# Continuous-Variable Assisted Thermal Quantum Simulation

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Simulation of a quantum many-body system at finite temperatures is crucially important but quite challenging. Here we present an experimentally feasible quantum algorithm assisted with continuous variable for simulating quantum systems at finite temperatures. Our algorithm has a time complexity scaling polynomially with the inverse temperature and the desired accuracy. We demonstrate the quantum algorithm by simulating a finite temperature phase diagram of the quantum Ising and Kitaev models. It is found that the important crossover phase diagram of the Kitaev ring can be accurately simulated by a quantum computer with only a few qubits and thus the algorithm may be implementable on current quantum processors. We further propose a protocol with superconducting or trapped ion quantum computers.

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*Introduction.*—Simulation of quantum many-body systems has been an incentive for building quantum computers [1]. Recent advances of scaling up quantum processors enable us to simulate steady states and dynamics of a quantum system at zero temperature to a larger size [2–5], and, remarkably, to make a simulation of quantum phase transition to be a reality [5,6]. However, simulation of a quantum many-body system at finite temperatures is even more challenging as the state in a quantum computer is usually a pure quantum state, while simulating a quantum system at finite temperatures requires us to simulate a kind of mixed states, namely, quantum thermal (Gibbs) states. The relevance of thermal states is ubiquitous, and its simulation is not only important for physics itself, such as understanding high-$T_c$ superconductivity [7], but also can provide quantum speedup for optimization [8].

Thermal quantum simulation (TQS) requires good control of both quantum coherence and temperature, which challenges the current quantum platforms. A quantum algorithm based on quantum phase estimation may involve a large number of auxiliary qubits and complicated quantum circuits, which is not suitable for near-term quantum simulators [9–12]. Recent hybrid quantum-classical variational algorithms require less quantum resources and are feasible in implementation [13–18], but should be trained for each Hamiltonian at every temperature and thus are not a general solution. Moreover, they wait for a guarantee of quantum advantages in time complexity.

An alternative way is to use continuous variables (CV and also called qumode) for encoding and processing high-density information by exploiting its infinite-dimensional Hilbert space [19,20]. Notably, a hybrid approach of incorporating both qubits and qumodes has been shown to have a potential advantage to make the best of both worlds [21–24]. Moreover, the mainstream platforms of quantum computers often have naturally existing continuous variables, such as motional modes of trapped ions [25,26] and cavity modes of superconducting circuits [27–30], making a hybrid variable approach physically realizable. This may enable us to design hybrid-variable quantum algorithms for TQS with both quantum advantage and feasible physical implementation.

In this Letter, we present a quantum algorithm for thermal quantum simulation assisted with an auxiliary qumode, which has a time complexity scaling polynomially with the inverse temperature $\beta$ and the desired accuracy $\epsilon$. The algorithm converts thermal information, encoded in the CV resource state parametrized with $\beta$, into the temperature of the quantum system. Moreover, by revealing an equivalence relation of the quantum algorithm, we further propose adaptive TQS, allowing TQS at varied $\beta$ with a proper-chosen resource state, which enables flexibility of algorithm design in practice. To show the power of adaptive TQS, we consider thermal states of two typical models, the quantum Ising model [31] and Kitaev ring [32], in the quantum critical regime, and demonstrate that our algorithm can accurately determine the crossover temperature. This indicates an interplay between quantum and thermal fluctuations, which underlines the quantum criticality at finite temperatures can be faithfully captured. An intriguing

 

result here is that the important crossover phase diagram [31] of the Kitaev model with periodic conditions (Kitaev ring) can be accurately simulated by a quantum computer with only a few qubits and thus the algorithm may be implementable on current quantum processors. We also propose an experimental protocol based on a superconducting or trapped ion quantum computer. Our work opens a new avenue for simulating finite temperature quantum systems by exploiting the power of continuous variables.

*Thermal quantum simulation.*—Consider a quantum system described by a Hamiltonian $H$, which can be mapped to a quantum computer with $N$ qubits. The energies and eigenstates of the Hamiltonian governed by the Schrödinger equation $H|u_n\rangle = E_n|u_n\rangle$ $(n = 0, 1, \ldots, D-1,$ where $D = 2^N)$. At a finite temperature $T = 1/\beta$, the system in equilibrium is in a quantum thermal state $\rho(\beta) = e^{-\beta H}/Z(\beta)$, where $Z(\beta) = \mathrm{Tr}e^{-\beta H}$ is the partition function. Our goal is to prepare a pure quantum state $|\psi(\beta)\rangle$ in an enlarger Hilbert space which has the property $\rho(\beta) = \mathrm{Tr}_A|\psi(\beta)\rangle\langle\psi(\beta)|$, where $\mathrm{Tr}_A$ denotes the partial trace of some ancillary degrees of freedom addressed later. One can verify that, partial trace of the first partite of the thermofield double (TFD) state defined as

$$|\psi(\beta)\rangle = \sum_n \frac{e^{-\beta E_n/2}}{\sqrt{\mathcal{Z}(\beta)}}|u_n^*\rangle_A \otimes |u_n\rangle_B \tag{1}$$

is just $\rho(\beta)$. We propose a quantum process as follows,

$$|\psi(\beta)\rangle = \sqrt{\mathcal{C}}I \otimes e^{-\beta H/2}|\psi(0)\rangle, \tag{2}$$

where $\mathcal{C}$ is a normalization factor. Here, $|\psi(0)\rangle = (1/\sqrt{D})\sum_n |n\rangle_A \otimes |n\rangle_B$ is an infinite temperature TFD which can be written as a product of $N$ copies of Bell state (see Supplemental Material for a derivation [33]), and thus is easy to prepare. The central task is then to construct $e^{-\beta H/2}$.

We introduce an auxiliary qumode to represent a nonunitary $e^{-\beta H/2}$ as an integral of unitary operators [20,39–41], which extends the linear-combination-of-unitary operator to the case of CV [8,39,42–45]. Note that

$$e^{-\beta h/2} = \int_{-\infty}^{\infty} dp R(\beta, p) e^{-ihp}, \qquad R(\beta, p) = \frac{2}{\pi}\frac{\beta}{\beta^2 + 4p^2} \tag{3}$$

holds for $h \geq 0$. It implies that we shall add a constant to $H$ to guarantee a nonnegative ground state energy in the algorithm. Then in the basis $\{|u_n\rangle\}$ that $H$ is diagonal, one can verify that

$$e^{-\beta H/2} = \int_{-\infty}^{\infty} dp R(\beta, p) e^{-iHp} \propto \langle 0_q|e^{-iH\hat{p}}|R(\beta)\rangle, \tag{4}$$

where $|R(\beta)\rangle = \sqrt{\beta\pi}\int_{-\infty}^{\infty} dp R(\beta, p)|p\rangle_p$. Here we denote $|p\rangle_p$ $(|q\rangle_q)$ as basis of continuous variable quadrature $\hat{p}$ $(\hat{q})$. Equation (4) shows a scheme that the nonunitary operator $e^{-\beta H/2}$ can be implemented on a quantum computer, assisted with an ancillary qumode. The qumode is prepared at $|R(\beta)\rangle$, evolves jointly with the system by $e^{-iH\hat{p}}$, and is finally projected onto $|0\rangle_q$. As the information related to temperature is encoded in $|R(\beta)\rangle$, we may call it as a resource state.

*Quantum algorithm.*—We now present the procedure of quantum algorithm for preparing thermal quantum simulation. The quantum algorithm is probabilistic since it postselects the quadrature $\hat{q}$ to zero. In practice, the measurement should have a finite precision, which reduces the accuracy while raises the success rate. We model this effect by projecting to a squeezing state $|0, s\rangle = s^{-\frac{1}{2}}\pi^{-\frac{1}{4}}\int dp|p\rangle_p e^{-p^2/2s^2}$, which squeezes the quadrature $\hat{q}$ by a factor $s$. The quantum algorithm, as illustrated in Fig. 1, has three steps: 1. *State preparation.* Prepare $N$ copies of Bell state, $|\psi(0)\rangle = \prod_{i=1}^{N} B_{i,i+N}$, where $B_{i,i+N} = (1/\sqrt{2})(|0_i 0_{i+N}\rangle + |1_i 1_{i+N}\rangle)$ is a Bell state. A qumode is initialized in a resource state $|R(\beta)\rangle$. The total system is in a state $|\Psi_0\rangle = |\psi(0)\rangle \otimes |R(\beta)\rangle$. Therefore, to simulate a Hamiltonian $H$ which is encoded in $N$ qubits, our scheme needs $2N$ qubits and one qumode. 2. *Unitary evolution.* A constant is added to $H$ to make positivity of the spectrum. Then the unitary evolution $I \otimes e^{-iH\hat{p}}$ is implemented and it couples the system with the qumode. The unitary can be decomposed with the Trotter-Suzuki formula, which will be discussed later. The state can be written as

$$|\Psi_1\rangle = \sum_n \int_{-\infty}^{\infty} dp \phi_n(\beta, p)|u_n^*\rangle_A \otimes |u_n\rangle_B \otimes |p\rangle_p, \tag{5}$$

where $\phi_n(\beta, p) = \sqrt{(\beta\pi/D)}R(\beta, p)e^{-E_n p}$. 3. *Projection.* Projecting the qumode onto a squeezing state $|0, s\rangle$, the unnormalized final state (discarding the qumode) is

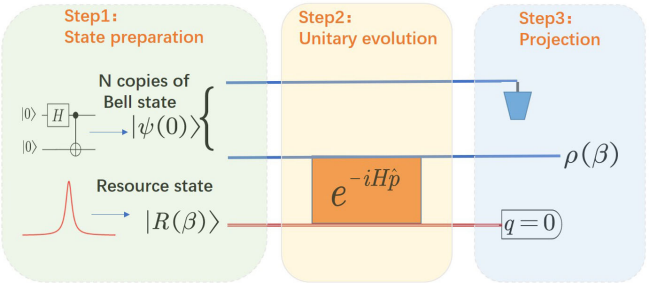


FIG. 1. An illustration of preparing quantum thermal state $\rho(\beta)$ from $N$ copies of Bell states, through coupling the system with a qumode by unitary evolution $e^{-iH\hat{p}}$. The qumode is initialed at the resource state $|R(\beta)\rangle$ and is finally projected onto $|0\rangle_q$. Thermal state $\rho(\beta)$ is obtained by discarding (tracing out) the additional $N$ ancillary qubits.

$$|\tilde{\psi}(\beta)\rangle = \sum_n a(E_i,\beta,s)|u_n^*\rangle_A \otimes |u_n\rangle_B, \tag{6}$$

where $a(E,\beta,s) = s^{-\frac{1}{2}}\pi^{-\frac{1}{4}}\int_{-\infty}^{\infty} dp\phi_n(\beta,p)e^{-(p^2/2s^2)}$. The success rate is $O[\mathcal{Z}(\beta)/(sD)]$.

Notably, at the limit of $s \to \infty$, $a(E,\beta,s) \propto e^{-\beta E/2}$, which exactly equals to the quantum thermal state at an inverse temperature $\beta$.

One issue of the quantum algorithm is that the resource state cannot be produced for free. To solve this problem, we reveal an equivalent relation of the quantum algorithm, which says that $\rho(\beta)$ can be simulated with different pairs of resource states and unitary evolutions, namely,

$$(R(\beta_0), e^{-iH\hat{p}(\beta/\beta_0)}) \mapsto \rho(\beta), \tag{7}$$

where $\beta_0$ is adjustable. The equivalent relation is a direct consequence of an invariance under $\beta \to a\beta$ and $H \to H/a$ in Eq. (4).

The equivalent relation allows us to use a fixed resource state to simulate the thermal state at varied $\beta$, which we call as adaptive TQS. From the perspective of quantum resource theory [46], the equivalent relation may reveal a conversion between static resource (preparing resource state) and dynamical resource (constructing unitary $e^{-iH\hat{p}}$) and their trade-off for thermal quantum simulation. It enriches the flexibility and feasibility of algorithmic implementation, as difficulties of resource state preparation and Hamiltonian evolution vary on different quantum platforms.

*Time complexity.*—We give a runtime analysis for a relative error $\epsilon$ in the partition function. As it is not practical to ignore the cost of preparing resource state (e.g., at $\beta \to 0, \infty$ limits), we consider adaptive TQS with a resource state $|R(\beta_0)\rangle$ that is easy to prepare. The runtime then relies on the circuit complexity of constructing the unitary operator $e^{-iH\hat{p}\beta/\beta_0}$ and the success rate.

For a Hamiltonian $H = \sum_{i=1}^{M} c_i H_i$ with local terms, one can refer to the Trotter-Suzuki formula [47] to decompose $e^{-iH\hat{p}\beta/\beta_0}$. Typically, it includes terms like evolutions of $\sigma_i^\alpha \hat{p}$, $\sigma_i^\alpha \sigma_{i+1}^\gamma \hat{p}$ $(\alpha,\gamma = x, y, z)$, which can be viewed as parity-dependent displacement operator and can be decomposed as basic gates of qubits and a hybrid gate $e^{i\theta\sigma^x\hat{p}}$ (see Supplemental Material [33]). The circuit complexity is $O(M^3\epsilon^{-1}\beta^2)$, and may be improved with more advanced techniques [48–50]. For a precision $\epsilon$, the squeezing factor should be $s = O(\epsilon^{-\frac{1}{2}})$. Using amplitude amplification [51], the success rate becomes $O\{\sqrt{[\mathcal{Z}(\beta)/(sD)]}\}$, and the algorithm should be run repeatedly with $O\{\sqrt{[D/\mathcal{Z}(\beta)]}\epsilon^{-\frac{1}{4}}\}$ times. In total, the time complexity is $O\{\sqrt{[D/\mathcal{Z}(\beta)]}M^3\beta^2\epsilon^{-\frac{5}{4}}\}$, which improves polynomially from methods using quantum phase estimation [10]. In addition, it is found that the quantum algorithm gives a bound from below for the partition function (see Ref. [33]). We emphasize that amplitude amplification is demanding for quantum resources, while TQS of physical models to be presented below may be implemented on the current quantum devices as the procedure of amplitude amplification is not involved.

*Demonstration with a single qubit.*—To warm up, we simulate the thermal state of a single qubit to highlight some features of the quantum algorithm. For the numeral simulation, we develop a classical simulator for hybrid-variable quantum computing based on the open-source Qutip [52]. The Hamiltonian is $H = g(\sigma_x + c)$ (here the conditions $g > 0$ and $c = 1$ enforce all eigenvalues are non-negative). After initialing the cavity mode into a resource state and preparing a Bell state, an unitary $e^{-ig(\sigma^x+1)\hat{p}t}$ ($t$ is the time of evolution) performs on the cavity mode and the system qubit, and finally the cavity mode is squeezed and projected onto zero photon. We use two approaches for preparing thermal states at $\beta = 1, 2, 3$. The first one fixes $t = 1/g$ and uses resource states $|R(\beta)\rangle$ with $\beta = 1, 2, 3$, respectively. The second is adaptive TQS, fixing the resource state $|R(\beta = 1)\rangle$ and using $t = 1, 2, 3$, respectively. Because of finite squeezing at the projection, those simulated thermal states can only approximate the exact thermal states. We use trace distance to measure the precision, $d_r(\beta) = \frac{1}{2}\mathrm{Tr}|\tilde{\rho}(\beta) - \rho(\beta)|$. In Fig. 2, we can see that the trace distance decreases rapidly with an increase of squeezing factor, at the cost of decreasing success rate, as expected. Using the adaptive TQS, the increasing of precision can be faster, and the trace distance can be small even at small $s$. Moreover, a moderate truncation of phonon number (e.g., up to 7 even-number Fock states) can reach a good precision (see Supplemental Material [33]). The above results indicate that we can use an adaptive approach with an approximated resource state for thermal quantum simulation. Remarkably, the one-qubit system reveals the mechanism of performance of TQS with truncation for different regimes of temperature, and can be quite informative for simulating the finite-temperature quantum many-body systems (see Supplemental Material [33] for more numerical results, analysis of general behavior, and a physical picture of the quantum algorithm).

*Simulation of the finite-temperature phase diagram.*—We now consider our TQS with two textbook models, the

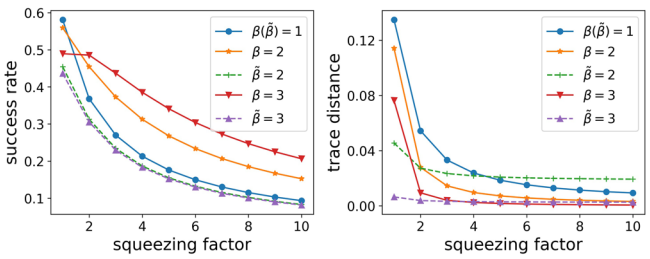


FIG. 2. Performance of preparing thermal states of the single qubit with two different approaches: $\beta$ ($\tilde{\beta}$) stands for results from TQS (adaptive TQS).

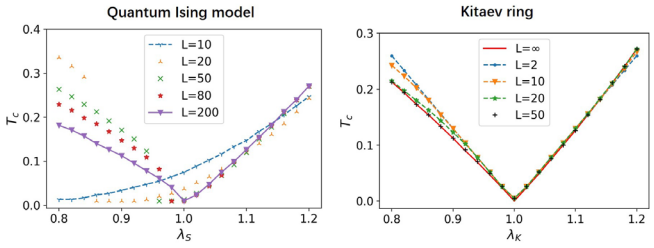


FIG. 3. Finite temperature phase diagram of the one-dimensional Kitaev ring and quantum Ising model.

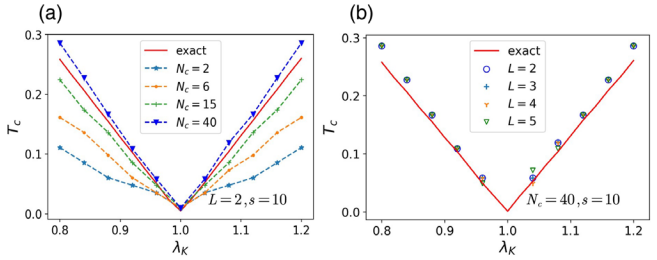


FIG. 4. Simulation of crossover temperature for the Kitaev ring in the quantum critical regime with adaptive TQS. (a) Crossover temperatures that use different truncating of photon number $N_c$ for the resource state $|R(\beta=4)\rangle$.(b) Crossover temperature for different lattice sizes, $L=2$, 3, 4, 5.

Kitaev ring (a spinless $p$-wave superconductor) [32] and the quantum Ising model [31]. The Hamiltonian of the Kitaev ring reads

$$H_K = -J\sum_{i=1}^{L}(c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger + \text{H.c.}) - \mu\sum_{i=1}^{L} c_i^\dagger c_i, \quad (8)$$

where fermionic operators $c_{L+1}=c_1$ as we consider the periodic condition. The model has a topological phase transition at $\lambda_K \equiv \mu/2J=1$. Using the Jordan-Wigner transformation, $c_i=\prod_{j=1}^{i-1}\sigma_j^z\sigma_i^-$, $c_i^\dagger=\sigma_i^+\prod_{j=1}^{i-1}\sigma_j^z$, $c_i^\dagger c_i=\frac{1}{2}(\sigma_i^z-1)$, the Hamiltonian of the Kitaev ring can be mapped into a spin model

$$H_S = -h\sum_{i}^{L}\sigma_i^z - J\sum_{i}^{L-1}\sigma_i^x\sigma_{i+1}^x - J\sigma_1^y P_L\sigma_L^y + E_0, \quad (9)$$

where $h=-(\mu/2)$, $P_L=\prod_{i=2}^{L-1}\sigma_i^z$ is a string operator, $E_0$ is added for assuring a non-negative spectrum (which is demanded for the quantum algorithm). The spin model $H_S$ becomes the quantum Ising model if $\sigma_1^y P_L\sigma_L^y$ is replaced by $\sigma_L^x\sigma_1^x$, and it has a phase transition at $\lambda_S \equiv h/J=1$. This difference between the Ising and Kitaev models has a big effect on the quantum criticality for small sizes, as addressed below. The finite-temperature phase diagrams of these two models in the infinite lattice size are the same, which have an important V-shape crossover structure [31] as shown in Fig. 3.

From numeral calculations (see Supplemental Material for details [33]), it is shown that almost $L\approx 80$ qubits are required for the quantum Ising chain to show well-shaped crossover temperatures, as seen in Fig 3, and $L$ should be larger when the system is closer to the QPT point. For the Kitaev ring, in contrast, the temperature crossovers are very close in shape for a quite large range even for small $L$. The subtle lies in that Kitaev ring always has an energy gap $\Delta=2J|1-\lambda_K|$, while the quantum Ising model will have low-lying in-gap states when $\lambda_S<1$, leading to small crossover temperatures for $\lambda_S<1$, which is obvious for $L=10$, 20. Thus, we refer to a small-size Kitaev ring for simulating a finite-temperature phase diagram with quantum computers.

To address the feasibility of physical implementation, we use the adaptive TQS for simulating thermal states of the Kitaev ring, using a resource state $|R(\beta=4)\rangle$ and a squeezing factor $s=10$. The crossover temperature for each $\lambda_K$ is determined by the temperature that maximizes the magnetic susceptibility $\chi_m$ (corresponding to the fluctuation of fermion number in the Kitaev ring), which can be obtained by measuring the magnetization $\mathcal{M}=(1/L)\sum_i \text{Tr}\rho(\beta)\sigma_i^z$ and then calculating the magnetic susceptibility $\chi_m=[(\partial\mathcal{M})/(\partial h)]$ using a finite difference. The results are plotted in Fig. 4. For $L=2$, we compare results of different truncation for the resource state ($N_c$ is the number of Fock basis of even-number photons), and it can be seen that the V-shape crossover temperature approaches the exact one when increasing $N_c$. We also simulate $L=2$, 3, 4, 5, which demonstrates very close crossover temperatures. Moreover, the near independence of $L$ holds even for small truncation $N_c$ (see Supplemental Material [33]). Therefore, a remarkable advantage of our quantum algorithm is that observation of the important crossover temperature phase diagram of the Kitaev ring needs only a few qubits.

*Experimental realization.*—We now discuss the physical implementation of the quantum algorithm, which relies on hybrid variable quantum computing. Promising candidates include trapped ions [25,26,53–55] and superconducting circuits [56–62], etc. We take the superconducting circuit system as an example, for their well controllable CV cavity mode and its coupling to the qubits. The scheme can be straightforwardly used in a trapped ion quantum computer.

First, the resource state can be expanded in a Fock space, $|R(\beta)\rangle=\sum_{n=0}^{\infty} r_n|2n\rangle$, where $r_n=\int_{-\infty}^{\infty} dq\sqrt{(\beta/2)}e^{-\beta|q|/2}H_{2n}(q)e^{-(q^2/2)}$ and $H_n(q)$ is the $n$th order Hermite function. With a truncation of photon number, the state can be prepared in a cavity by superposing even-number photons. We demonstrate in the Supplemental Material [33] that the resource states can be feasibly realized with two schemes. It can be achieved with a sequence of qubit rotation and Jaynes-Cummings type qubit-cavity coupling [62,63], or using the number-dependent arbitrary phase gate and displacement operator in the dispersive regime [59,64]. An alternative method is optimal quantum control, which uses a sequence of well-designed pulses to generate required

superposed Fock states. This approach has been widely applied for bosonic codes [65,66]. As a concrete example, we demonstrate in the Supplemental Material [33] that the resource state around $\beta = 4$ can be approximated with a few components of small number photons, and can be experimentally realized with both approaches. Thus, we can choose one such resource state and use it for adaptive TQS. Second, construction of $e^{-iH\hat{p}t}$ can be compiled into basic qubit gates and only one hybrid variable gate $e^{i\theta\sigma^x\hat{p}}$, as discussed before. All are standard quantum operations in the superconducting circuit system, and remarkably, the hybrid gate $e^{i\theta\sigma^x\hat{p}}$ can be readily realized in the strong coupling limit [67–69]. Third, projection onto a squeezing state $|0, s\rangle$ can be implemented by first performing a squeezing on the CV mode, and then postselecting the CV mode to the vacuum state (zero photon state). Further, we can measure the system to access the thermal state by quantum state tomography, or studying the quantum statistical mechanism by measuring physical quantities, such as heat capacity, magnetic susceptibility, etc. As for the Kitaev ring, we note that the evolution of the nonlocal term $\sigma_1^y P_L \sigma_L^y \hat{p}$ can be constructed efficiently (see Supplemental Material [33]). Thus, all the above well-developed quantum operations can render a feasible implementing protocol for thermal quantum simulation of the Kitaev ring, to illuminate the novel quantum critical regime on small quantum processors (we have analyzed the experimental requirements and feasibility in a minimal Kitaev ring with $L = 3$, see Ref. [33]).

*Summary.*—We have proposed a quantum algorithm for thermal quantum simulation assisted with an auxiliary CV resource state. We have confirmed its power by simulating finite-temperature phase diagram of the Kitaev ring, and found that the important crossover phase diagram of the model can be accurately determined by a quantum computer with only a few qubits. Thus, our work may pave the way for studying finite temperature quantum systems in experiments.

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