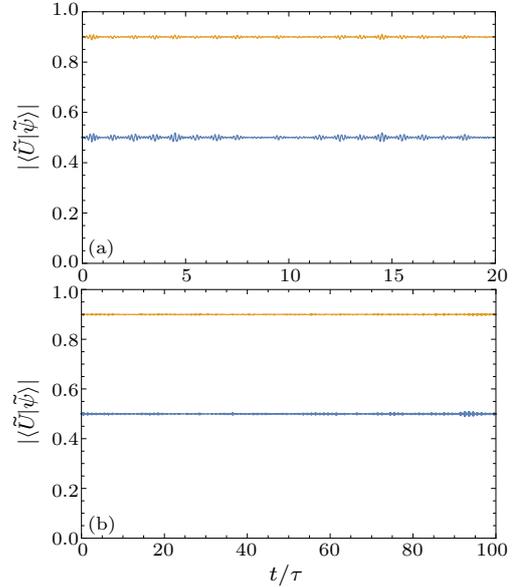


Fig. B1. The error can also be described by $|\langle \tilde{U} | \tilde{\psi} \rangle|$, the product of the normalized actual state of (B1) \tilde{U} and $\mathcal{M}(t)$'s exact ground state $\tilde{\psi}$. The orange line and blue line indicate the two initial conditions, where the initial similarity $|\langle \tilde{U} | \tilde{\psi} \rangle| = 0.9$ and 0.5 . The similarity is almost unchanging with t for both the cases. In our computation, we set (a) $L = 20$, $\tau = 40$ and $\eta = 4$; (b) $L = 100$, $\tau = 40$ and $\eta = 4$.

In the above discussion, we have discussed with the assumption that $U(t)$ is initially close to the ground state (B10) but we have not discussed how to achieve this. Equation (B10) is the ground state only when the dynamical (B9) is defined on the entire real axis $s \in \mathbb{R}$

while $U(t)$ is defined only on the interval $s \in [0, L]$. In addition, the $\psi(x, t)$ slightly differs from the exact ground state $\tilde{\psi}(t)$ of $\mathcal{M}(t)$. We notice that the ground state of (B9) is bounded near the potential well, and fades exponentially with s . So, when $s = t/\tau$ is far enough from 0 and L , Eq. (B10) will become a very good approximation and $\psi(x, t)$ is also very close to $\tilde{\psi}(x)$ after discretization and normalization. Therefore, when s is far enough from 0 and L , the error between $\tilde{\psi}$ and \tilde{U} will not grow with t .

Before $s = t/\tau$ evolves far enough from 0 or too close to L , we need a large τ to reduce the error between $\tilde{\psi}$ and \tilde{U} . The τ is independent of L because $\mathcal{M}(t)$ has a lower bound only related with η for the ground energy gap. Since these two processes are only related with the first and last several qubits, once τ is set, the error will not change with the gate number L . Thus, the evolution from $H_I(0)$ to $H_I(L\tau)$ does bring error, but the error is controlled by τ . This is confirmed by our numerical result in Fig. B1 for different

initial errors. In Fig. B1, we have presented two sets of results, one for $L = 20$ and the other for $L = 100$, to show that the error does not grow with L (the size of the problem).

References

- [1] Nielsen M A and Chuang I L 2000 *Quantum Computation and Quantum Information* (Cambridge: Cambridge University Press)
- [2] Farhi E, Goldstone J, Gutmann S and Sipser M 2000 [arXiv:quant-ph/0001106v1](https://arxiv.org/abs/quant-ph/0001106v1)
- [3] Zhang Q, Gong J and Wu B 2014 *New J. Phys.* **16** 123024
- [4] Aharonov D, van Dam W, Kempe J, Landau Z, Lloyd S and Regev O 2007 *SIAM J. Comput.* **37** 166
- [5] van Dam W, Mosca M and Vazirani U 2001 *Proceedings 2001 IEEE International Conference on Cluster Computing (Las Vegas, Nevada, USA 14–17 October 2001)* p 279
- [6] Kitaev A Y, Shen A H and Vyalii M N 2002 *Classical and Quantum Computation* (Rhode Island: American Mathematical Society)
- [7] Diener R B, Wu B, Raizen M G and Niu Q 2002 *Phys. Rev. Lett.* **89** 070401