

Scattering phase shift in quantum mechanics on quantum computers: Non-Hermitian systems and imaginary-time simulations

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To overcome the fast oscillatory behavior of correlation functions for extracting scattering phase shift in real-time quantum simulations encountered in the work of Guo *et al.* [*Phys. Rev. D* **113**, 054512 (2026)], we propose and test two solutions in the present work. One is to simulate Hermitian systems in imaginary time, and the other is to simulate non-Hermitian systems in real time. We demonstrate that both approaches lead to the problem of nonunitary quantum evolution that can be solved by combining two quantum algorithms: block encoding and Hadamard test. The combined quantum algorithm does not require midcircuit measurements or adjustment of the input parameters of the Hamiltonian and can be easily implemented on quantum computers. Numerical tests on quantum simulators show that both approaches agree with exact solutions for a sufficiently long time before the signal is lost in statistical fluctuations. The results bode well for using non-Hermitian and imaginary-time simulations to circumvent oscillations inherent in real-time simulation of other quantum systems. In particular, the non-Hermitian approach shows a decisive advantage over the imaginary-time one on the number of required ancillary qubits, and hence is more practical to scale up.

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I. INTRODUCTION

Scattering is an indispensable tool in our understanding of interactions in nature, from the original Rutherford experiment on the structure of the atom to modern experiments in nuclear and particle physics.

The promise of quantum computing to solve scattering problems is drawing increasing attention. Various ideas have been proposed in nuclear physics and lattice QCD in general [1–4], and

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scattering, in particular [5–13]. Additionally, there have been developments on the subject of reaction processes in quantum simulations, such as combined variational quantum eigensolver and Lüscher- or Busch-Englert-Rzażewski-Wilkens-like formula approach in Refs. [9,14], measuring phase shift by wave packet time delay [15], reconstructing scattering amplitudes through the coupling of the particle with an ancillary spin-1/2 [16], radiative processes [17], and other ideas, e.g., Refs. [13,18].

In a previous study [19], we explored the feasibility of extracting scattering phase shift on quantum computers in one-dimensional (1D) quantum mechanics using the integrated correlation function (ICF) formalism [20] and were faced with the challenge of fast oscillatory behavior typically encountered in real-time quantum simulations. Different ideas have been proposed to mitigate the issue by postdata analysis (see, e.g., Refs. [21,22]). We explored two such methods, one is $E \rightarrow E + i\epsilon$ prescription, and the other is the $L \rightarrow iL$ rotation, where E refers to the energy of a quantum system and L is the size of periodic box for a trapped system. We showed that both methods allow the extraction of infinite volume phase shifts, with the $L \rightarrow iL$ rotation being more effective than the $E \rightarrow E + i\epsilon$ prescription. Additional postdata processing approaches include averaging either in time or energy bins [21,22]. However, iL rotation yields a non-Hermitian Hamiltonian; the question of how to deal with quantum simulation of a non-Hermitian Hamiltonian system on unitary-gate based quantum hardware was left unanswered.

The goal of the present work is to expand the discussion of our previous work in Ref. [19] to explore the real-time quantum simulation of non-Hermitian systems. The same quantum algorithm can be applied to imaginary-time evolution of a quantum system as well; hence, the imaginary-time quantum simulation is also studied in this work. We will employ the same 1D quantum mechanical setup with the same contact interaction as in Ref. [19]. We consider two possibilities. One is to rotate time and simulate the system in imaginary time. If the Hamiltonian is independent of time, it stays Hermitian. This approach is the one widely adopted in Monte Carlo simulations in lattice QCD and other quantum field theories. Except here we are not performing Monte Carlo, but imaginary-time quantum evolution. The other possibility is to rotate space and simulate the system in real time. The rotation in space $L \rightarrow iL$ renders the system Hamiltonian non-Hermitian. In both cases, we are left with the challenge of how to devise quantum algorithms and circuits to carry out time evolution of nonunitary operators. We will show that both imaginary-time quantum simulation of the integrated correlation function and real-time quantum simulation of a non-Hermitian system can be realized by using Hadamard test algorithm [23] combined with block encoding method used for imaginary-time evolution in Refs. [24–26].

The paper is organized as follows. In Sec. II, the integrated correlation function formalism in 1D quantum mechanical scattering is outlined. In Sec. III, the quantum algorithm for trace of nonunitary operators is presented along with their quantum circuits. In Sec. IV, numerical tests on quantum simulators are discussed. The optimization of quantum circuits for real-time non-Hermitian quantum simulation is given in Sec. V, followed by summary and outlook in Sec. VI.

II. SUMMARY OF INTEGRATED CORRELATION FUNCTION APPROACH TO 1D QUANTUM MECHANICAL SCATTERING

In this section, we give a brief outline of the essential elements in the integrated correlation function approach to the scattering problem in 1D quantum mechanics. The complete discussion can be found in Ref. [19].

A. Hamiltonian matrix

As discussed in Refs. [19–21,27–30], the infinite volume elastic scattering phase shift, $\delta(\epsilon)$, is related to the difference of integrated correlation functions in a trap through a weighted integral,

$$\Delta C(\tau) = C(\tau) - C_0(\tau) \xrightarrow{\text{trap} \rightarrow \infty} \frac{i\tau}{\pi} \int_0^\infty d\epsilon \delta(\epsilon) e^{-i\epsilon\tau}, \quad (1)$$

where $C(t)$ and $C_0(t)$ are the ICF for interacting and noninteracting particles in the trap. In quantum mechanics, the integrated correlation function is associated with the Hamiltonian of nonrelativistic two-particle system in the trap,

$$C(t) = \text{Tr}[e^{-i\hat{H}t}]. \quad (2)$$

The same holds for noninteracting integrated correlation function $C_0(t)$.

The discretized Hamiltonian matrix for a particle interacting with a contact interaction potential placed at center of a periodic box is written as [19]

$$\hat{H} = -\frac{1}{2ma^2} \sum_{\alpha=0}^{2^\Gamma-1} (|\alpha\rangle\langle\alpha+1| + |\alpha+1\rangle\langle\alpha|) + \sum_{\alpha=0}^{2^\Gamma-1} \left(\frac{1}{ma^2} + V(x_\alpha) \right) |\alpha\rangle\langle\alpha|, \quad (3)$$

where Γ denotes the number of qubits, m is the mass of particle, and $|\alpha\rangle$ is shorthand notation of discretized position $|x_\alpha\rangle$ basis. The position $x \in [-\frac{L}{2}, \frac{L}{2}]$ in a periodic box of length L is discretized to $x_\alpha = -\frac{L}{2} + a\alpha$, where $a = \frac{L}{2^\Gamma}$ is lattice spacing and $\alpha \in [0, 1, \dots, 2^\Gamma - 1]$. The periodic boundary condition requires $|2^\Gamma\rangle = |0\rangle$. The contact interaction potential is defined by

$$V(x_\alpha) = \begin{cases} \frac{V_0}{2a}, & \alpha \in [\frac{2^\Gamma}{2} - 1, \frac{2^\Gamma}{2}], \\ 0, & \text{otherwise,} \end{cases} \quad \xrightarrow[2^\Gamma \rightarrow \infty]{a \rightarrow 0} V_0 \delta(x). \quad (4)$$

The analytic solution of infinite volume scattering phase shift for the contact potential is given by

$$\delta(E) = \cot^{-1} \left(-\frac{\sqrt{2mE}}{mV_0} \right), \quad (5)$$

which leads to the analytic expression of right-hand side of Eq. (1),

$$\Delta C(t) \xrightarrow{\text{trap} \rightarrow \infty} \frac{1}{2} \text{erfc} \left(mV_0 \sqrt{\frac{it}{2m}} \right) e^{(mV_0)^2 \frac{it}{2m}} - \frac{1}{2}. \quad (6)$$

It is a fast oscillatory, complex-valued function in real time. Its version in imaginary time can be obtained by an analytic continuation $t \rightarrow -i\tau$, which causes $\Delta C(\tau)$ to be positive if the interaction is attractive ($V_0 < 0$), and negative if it is repulsive ($V_0 > 0$) (see Ref. [19]).

B. Quantum circuits for the Hamiltonian

The quantum circuits for the Hamiltonian matrix in Eq. (3) are given in Sec. III in Ref. [19] (also see, e.g., Ref. [31]). For the purposes of this work, we need to express the entire Hamiltonian matrix in Pauli basis. Starting with the even-odd decomposition plus interaction,

with $\hat{H} = \hat{H}_a + \hat{H}_b + \hat{H}_v$,

$$\begin{aligned} \hat{H}_a &= -\frac{1}{2ma^2} \sum_{\alpha=0}^{2^{\Gamma-1}-1} (|2\alpha\rangle\langle 2\alpha+1| + |2\alpha+1\rangle\langle 2\alpha|), \\ \hat{H}_b &= -\frac{1}{2ma^2} \sum_{\alpha=0}^{2^{\Gamma-1}-1} (|2\alpha+1\rangle\langle 2\alpha+2| + |2\alpha+2\rangle\langle 2\alpha+1|), \\ \hat{H}_v &= \sum_{\alpha=0}^{2^\Gamma-1} \left(\frac{1}{ma^2} + V(x_\alpha) \right) |\alpha\rangle\langle\alpha|. \end{aligned} \quad (7)$$

For $\hat{H}_a$, the Pauli expansion is simply the tensor product of X gate and identity gates: $I_\Gamma \otimes \cdots \otimes I_2 \otimes X_1$. For $\hat{H}_v$, it was worked out in Eq. (33) of Ref. [19].

For $\hat{H}_b$, the Pauli expansion is more complicated, with expression

$$\hat{H}_b = -\frac{1}{2ma^2} \left[\sum_{k=2}^{\Gamma} \frac{1}{2^{k-2}} \sum_S (-1)^{\frac{|S|}{2}} I^{\otimes(\Gamma-k)} \otimes (X_k - I_k) \otimes P_{k-1}(S) \right], \quad (8)$$

where the inner sum is over all even sized subsets of $\{1, \dots, k-1\}$ and

$$P_{k-1}(S) = M_{k-1}(S) \otimes \cdots \otimes M_1(S), \quad M_j(S) = \begin{cases} Y_j, & j \in S, \\ X_j, & j \notin S. \end{cases} \quad (9)$$

The derivation is given in Appendix.

In general, the Pauli expansion is a lengthy and tedious process, but for few-qubit systems, the Hamiltonian matrix takes fairly simple forms. For one qubit, it is given by X and I gates,

$$\hat{H} = -\frac{1}{ma^2} X + \left(\frac{1}{ma^2} + \frac{V_0}{2a} \right) I, \quad (10)$$

and for two qubits by X , I , and Z gates,

$$\hat{H} = -\frac{1}{2ma^2} [I_2 \otimes X_1 + X_2 \otimes X_1] - \frac{V_0}{4a} Z_2 \otimes Z_1 + \left(\frac{1}{ma^2} + \frac{V_0}{4a} \right) I_2 \otimes I_1. \quad (11)$$

Under the $L \rightarrow iL$ rotation, the Hamiltonian matrix becomes non-Hermitian,

$$\hat{H}^{(iL)} = \frac{1}{ma^2} X - \left(\frac{1}{ma^2} + i \frac{V_0}{2a} \right) I, \quad (12)$$

for one qubit, and

$$\hat{H}^{(iL)} = \frac{1}{2ma^2} [I_2 \otimes X_1 + X_2 \otimes X_1] + i \frac{V_0}{4a} Z_2 \otimes Z_1 - \left(\frac{1}{ma^2} + i \frac{V_0}{4a} \right) I_2 \otimes I_1 \quad (13)$$

for two qubits. The non-Hermitian Hamiltonian has the general form

$$\hat{H}^{(iL)} = H_1 + iH_2, \quad (14)$$

where H_1 is Hermitian and iH_2 is anti-Hermitian. Both H_1 and H_2 are Hermitian matrices.

III. QUANTUM ALGORITHM FOR TRACE OF NONUNITARY OPERATORS

Symbolically, we can suppress the real-time oscillatory operator e^{-iHt} in two ways. One is by rotating to imaginary time $t \rightarrow -i\tau$, so $e^{-iHt} \rightarrow e^{-H\tau}$. The Hermitian Hamiltonian is untouched. The other is by rotating space $L \rightarrow iL$, so $e^{-iHt} \rightarrow e^{-iH^{(iL)}t} \rightarrow e^{-iH_1t} e^{H_2t}$. In both cases, we must deal with the problem of a nonunitary operator: $e^{-H\tau}$ in imaginary-time evolution or e^{H_2t} in real-time evolution. Whether it is an exponential growth or decay depends on whether it is a bound or a scattering state in the system.

A. Trace of nonunitary operator

The problem boils down to taking the trace of a nonunitary operator A ,

$$\text{Tr}[A] = \sum_{\alpha} \langle \alpha | A | \alpha \rangle, \quad (15)$$

which can be accomplished by combining two quantum algorithms [23]: block encoding and Hadamard test.

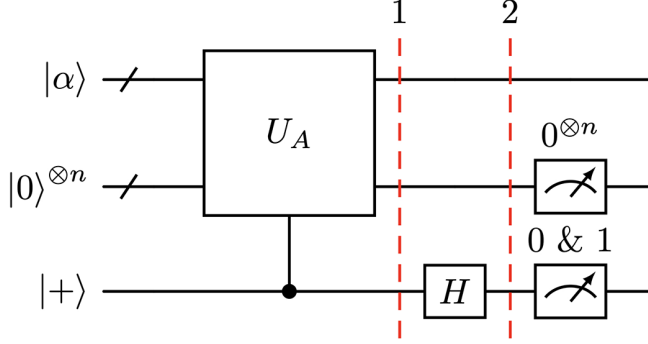


FIG. 1. Quantum circuit for computing real part of $\langle \alpha | \frac{A^\dagger + A}{2} | \alpha \rangle$, where nonunitary operator A is block encoded in unitary operator U . $|+\rangle$ refers to the linear superposition state $H|0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}$.

First, the nonunitary operator A has to be block encoded in a unitary matrix U_A with n ancillary qubits,

$$U_A = \begin{pmatrix} A & \cdot \\ \cdot & \cdot \end{pmatrix}, \quad (16)$$

which can then be projected to the nonunitary sector,

$$U_A(|\alpha\rangle \otimes |0\rangle^{\otimes n}) = A|\alpha\rangle \otimes |0\rangle^{\otimes n} + \dots, \quad (17)$$

discarding everything else from the non- A elements in the U_A matrix, as represented by the ellipsis. The implementation of block encoding for real-time evolution of non-Hermitian Hamiltonian systems or imaginary-time evolution of Hermitian systems will be discussed in Secs. III B and III C.

Next, combining with Hadamard test algorithm [23] allows us to evaluate $\text{Tr}[A]$. For the real part, starting with quantum circuit in Fig. 1, the quantum state at step 1 is given by

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}|\alpha\rangle \otimes |0\rangle^{\otimes n} \otimes |0\rangle + \frac{1}{\sqrt{2}}A|\alpha\rangle \otimes |0\rangle^{\otimes n} \otimes |1\rangle + \dots. \quad (18)$$

Applying another Hadamard gate on the last ancillary qubit for Hadamard test algorithm at step 2 then yields

$$|\psi_2\rangle = \frac{1+A}{2}|\alpha\rangle \otimes |0\rangle^{\otimes n} \otimes |0\rangle + \frac{1-A}{2}|\alpha\rangle \otimes |0\rangle^{\otimes n} \otimes |1\rangle + \dots. \quad (19)$$

Measurements will be carried out on $n+1$ ancillary qubits (n for block encoding and one for Hadamard test algorithm), only keeping zeros on all n ancillary qubits for block encoding, and both zero (labeled as 0) and one (labeled as 1) for ancillary qubit for the Hadamard test algorithm. The probability difference is given by

$$P_\alpha(0) - P_\alpha(1) = \langle \alpha | \frac{A^\dagger + A}{2} | \alpha \rangle, \quad (20)$$

where $P_\alpha(0)$ and $P_\alpha(1)$ refer to the probabilities of finding all n ancillary qubits at zero states and the ancillary qubit for Hadamard test algorithm at state zero and state one, respectively.

Finally, by summing over all the $|\alpha\rangle$ basis states and using $\text{Tr}[A^\dagger] = \text{Tr}[A^*]$, we find

$$\sum_\alpha [P_\alpha(0) - P_\alpha(1)] = \text{Re}(\text{Tr}[A]). \quad (21)$$

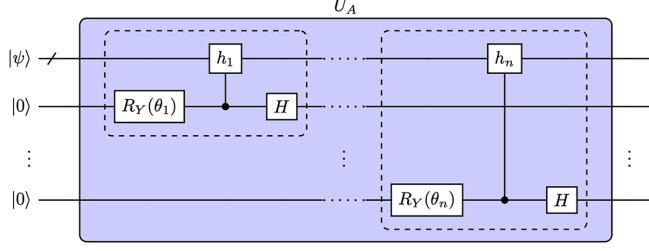


FIG. 2. Block encoding quantum circuit for unitary evolution of non-Hermitian system in real time [see Eqs. (25)–(29)].

Similarly, by inserting a S gate in front of the Hadamard gate in Fig. 1, the imaginary part can be measured by

$$\sum_{\alpha} [P_{\alpha}(1) - P_{\alpha}(0)] = \text{Tr} \left[\frac{A - A^{\dagger}}{2i} \right] = \text{Im}(\text{Tr}[A]). \quad (22)$$

B. Block encoding for real-time evolution of non-Hermitian systems

Here, we detail how to implement block encoding for the non-Hermitian Hamiltonian in real-time evolution arising from the $L \rightarrow iL$ rotation, using a technique developed in Refs. [24–26]. In general, a non-Hermitian Hamiltonian can be split into two groups (Hermitian and anti-Hermitian) in Pauli strings,

$$\hat{H} = \sum_i c_i \hat{h}_i + i \sum_{j=1}^n c_j \hat{h}_j, \quad (23)$$

where all the coefficients c_i are real, and all $\hat{h}_i$'s are tensor products of Pauli gates and are Hermitian. We have assumed n terms in the anti-Hermitian operator group, but kept open the number of terms in the Hermitian operator group.

Using the Hamiltonian in Eq. (23), the real-time evolution of a non-Hermitian system with a single step δt is given by

$$e^{-i\hat{H}\delta t} \simeq \left(\prod_i e^{-ic_i \hat{h}_i \delta t} \right) \left(\prod_{j=1}^n e^{c_j \hat{h}_j \delta t} \right), \quad (24)$$

where the terms in the first bracket are all unitary operators, but the terms in the second bracket are all nonunitary operators and have to be block encoded into unitary operators by using ancillary qubits.

The quantum circuit of block encoding a single step of time evolution operator, $e^{-i\hat{H}\delta t}$ in Eq. (24), into unitary operation, $U_A(|\psi\rangle \otimes |0\rangle^{\otimes n})$, is given in Fig. 2, where

$$|\psi\rangle = \prod_i e^{-ic_i \hat{h}_i \delta t} |\alpha\rangle \quad (25)$$

are pure unitary operations that do not require block encoding. The nonunitary operator A in Fig. 2 requires ancillary qubits for block encoding and is defined by

$$A = \prod_{j=1}^n \frac{e^{c_j \hat{h}_j \delta t}}{\sqrt{2(\alpha_j^2 + \beta_j^2)}}, \quad (26)$$

where

$$\alpha_j = \cosh(c_j \delta t), \quad \beta_j = \sinh(c_j \delta t). \quad (27)$$

Each nonunitary operator for a single time evolution step, $e^{c_j \hat{h}_j \delta t}$, requires one ancillary qubit for block encoding into a unitary operation, and n nonunitary operators require n ancillary qubits. The extra normalization factors $\frac{1}{\sqrt{2(\alpha_j^2 + \beta_j^2)}}$ in Eq. (26) for each $e^{c_j \hat{h}_j \delta t}$ term are generated by the $R_Y(\theta_j)$ gate in block encoding process:

$$R_Y(\theta_j) = \begin{bmatrix} \frac{\alpha_j}{\sqrt{\alpha_j^2 + \beta_j^2}} & \frac{\beta_j}{\sqrt{\alpha_j^2 + \beta_j^2}} \\ -\frac{\beta_j}{\sqrt{\alpha_j^2 + \beta_j^2}} & \frac{\alpha_j}{\sqrt{\alpha_j^2 + \beta_j^2}} \end{bmatrix}, \quad (28)$$

where the rotation angles are defined by

$$\theta_j = -2 \cos^{-1} \left(\frac{\alpha_j}{\sqrt{\alpha_j^2 + \beta_j^2}} \right). \quad (29)$$

The block encoding method given in Fig. 2 can be implemented for N -step time evolution via the trotterization approximation,

$$e^{-i\hat{H}t} \simeq \left[\left(\prod_i e^{-ic_i \hat{h}_i \delta t} \right) \left(\prod_{j=1}^n e^{c_j \hat{h}_j \delta t} \right) \right]^N, \quad t = N\delta t. \quad (30)$$

Therefore, $n \times N$ ancillary qubits are needed for block encoding of nonunitary operators, and the number of required ancillary qubits increases linearly as time increases.

C. Block encoding for imaginary-time evolution of Hermitian systems

As discussed earlier, evolution of Hermitian Hamiltonian in imaginary time involves $e^{-H\delta\tau}$, and evolution of non-Hermitian Hamiltonian in real time involves $e^{-iH_1\delta t} e^{H_2\delta t}$. They are mathematically equivalent as far as the nonunitary part is concerned: $e^{-H\delta\tau}$ versus $e^{H_2\delta t}$. So the same block encoding procedure in the previous section applies, absent of the unitary part $e^{-iH_1\delta t}$ and with a sign difference.

IV. NUMERICAL TEST

In this section, we put both approaches (imaginary time and non-Hermitian) to numerical testing on a quantum simulator using the exact solutions as a measuring stick. We are limited to small systems because of the computational demand to run the quantum circuits.

A. Imaginary-time quantum simulation of integrated correlation function

In imaginary time, the difference of integrated correlation functions takes the form

$$C(\tau) - C_0(\tau) = \text{Tr}[e^{-\hat{H}\tau} - e^{-\hat{H}_0\tau}], \quad (31)$$

which is real valued. The imaginary part is completely removed by Wick rotation $\tau = it$. We will construct quantum circuits to simulate both the one-qubit Hamiltonian in Eq. (10) and two-qubit Hamiltonian in Eq. (11).

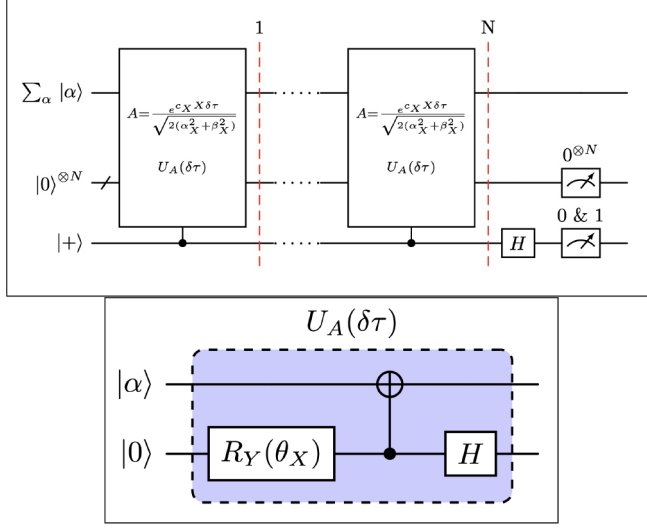


FIG. 3. Quantum circuits for computing imaginary-time evolution of single-qubit system of Eq. (33) (upper panel), and the block encoding of nonunitary operator A into $U_A(\delta\tau)$ (lower panel).

1. Single-qubit Hamiltonian system

The one-qubit Hamiltonian has only two terms. The second term in Eq. (10) with an identity gate yields a trivial factor, which can be pulled out from the trace:

$$\Delta C(\tau) = e^{-\frac{1}{ma^2}\tau} (e^{-\frac{V_0}{2a}\tau} - 1) \text{Tr}[(e^{c_X X \delta\tau})^N], \quad (32)$$

where $\tau = N\delta\tau$ and $c_X = \frac{1}{ma^2}$. So we will only compute the nontrivial trace term in Eq. (32) in quantum simulation to reduce computation cost.

In Fig. 3, we show the block encoding quantum circuits for computing trace of nonunitary operator $e^{c_X X \tau}$ modified by extra normalization factors that are associated to the input $c_X \delta\tau$,

$$\sum_{\alpha} \langle \alpha | A^N | \alpha \rangle, \quad \text{with} \quad A = \frac{e^{c_X X \delta\tau}}{\sqrt{2(\alpha_X^2 + \beta_X^2)}}, \quad (33)$$

where

$$\alpha_X = \cosh(c_X \delta\tau), \quad \beta_X = \sinh(c_X \delta\tau). \quad (34)$$

The $R_Y(\theta_X)$ rotation angle θ_X is defined in Eq. (29).

In this circuit, a single qubit is used for the computation of $\sum_{\alpha} |\alpha\rangle$. Each time step requires one ancillary qubit for block encoding $e^{c_X X \delta\tau}$ into a unitary operation. Thus, N time steps require N ancillary qubits for block encoding of the $(e^{c_X X \delta\tau})^N$ operator. Adding another ancillary qubit for computing the expectation value $\langle \alpha | (e^{c_X X \delta\tau})^N | \alpha \rangle$ (Hadamard test), a total of $N + 1$ ancillary qubits are needed for quantum simulation of the quantity defined in Eq. (33). As the number of time steps N is increased, the quantum circuit grows linearly in size both vertically (ancillary qubits) and horizontally (time evolution). Only 0s are kept in the measurement of N ancillary qubits for block encoding, and both 0 and 1 are kept for the measurement of the additional ancillary qubit for the Hadamard test algorithm. The probabilities of $N + 1$ ancillary qubits in the state of $|0\rangle^{\otimes N} \otimes |0\rangle$ and $|0\rangle^{\otimes N} \otimes |1\rangle$ for each $|\alpha\rangle$ are labeled as $P_{\alpha}(0)$ and $P_{\alpha}(1)$, respectively, and the sum of the differences

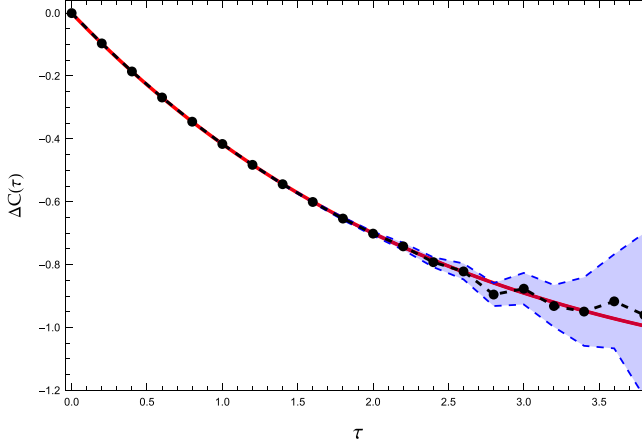


FIG. 4. Imaginary-time simulation of $\Delta C(\tau)$ for the one-qubit system in Eq. (10). Red curve is the exact solution. The black dots and blue band represent quantum simulator results for the mean value and two-standard-error band generated from 100 trials, each with 100 000 shots. The model parameters are $m = 1$, $a = 4$, and $V_0 = 2$. The time step is $\delta\tau = 0.2$.

is related to $\Delta C(\tau)$ by

$$\Delta C(\tau) = e^{-\frac{1}{ma^2}\tau} \left(e^{-\frac{V_0}{2a}\tau} - 1 \right) \left(\sqrt{2(\alpha_X^2 + \beta_X^2)} \right)^N \sum_{\alpha} (P_{\alpha}(0) - P_{\alpha}(1)). \quad (35)$$

In Fig. 4, we show the comparison of quantum simulator results for $\Delta C(\tau)$ versus the exact solution that is obtained by solving Eq. (31) directly. The model parameters are chosen as $m = 1$, $a = 4$, $V_0 = 2$, and hence $L = 2a$ according to $a = \frac{L}{2}$. We observe no oscillatory behavior in imaginary-time simulation results, and the agreement with the exact solution extends to over ten time steps before the signal is lost in statistical fluctuations. As the number of time steps goes up, more statistics are needed in the simulation. One hundred trials of 100 000 shots each are used in this example. The quantum simulator assumes error-free quantum hardware so only statistical errors are accounted for.

2. Two-qubit Hamiltonian system

For the two-qubit system Hamiltonian given in Eq. (11), the integrated correlation function with a contact interaction in imaginary time is given by

$$C(\tau) = e^{-\left(\frac{1}{ma^2} + \frac{V_0}{4a}\right)\tau} \text{Tr} \left[\left(\prod_{j=1}^3 e^{c_j \hat{h}_j \delta\tau} \right)^N \right], \quad (36)$$

where all c 's and h 's are given by

$$c_1 = c_2 = \frac{1}{2ma^2}, \quad c_3 = \frac{V_0}{4a}, \quad \hat{h}_1 = I_2 \otimes X_1, \quad \hat{h}_2 = X_2 \otimes X_1, \quad \hat{h}_3 = Z_2 \otimes Z_1. \quad (37)$$

In Fig. 5, we show the block encoding quantum circuits for computing

$$\sum_{\alpha} \langle \alpha | A^N | \alpha \rangle, \quad \text{with} \quad A = \prod_{j=1}^3 \frac{e^{c_j \hat{h}_j \delta\tau}}{\sqrt{2(\alpha_j^2 + \beta_j^2)}}, \quad (38)$$

where α_j and β_j are related to $c_j \delta\tau$ by Eq. (27). Two qubits are used for the computation of $\sum_{\alpha} |\alpha\rangle$. Three ancillary qubits are needed to block encode three $\prod_{j=1}^3 e^{c_j \hat{h}_j \delta\tau}$ nonunitary operators into a

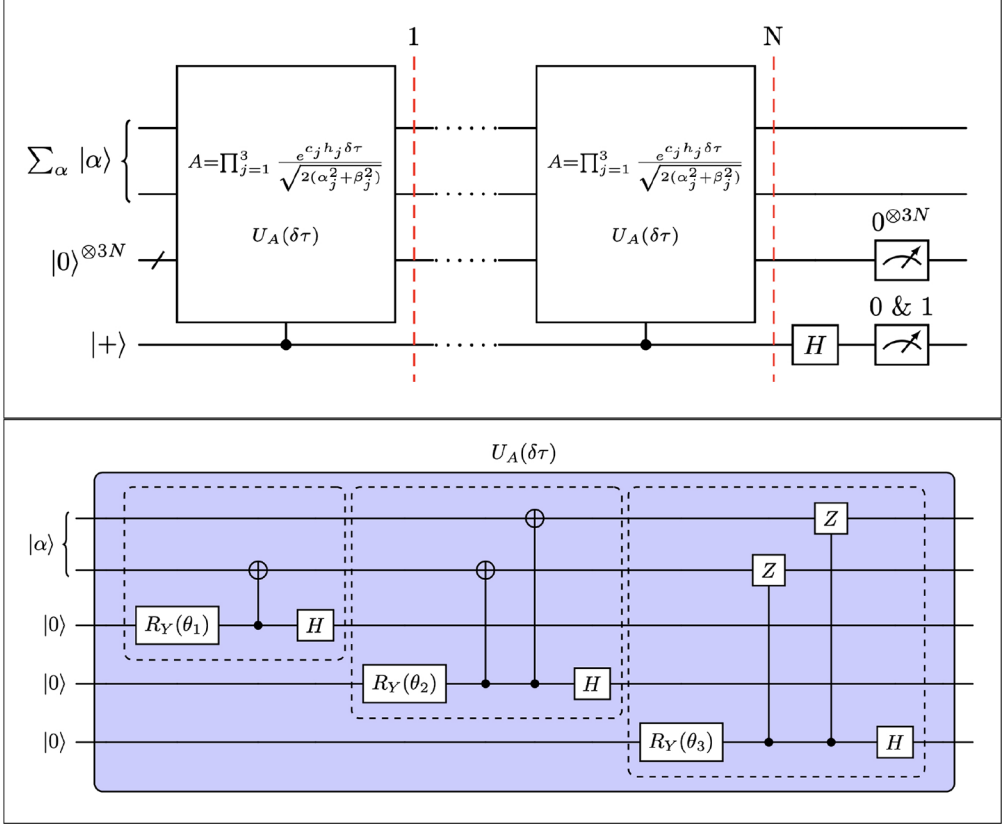


FIG. 5. Quantum circuits for computing imaginary-time evolution of two-qubit system of Eq. (38) (upper panel) and the block encoding of nonunitary operator A into $U_A(\delta\tau)$ (lower panel).

unitary operation U_A for a single time step; thus, a total of $3N + 1$ ancillary qubits are required for N time steps for imaginary-time quantum simulation of a two-qubit Hamiltonian system.

The measurements on the $3N + 1$ ancillary qubits yield

$$C(\tau) = e^{-\left(\frac{1}{ma^2} + \frac{V_0}{4a}\right)\tau} \left(\prod_{j=1}^3 \sqrt{2(\alpha_j^2 + \beta_j^2)} \right)^N \times \sum_{\alpha} (P_{\alpha}(0) - P_{\alpha}(1)). \quad (39)$$

The noninteracting $C_0(\tau)$ can be obtained by setting $V_0 = 0$ (thus, $c_3 = 0$) in the procedure for the interacting case. In Fig. 6, we show the comparison between quantum simulator results and the exact solutions, where the lattice spacing a is adjusted to $4/3$; the rest of model parameters are kept the same as in the one-qubit case. The agreement extends to about five time steps and then is spoiled by statistical errors. This is expected because it requires $3N + 1$ ancillary qubits as opposed to $N + 1$ in the one-qubit case under the same statistics.

B. Real-time quantum simulation of integrated correlation function under $L \rightarrow iL$ rotation

Under the $L \rightarrow iL$ rotation, the single-qubit non-Hermitian Hamiltonian $\hat{H}^{(iL)}$ can be found in Eq. (12). The identity gate term yields a trivial factor that can be pulled out in the integrated correlation function calculation. The X gate term is Hermitian that yields a unitary operator in quantum simulation and does not require block encoding. Such scenarios have been considered in

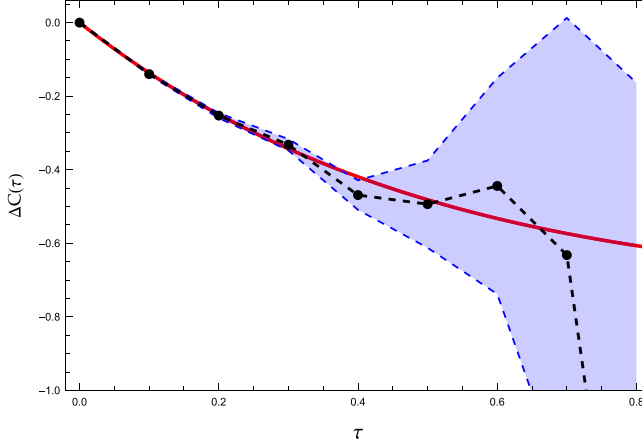


FIG. 6. Similar to Fig. 4, but for the two-qubit system Hamiltonian in Eq. (11). The model parameters are $m = 1$, $a = 4/3$, $V_0 = 2$, and $\delta\tau = 0.1$.

Ref. [19]. Here, we focus on the two-qubit system Hamiltonian given in Eq. (13), which presents the case study of a non-Hermitian system in real-time quantum simulation. The integrated correlation function $C(t) = \text{Tr}[e^{-i\hat{H}^{(iL)}t}]$ for the interacting Hamiltonian in Eq. (13) can be expressed as

$$C(t) = \text{Tr} \left[\left(e^{c_3 \hat{h}_3 \delta t} \prod_{j=1}^2 e^{-ic_j \hat{h}_j \delta t} \right)^N \right] e^{i(\frac{1}{ma^2} + i\frac{V_0}{4a})t}, \quad (40)$$

where all c 's and $\hat{h}$'s are defined in Eq. (37). $\prod_{j=1}^2 e^{-ic_j \hat{h}_j \delta t}$ is a unitary operator and does not require block encoding. However, the nonunitary operator $e^{c_3 \hat{h}_3 \delta t}$ has to be block encoded into a unitary operation that requires one ancillary qubit for each time step. Thus, N time steps require a total of $N + 1$ ancillary qubits for quantum simulation of the two-qubit non-Hermitian Hamiltonian $\hat{H}^{(iL)}$ system.

In Fig. 7, we give the quantum circuits for computing

$$\sum_{\alpha} \langle \alpha | \left(A \prod_{j=1}^2 e^{-ic_j \hat{h}_j \delta t} \right)^N | \alpha \rangle, \quad \text{with} \quad A = \frac{e^{c_3 \hat{h}_3 \delta t}}{\sqrt{2(\alpha_3^2 + \beta_3^2)}}, \quad (41)$$

where α_3 and β_3 are related to $c_3 \delta t$ by definition in Eq. (27). Two qubits are used for the computation of $\sum_{\alpha} |\alpha\rangle$. One ancillary qubit is needed to block encode the $e^{c_3 \hat{h}_3 \delta t}$ nonunitary operator into a unitary operation U_A for a single time step; thus, a total of $N + 1$ ancillary qubits are required for N time steps. Unlike the imaginary-time circuit in Fig. 6, the non-Hermitian circuit requires an extra step to handle the unitary operator $\prod_{j=1}^2 e^{-ic_j \hat{h}_j \delta t}$.

The measurements on the $N + 1$ ancillary qubits yield

$$C(t) = e^{i(\frac{1}{ma^2} + i\frac{V_0}{4a})t} \left(\sqrt{2(\alpha_3^2 + \beta_3^2)} \right)^N \sum_{\alpha} (P_{\alpha}(0) - P_{\alpha}(1)). \quad (42)$$

Similarly, the noninteracting $C_0(t)$ can be obtained by setting $V_0 = 0$ in the procedure for the interacting case. In Fig. 8, we show the comparison between quantum simulator results and the exact solution using the same model parameters and one hundred trials of 100 000 shots each. The

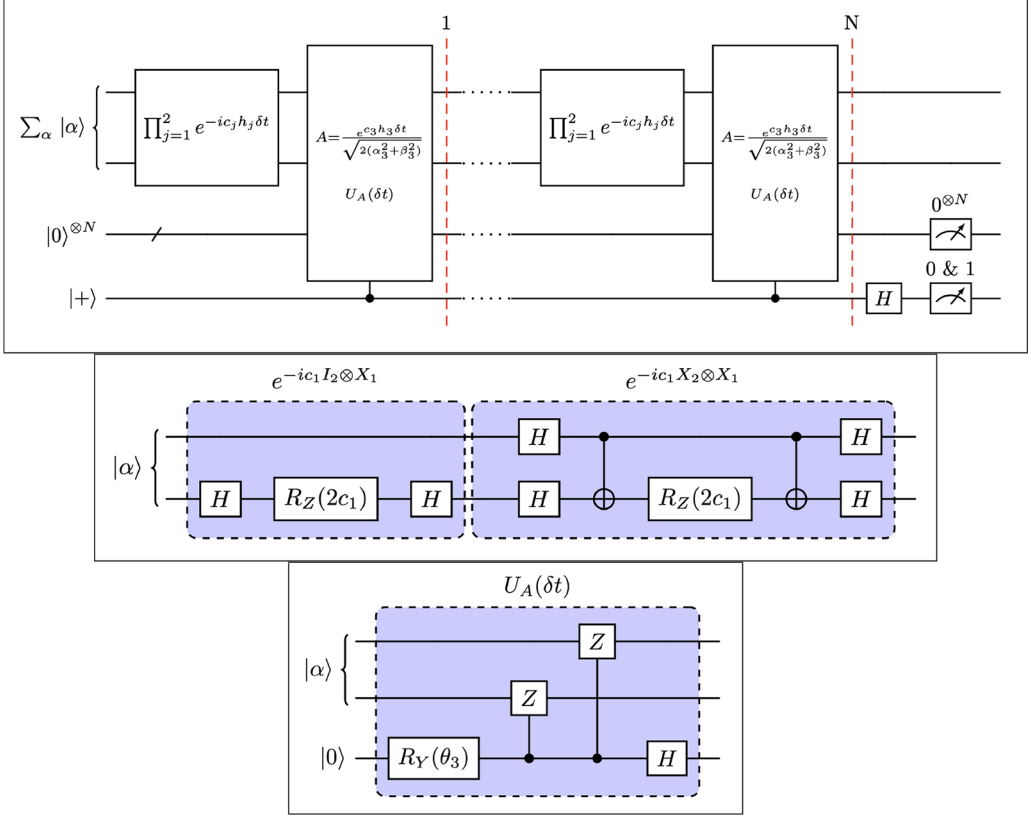


FIG. 7. Quantum circuits for computing real-time evolution of two-qubit non-Hermitian system of Eq. (41) (upper panel), unitary operator $\prod_{j=1}^2 e^{-ic_j h_j \delta t}$ (mid panel), and the block encoding of nonunitary operator A into $U_A(\delta \tau)$ (lower panel).

exact result is obtained by solving

$$C(t) - C_0(t) = \text{Tr}[e^{-i\hat{H}^{(IL)}t} - e^{-i\hat{H}_0^{(IL)}t}] \quad (43)$$

directly for the Hamiltonian in Eq. (13). We see that the agreement extends to around 15 time steps in the real part and about 10 steps in the imaginary part. This is much better than the two-qubit case for imaginary-time evolution under the same conditions. The reason is simply that the non-Hermitian circuit requires fewer ancillary qubits than in the imaginary-time circuit.

V. QUANTUM CIRCUITS OPTIMIZATION FOR REAL-TIME NON-HERMITIAN QUANTUM SIMULATION

As demonstrated in Sec. IV, overall performance of each time step depends heavily on the number of required ancillary qubits to embed the anti-Hermitian part of Hamiltonian into unitary operations. In a rough estimate, the success probability in both the imaginary-time and the non-Hermitian approaches is proportional to $1/2^n$, where n is the number of ancillary qubits required for block encoding. Though non-Hermitian real-time quantum simulation with $L \rightarrow iL$ rotation approach reduced the number of required ancillary qubits compared with imaginary-time simulation, fundamentally, it still faces the challenge of inefficiency and practicality in scaling up the size of a quantum system.

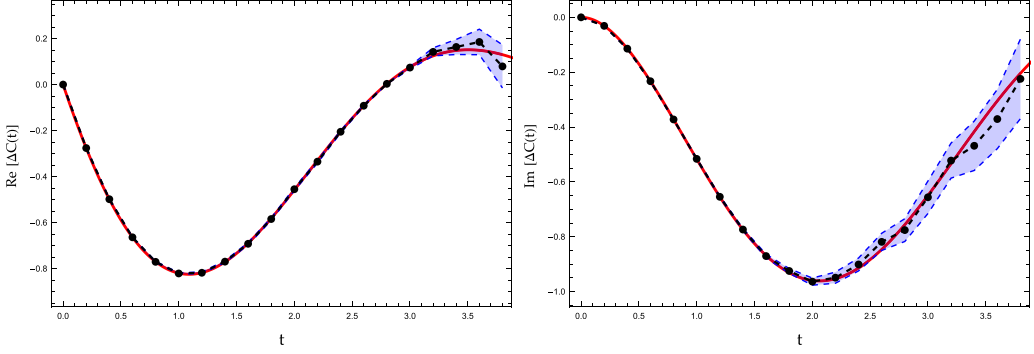


FIG. 8. Real-time quantum simulation of real (left) and imaginary (right) parts of $\Delta C(t)$ for the two-qubit non-Hermitian system in Eq. (13). Red curve is the exact solution. The black dots and blue band represent quantum simulator results for the mean value and two-standard-error band generated from 100 trials, each with 100 000 shots. The model parameters are $m = 1$, $a = 4/3$, $V_0 = 2$, and $\delta t = 0.2$.

In this section, we show that the quantum circuits in non-Hermitian real-time quantum simulation with $L \rightarrow iL$ rotation approach can be drastically improved and only a single ancillary qubit is required for block encoding in each time step, resulting in a distinct advantage over the imaginary-time approach. With the $L \rightarrow iL$ rotation, the only anti-Hermitian terms in Eq. (7) are from the interaction potential term:

$$V^{(iL)}(x_\alpha) = \begin{cases} -i\frac{V_0}{2a}, & \alpha \in \left[\frac{2\Gamma}{2} - 1, \frac{2\Gamma}{2}\right], \\ 0, & \text{otherwise,} \end{cases} \quad (44)$$

and $e^{-i\hat{V}^{(iL)}\delta t}$ matrix is a diagonal nonunitary matrix,

$$e^{-i\hat{V}^{(iL)}\delta t} = \begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & e^{-\frac{V_0\delta t}{2a}} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & e^{-\frac{V_0\delta t}{2a}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & 0 & \cdots & 1 \end{bmatrix}. \quad (45)$$

It turns out that for a diagonal nonunitary matrix, the insertion of nonunitary terms such as $e^{-\frac{V_0\delta t}{2a}}$ into the certain locations of a diagonal matrix can be accomplished more efficiently than the method used in Sec. III B by breaking up $\hat{V}^{(iL)}$ into the sum of Pauli strings: $\sum_j c_j \hat{h}_j$ in Eq. (23), and then block encoding each term with one ancillary qubit into unitary operations.

Using a two-qubit system as an example, the block encoding of a diagonal matrix

$$A = \begin{bmatrix} e^{-v_0\delta t} & 0 & 0 & 0 \\ 0 & e^{-v_1\delta t} & 0 & 0 \\ 0 & 0 & e^{-v_2\delta t} & 0 \\ 0 & 0 & 0 & e^{-v_3\delta t} \end{bmatrix} \quad (46)$$

can be accomplished with a single ancillary qubit and four controlled- R_y rotation gates in Fig. 9. The rotation angles in Fig. 9 are defined by

$$\theta_\alpha = 2 \cos^{-1}(e^{-v_\alpha\delta t}), \quad \alpha \in [0, 3], \quad (47)$$

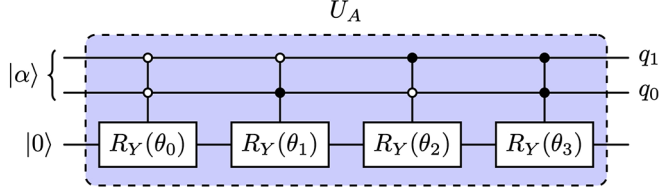


FIG. 9. Quantum circuits for the block encoding of a diagonal nonunitary operator A in Eq. (46) into U_A .

where we have assumed that v_i 's are all positive and the potential is repulsive. The controlled- $R_Y(\theta_\alpha)$ rotation gate inserts a factor $e^{-v_\alpha \delta t}$ into the diagonal matrix at location α by using a combination of both states 0 and 1 in two qubits that is the exact binary representation of α .

If v_i 's are all negative and the potential is attractive, then we need to block encode the diagonal matrix,

$$B = \begin{bmatrix} e^{|v_0|\delta t} & 0 & 0 & 0 \\ 0 & e^{|v_1|\delta t} & 0 & 0 \\ 0 & 0 & e^{|v_2|\delta t} & 0 \\ 0 & 0 & 0 & e^{|v_3|\delta t} \end{bmatrix}, \quad (48)$$

with the value of all elements greater than 1. First of all, by pulling a common factor $e^{\sum_{\alpha=0}^3 |v_\alpha| \delta t}$ out of matrix, we can turn it into a diagonal matrix that has all the value of matrix elements less than 1 and can be embedded into a unitary operation by using controlled- R_Y rotation gates. Hence, the matrix,

$$A = e^{-\sum_{\alpha=0}^3 |v_\alpha| \delta t} B, \quad (49)$$

can be block encoded using the quantum circuit in Fig. 9, where all the angles are now defined by

$$\theta_\alpha = 2 \cos^{-1} \left(e^{-\sum_{\beta \neq \alpha} |v_\beta| \delta t} \right), \quad \alpha \in [0, 3]. \quad (50)$$

The common factor $e^{\sum_{\alpha=0}^3 |v_\alpha| \delta t}$ can be installed at the end of quantum simulation at each time step.

In the cases that v_i 's are a mixture of negative and positive values, the diagonal matrix again can be turned into a diagonal matrix with the value of all elements less than 1 by pulling out a common factor as in the attractive potential case.

Circling back to the quantum mechanical model with the expression $e^{-i\hat{V}^{(IL)}\delta t}$ given in Eq. (45), without losing generality, again using a two-qubit system as a simple example, the integrated correlation function,

$$C(t) = \text{Tr} \left[\left(e^{-i\hat{V}^{(IL)}\delta t} \prod_{j=1}^2 e^{-ic_j \hat{h}_j \delta t} \right)^N \right] e^{i\frac{1}{m\alpha^2}t}, \quad (51)$$

can be computed by using the quantum circuit in Fig. 10, where we have assumed that the potential is repulsive and $c_{1,2}$ and $\hat{h}_{1,2}$ are defined in Eq. (37). By using controlled- R_Y rotation gates to insert $e^{-v_\alpha \delta t}$ into a diagonal matrix $e^{-\hat{V}^{(IL)}\delta t}$ as described above, now regardless of the system size, only a single ancillary qubit is required for each time step for block encoding $e^{-\hat{V}^{(IL)}\delta t}$ into unitary-gate operations. With N steps, a total of N ancillary qubits are needed for block encoding, which is equivalent to the midcircuit measurement at each time step.

VI. SUMMARY AND OUTLOOK

In this work, we explored two proposals to suppress the oscillatory behavior in real-time simulation of quantum systems. We use the same simple case study of integrated correlation scattering

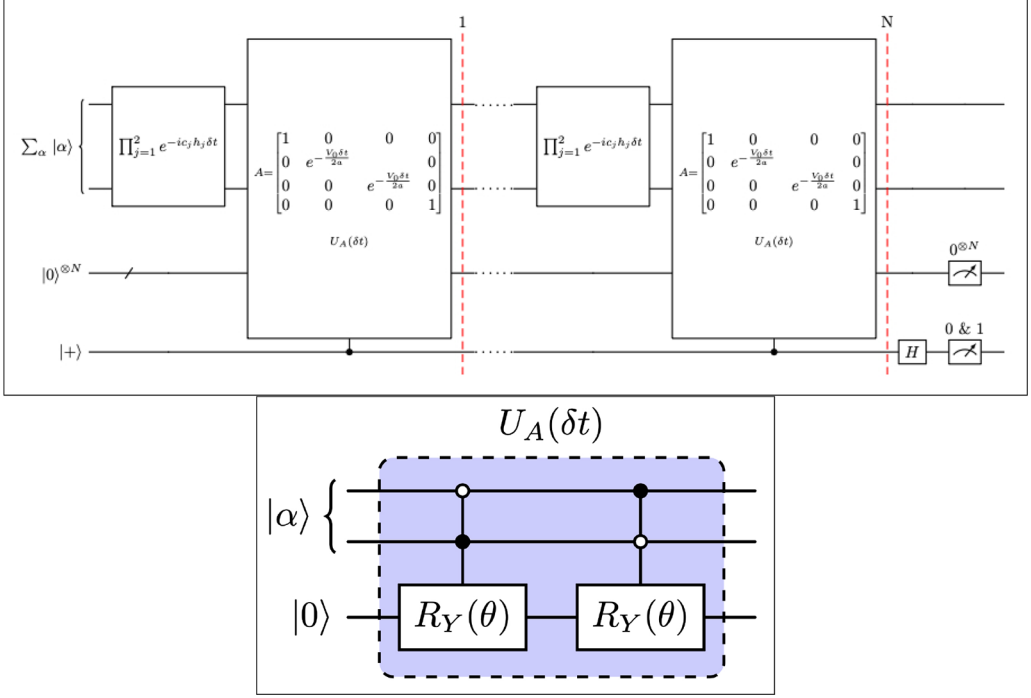


FIG. 10. Quantum circuits for computing real-time evolution of two-qubit non-Hermitian system of Eq. (51) (upper panel), unitary operator $\prod_{j=1}^2 e^{-ic_j h_j \delta t}$ are same as the quantum circuit in the mid panel in Fig. 7, and the block encoding of nonunitary operator $A = e^{-i\hat{V}^{(L)} \delta t}$ into $U_A(\delta \tau)$ (lower panel). The angle θ in lower panel is defined by $\theta = 2 \cos^{-1}(e^{-\frac{V_0 \delta t}{2a}})$.

formalism in 1D quantum mechanics as in Ref. [19]. One proposal is to simulate a non-Hermitian system in real time, and the other is to simulate a Hermitian system in imaginary time. Both proposals lead to the problem of quantum simulation of a nonunitary operator.

We showed that combining two quantum algorithms (Hadamard test [23] and block encoding [24–26]) can work in both cases. The combined quantum algorithm has a simple form and can be easily implemented. It does not require midcircuit measurement and the only input is the parameters in the Hamiltonian. The algorithm does require that imaginary-time Hamiltonian and the anti-Hermitian part of the non-Hermitian Hamiltonian [see Eq. (14)] be expressed in terms of Pauli strings for block encoding.

In terms of computational demand, the size and length of the quantum circuits grow linearly as the number of time steps increases in both approaches. Even for small-size Hamiltonian systems, running tests on local quantum simulators becomes a computational challenge after 10–20 steps. We constructed one-qubit and two-qubit Hamiltonian systems to numerically test the ideas against exact solutions. In both cases, we observe good agreement with the exact solutions to reasonably long times before the signal is overwhelmed by statistical fluctuations.

The non-Hermitian simulation does have a computational advantage over the imaginary-time one. Comparing at the two-qubit Hamiltonian level, there are three nonunitary terms in imaginary-time Hermitian simulation that need to be block encoded, versus only one term in real-time non-Hermitian simulation. Block encoding of each nonunitary term introduces one extra ancillary qubit to make it into a unitary operation. Hence, the cost of imaginary-time quantum simulation is 3 times higher than that of non-Hermitian one.

The success probability in both the imaginary-time and the non-Hermitian approaches is proportional to $1/2^n$, where n is the number of ancillary qubits required for block encoding. This

makes the simulations appear costly and impractical at scale. Fortunately, the quantum circuits for real-time non-Hermitian quantum simulations can be optimized so that only a single ancillary qubit is required for block encoding nonunitary diagonal $e^{-i\hat{V}^{(iL)}\delta t}$ matrix for each time step. Hence, even without amplitude amplification algorithms, the correlation function can be computed fairly accurately up to at least ten steps with 100 000 shots. The $L \rightarrow iL$ rotation approach definitely boosts our confidence for the practicality of quantum simulation at scale. How the $L \rightarrow iL$ rotation works in other field theory models, such as the ϕ^4 theory, and whether the quantum simulation of a non-Hermitian system is practical in general are not clear at this stage and deserve further study.

Looking forward, although the work performed here is limited to a simple quantum mechanical model and small systems, we expect the imaginary-time and non-Hermitian approaches to be helpful in simulation of other quantum systems on quantum computers. Finally, it should be mentioned that the computational challenge mentioned above is due to running quantum simulators on classical computers. If the circuits are executed on fault-free quantum hardware, quantum advantage is expected.

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX: DERIVATION OF THE PAULI BASIS EXPRESSION FOR $\hat{H}_b$

In this Appendix, we derive the Pauli basis representation of

$$B_\Gamma = \sum_{\alpha=0}^{2^{\Gamma-1}-1} (|2\alpha+1\rangle\langle 2\alpha+2| + |2\alpha+2\rangle\langle 2\alpha+1|), \quad (\text{A1})$$

where we identify $|2^\Gamma\rangle \equiv |0\rangle$, so that $\hat{H}_b$ is obtained by multiplying by $\frac{-1}{2ma^2}$. Here, the computational basis is ordered in bitwise representation as

$$|\alpha\rangle = |b_\Gamma \cdots b_1\rangle, \quad \alpha = \sum_{j=1}^{\Gamma} 2^{j-1} b_j, \quad (\text{A2})$$

with b_1 the least significant bit.

The operator in Eq. (A1) swaps the basis-state pairs

$$0 \leftrightarrow 2^\Gamma - 1, \quad 1 \leftrightarrow 2, \quad \dots, \quad 2^\Gamma - 3 \leftrightarrow 2^\Gamma - 2. \quad (\text{A3})$$

If we split the basis according to the most significant bit by setting $|b, \mu\rangle \equiv |b\rangle \otimes |\mu\rangle$, where $b \in \{0, 1\}$ and $|\mu\rangle$ denotes the last $\Gamma - 1$ qubits, then away from $\mu = 0$ and $\mu = 2^{\Gamma-1} - 1$, the pairings in Eq. (A3) are identical in the $b = 0$ and $b = 1$ halves for the respective $(\Gamma - 1)$ -qubit actions on $|\mu\rangle$. The only changes occur at the corners with

$$|0\rangle \otimes |0^{\Gamma-1}\rangle \leftrightarrow |1\rangle \otimes |1^{\Gamma-1}\rangle, \quad |0\rangle \otimes |1^{\Gamma-1}\rangle \leftrightarrow |1\rangle \otimes |0^{\Gamma-1}\rangle.$$

This means that we can recover the operator B_Γ by starting from two copies of the $(\Gamma - 1)$ -qubit operator $B_{\Gamma-1}$ and replacing the two internal corner swaps by two half swaps.

In terms of a matrix expression, we can write this by defining $W_n = |0^n\rangle\langle 1^n| + |1^n\rangle\langle 0^n|$ and writing

$$B_n = \begin{pmatrix} B_{n-1} - W_{n-1} & W_{n-1} \\ W_{n-1} & B_{n-1} - W_{n-1} \end{pmatrix} \quad (\text{A4})$$

or equivalently, $B_n = I_n \otimes B_{n-1} + (X_n - I_n) \otimes W_{n-1}$, with $B_1 = X_1$.

For one qubit,

$$|0\rangle\langle 1| = \frac{X + iY}{2}, \quad |1\rangle\langle 0| = \frac{X - iY}{2}.$$

And so

$$W_n = |0^n\rangle\langle 1^n| + |1^n\rangle\langle 0^n| = \frac{1}{2^n} [(X_n + iY_n) \otimes \cdots \otimes (X_1 + iY_1) \quad (\text{A5})$$

$$+ (X_n - iY_n) \otimes \cdots \otimes (X_1 - iY_1)]. \quad (\text{A6})$$

For each subset $S \subseteq \{1, \dots, n\}$, if we define

$$P_{k-1}(S) = M_{k-1}(S) \otimes \cdots \otimes M_1(S), \quad M_j(S) = \begin{cases} Y_j, & j \in S, \\ X_j, & j \notin S. \end{cases} \quad (\text{A7})$$

Then, choosing Y_j exactly on the subset S contributes coefficient $i^{|S|}$ from the first product in Eq. (A6) and $(-i)^{|S|}$ from the second after expanding these binomials. Hence, the coefficient of $P_n(S)$ in W_n is $\frac{1}{2^n}(i^{|S|} + (-i)^{|S|})$. If $|S|$ is odd, this vanishes, whereas if $|S| = 2r$ is even, then $i^{|S|} + (-i)^{|S|} = 2(-1)^r = 2(-1)^{\frac{|S|}{2}}$. Together with the recursion for B_n , this iterates to the expression [Eq. (8)] for $\hat{H}_b$.

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