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# Simulation of classical thermal states on a quantum computer: A transfer-matrix approach

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We present a hybrid quantum-classical algorithm to simulate thermal states of classical Hamiltonians on a quantum computer. Our scheme employs a sequence of locally controlled rotations, building up the desired state by adding qubits one at a time. We identified a class of classical models for which our method is efficient and avoids potential exponential overheads encountered by Grover-like or quantum Metropolis schemes. Our algorithm also gives an exponential advantage for two-dimensional Ising models with magnetic field on a square lattice, compared with the previously known Zalka's algorithm.

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Simulation of a finite-temperature physical system with a controllable quantum device is one of the most important goals of quantum simulation [1,2]. Classical Markov-Chain Monte Carlo (MCMC) algorithms are powerful tools for sampling Gibbs distributions. They are efficient provided that the gap $\Delta$ of the transition matrix is nonvanishing; the running time typically scales as $\tau \sim O(1/\Delta)$. A quantum generalization [3] of MCMC has recently been explored by the quantum information community due to the connection to quantum walks [4]. Richter [5] developed a method for sampling from the Gibbs distribution for periodic lattices. Somma *et al.* [6] combined quantum walk and quantum Zeno effect to achieve quantum speedup. Wocjan and Abeyesinghe [7] improved it by using fixed point quantum search. Generally, these quantum algorithms allow the running time to scale as $\tau \sim O(1/\sqrt{\Delta})$, a quadratic speedup compared with the classical counterparts. However, for many problems of practical interest, such as optimization problems and spin glasses, the gap $\Delta$ may become exponentially small when the system size increases, making it unpractical to use MCMC algorithms for solving them (see Fig. 1). Therefore, gap-independent methods are more desirable for solving these problems.

A class of gap-independent methods is called *belief propagation* [8], which generalizes the transfer matrix methods in statistical physics. For problems involving a regular geometry, it can be very efficient. This property will be exploited in this Rapid Communication, where a different way for obtaining samples from the thermal state is discussed. This approach is a generalization of the state preparation method by Lidar and Biham [9] and Zalka [10]. We show that in some cases, the structure of the system under investigation allows for large speedups over the general methods. This is because the cost of our method is independent of the temperature and the gap size.

Our proposed strategy is to construct a *coherent encoding of a thermal state* (CETS) $|\psi_{\mathrm{CETS}}\rangle$ directly, rather than sampling from the thermal probability distribution:

$$|\psi_{\mathrm{CETS}}\rangle = \sum_s \sqrt{e^{-\beta H(s)}/Z}|s\rangle, \tag{1}$$

where $s = \{0,1\}^N$, $\beta \equiv 1/k_B T$ is the inverse temperature, $H(s)$ is the eigenenergy of some classical spin Hamiltonian for the $N$-spin configuration $s = s_1 s_2 \cdots s_N$, and $Z$ is the partition function. This CETS can be transformed into the corresponding thermal state

$$\rho_{\mathrm{th}} = e^{-\beta H}/\mathrm{Tr}(e^{-\beta H}) \tag{2}$$

by including a set of $N$ ancilla qubits, performing bit-by-bit controlled-NOT (CNOT) transformations such that

$$|s\rangle \otimes |0\cdots 0\rangle_A \rightarrow |s\rangle \otimes |s\rangle_A, \tag{3}$$

and tracing over the ancilla system. However, for some applications, such as the partition functions estimation in [11], it is preferable to use the CETS directly. With the CETS, all the thermal properties can be extracted. In Ref. [2], several efficient methods of measurement applicable to CETS are outlined. For completeness, in the appendix [12], we include a self-contained description of the measurement methods, and consider how randomness can be introduced efficiently.

We will present a method for preparing the CETS of a classical Hamiltonian from the initial state $|0\cdots 0\rangle$ by a sequence of locally controlled rotations. Zalka's approach [10], as applied to discrete cases [13], allows for preparing the CETS by adding qubits one by one, and performing a rotation (controlled by *all* of the previous qubits) on each new qubit as

$$|s_1 \cdots s_k\rangle|0\rangle \rightarrow |s_1 \cdots s_k\rangle(\cos\theta_s|0\rangle + \sin\theta_s|1\rangle), \tag{4}$$

where $\cos^2\theta_s$ is the conditional probability of $s_{k+1} = 0$, given that the first $k$ spins are in a particular configuration $s_1 s_2 \cdots s_k$. The problem here is that in general, this requires the knowledge (or efficient calculation) of $O(2^N)$ conditional probabilities. Thus, Zalka's method is efficient only when the probability distributions are efficiently integrable [14]. Here we focus on the cases where the controlled rotations are local, i.e., they depend only on a few previous qubits. This in turn allows efficient computation of the respective rotation angles.

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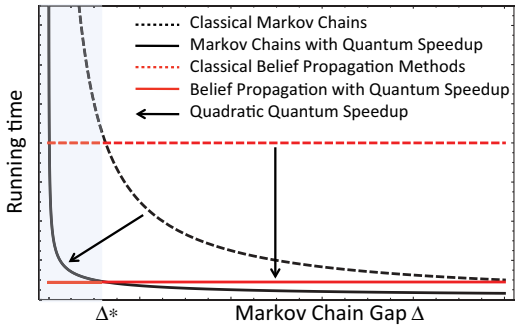


FIG. 1. (Color online) The running time $\tau \sim O(1/\Delta)$ of Markov chain methods, limited by the gap $\Delta$ of the Markov matrix. A quantum quadratic speedup $\tau \sim O(1/\sqrt{\Delta})$ (black solid line) relative to classical Markov chains (black dashed line) can be achieved by a quantum computer. Below some critical gap size $\Delta < \Delta^*$, Markov chain methods become inefficient (shaded region), and classical belief propagation methods (red dashed line), including transfer matrix methods (which are gap independent), become more efficient. Combined with quantum amplitude amplification, a further quantum speedup is possible (red solid line).

*Real-space renormalization.* This method is also related to the renormalization group method [15], which idea is to integrate out some degrees of freedom (coarse-graining) in the partition function $Z$, and describe the subsystem with a similar system with modified (renormalized) couplings. As an example, consider a linear chain of three spins [Fig. 2(a)]. The partition function after eliminating spin 3 [cf. Eq. (21)],

$$Z = \Lambda(\beta) \sum_{s_1,s_2} e^{B(\beta)s_1 s_2}, \tag{5}$$

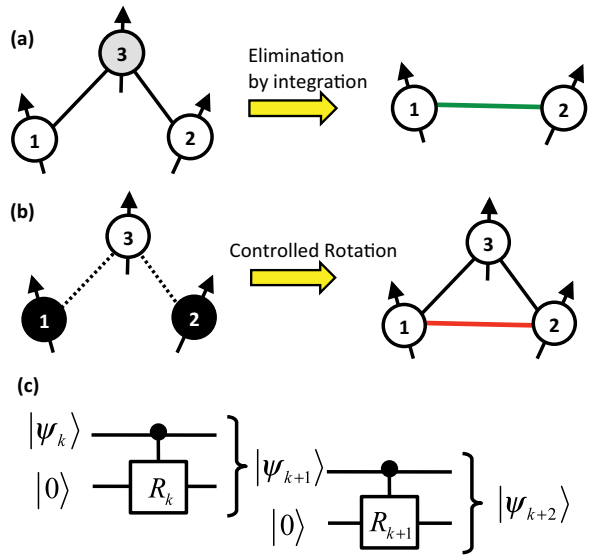


FIG. 2. (Color online) Real space renormalization approach for preparing the coherent encoding of a thermal state (CETS). (a) Spin 3 is eliminated by integration, inducing an effective interaction (green bond) between spin 1 and spin 2. (b) A controlled rotation is performed on spin 3, inducing an effective interaction (red bond) between spin 1 and spin 2. (c) A quantum circuit demonstrating the sequential construction of the full thermal state.

is proportional to that of spin 1 and spin 2 interacting with an effective interaction $-B(\beta)/\beta$. In contrast to this conventional renormalization treatment, where the degrees of freedom of the physical systems are progressively reduced, our method works in a reverse fashion: at each step, we *increase* the number of degrees of freedom, and then perform a controlled rotation (Fig. 2(b)), which also changes the effective interaction of spins 1 and 2.

We next define a sequential method for preparing a CETS for a generalized Ising Hamiltonian of $N$ classical spins which has multiple spin-spin coupling constants:

$$H_s = \sum_j A_j s_j + \sum_{ij} B_{ij} s_i s_j + \sum_{ijk} C_{ijk} s_i s_j s_k + \cdots. \tag{6}$$

Our goal is to investigate how a CETS can be constructed by locally controlled quantum rotations. Suppose we are given a CETS as defined in Eq. (1) of $k$ spins $|\psi_k\rangle$ for the Hamiltonian given by Eq. (6), and an additional qubit initialized in the state $|0\rangle$ that will become spin $k+1$ of our CETS. Let us define the rotation angle $\theta_s$ by

$$\cos\theta_s \equiv \sqrt{e^{-\beta m_s}/W_s}, \tag{7}$$

where $W_s \equiv e^{-\beta m_s} + e^{\beta m_s} = 2\cosh(\beta m_s)$, and

$$m_s \equiv m(s_1,\ldots,s_k) \tag{8}$$

is a function (to be determined later) of the spin variables of the first $k$ spins. After performing a controlled rotation (4) on spin $k+1$, with angles given by Eq. (7), we obtain a CETS $|\psi_{k+1}\rangle$ of a new $(k+1)$-spin Hamiltonian

$$H_{k+1} = \tilde{H}_k + m_s s_{k+1}. \tag{9}$$

To justify this statement, rewrite $W$ in Eq. (7) as

$$W_s = e^{-\beta m_s} + e^{\beta m_s} = \Lambda_k e^{-\beta(H_k - \tilde{H}_k)}, \tag{10}$$

for some constant $\Lambda_k$ and some $k$-spin Ising spin Hamiltonian $\tilde{H}_k$ (with possible higher order interactions). The state that we get from $|\psi_k\rangle|0\rangle$ by the controlled rotation (7) is $\sum_s \sqrt{F(s)}|s\rangle$ with $F(s) \equiv F(s_1,s_2,\ldots,s_n)$ given by

$$F(s) = \frac{e^{-\beta H_k}}{Z_k}\frac{e^{-\beta m_s s_{k+1}}}{W_s} = \frac{e^{-\beta(\tilde{H}_k + m_s s_{k+1})}}{Z_k \Lambda_k}, \tag{11}$$

i.e., a CETS for the Hamiltonian (9). Moreover, the new normalization constant is the same as the partition function $Z_{k+1}$ for the system with Hamiltonian (9) and can be obtained simply by

$$Z_{k+1} = \Lambda_k Z_k. \tag{12}$$

The term $\tilde{H}_k$ in (9) is an Ising Hamiltonian of the form (6) for the first $k$ spins, but associated with a different set of renormalized couplings $\{\tilde{A}_j, \tilde{B}_{ij}, \tilde{C}_{ijk}, \ldots\}$. Finally, the constant $\Lambda_n$ can be shown to be the geometric mean of the left-hand side of (10)

$$\Lambda_k = 2\prod_{m_s}[\cosh(2\beta m_s)]^{1/2^k}. \tag{13}$$

This is reminiscent of formulas which appear in classical algorithms such as belief propagation [8] for calculating some thermal properties of some spin systems. The controlled

rotation is therefore the crucial element of our renormalization step. Using our method iteratively as shown in Fig. 2(c), we can generate the CETS of a particular spin Hamiltonian. In general, $\tilde{H}_k$ could contain up to $k$-local interaction terms. If all the terms in $\tilde{H}_k$ involve at most $t$ spins, we call this a *t-renormalizable* operation.

*Finite-range interactions and belief propagation.* As a general construction, we consider spin chains with finite-range interactions involving $z$ neighboring spins. The computational complexity of this approach generally scales exponentially in $z$. As an example, consider two groups of spins $s$ and $t$, each can be considered as a $2^z$-dimensional system. The Hamiltonian is of the form

$$H = H_s + H_t + H_{st}, \tag{14}$$

where $H_s$ and $H_t$ are the internal interaction terms for spins within group $s$ and $t$, and $H_{st}$ contains the interactions between the groups. We start with preparing the state of the group $s$ as

$$\frac{1}{\sqrt{M}} \sum_s \sqrt{e^{-\beta H_s} \gamma_s} |s\rangle, \tag{15}$$

where $M$ is a normalization constant, and $\gamma_s$ is a function of the spins $s$ to eliminate renormalization effects induced by the spins in group $t$. The group $t$ is initialized in the state $|0 \cdots 0\rangle$. We choose the controlled rotation

$$|s\rangle|0 \cdots 0\rangle \to |s\rangle \sum_t \sqrt{e^{-\beta(H_t + H_{st})}(\gamma_t/\gamma_s)} |t\rangle, \tag{16}$$

with $\gamma_t$ determined by the next group of spins to be included in the preparation procedure. If group $t$ is the last group, then all $\gamma_t$ are equal to 1. To ensure unitarity of this operation, we require

$$\gamma_s = \sum_t \gamma_t e^{-\beta(H_t + H_{st})}, \tag{17}$$

which is a recursion relation typically encountered in belief propagation [8] problems. For a group of $z$ spins, and a given set of $\gamma_t$, the sum involves $O(2^z)$ terms, scaling exponentially in $z$. To perform the multi-qubit rotation, we can apply Zalka's algorithm [10], which requires the computation of $O(2^z)$ rotation angles, and a polynomial number of subsequent quantum operations. To save computational resource for large $z$, it is more efficient to determine the angles for rotation "on the fly." This can be achieved by the quantum amplitude amplification algorithm [16] calculated with some ancilla qubits.

We can apply this approach to an $N \times N$ square lattice of Ising spins with nonuniform couplings and arbitrary local magnetic fields. We make a group for each row of $z = N$ spins. In the worst case scenario, the number of required operations in the above approach then scales[1] as $O(2^{2N})$, which becomes $O(2^N)$ after combining with the amplitude amplification algorithm. This is still an exponential algorithm, but nevertheless with an exponential speed up over the direct application of Zalka's algorithm, whose complexity scales as $O(2^{N^2})$, as it requires the preparation of a probability distribution with $2^{N^2}$ amplitudes. However, for the uniform two-dimensional Ising model without magnetic fields, an efficient $t$-renormalizable approach might exist, as classical polynomial algorithms exist for this problem [17].

*Building blocks for frustrated magnets and spin ice.* As another example, we show how to generate a CETS of a triangle plaquette of three Ising spins by a 2-renormalizable operation. Our goal is to prepare a CETS of three spins (see Fig. 2(b)) for the Hamiltonian

$$H_3 = J(s_1 s_2 + s_1 s_3 + s_2 s_3). \tag{18}$$

Let us start with two qubits initialized as

$$\frac{1}{\sqrt{M}} \sum_{s_1, s_2 = \{0,1\}} \sqrt{\gamma_{s_1 s_2} e^{-\beta J s_1 s_2}} |s_1 s_2\rangle, \tag{19}$$

where $M$ is a normalization constant and $\gamma_{s_1 s_2} > 0$ is some positive function of $s_1$ and $s_2$ to be determined later. Let us add a third qubit in the state $|0\rangle$ to the system, and act with the controlled rotation (7) depending on the values of the first two qubits. When we choose

$$m_s = J(s_1 + s_2) \tag{20}$$

for some constant $J$, we can use the well-known result in renormalizing the one-dimensional Ising chain [15], and write

$$W_s = e^{-\beta J(s_1 + s_2)} + e^{\beta J(s_1 + s_2)} = \Lambda e^{\beta B s_1 s_2}, \tag{21}$$

where the coefficients $\Lambda$ and $B$ are

$$\begin{aligned} \Lambda &= 2\sqrt{\cosh(2\beta J)}, \\ B &= (1/2\beta) \ln \cosh(2\beta J). \end{aligned} \tag{22}$$

Observe now that if we chose $\gamma_{s_1 s_2} = \Lambda e^{\beta B s_1 s_2}$ when preparing the first two qubits, applying the controlled rotation of the third qubit eliminates this factor. Consequently, this operation produces the CETS for the three-spin Ising cycle $H_3$. We will discuss more examples in the appendix [12].

*Connection to matrix product state (MPS) representation.* Many-body quantum states can be expressed in the form of matrix product states (MPS) [18,19]; our CETS is of no exception. The representation in terms of MPS,

$$|\psi_{\mathrm{MPS}}\rangle = \sum_s \mathrm{tr}\{A^{(1)}_{s_1} A^{(2)}_{s_2} \cdots A^{(n)}_{s_n}\} |s_1 s_2 \cdots s_n\rangle, \tag{23}$$

where $A^1_{s_1}$ is a vector and the rest of the $A$'s are matrices, is closely related to the classical algorithm called the density matrix renormalization group (DMRG) [20]. In the practical implementation of DMRG algorithms, the matrices $A$ are truncated to a constant size ($m \times m$ where $m \ll 2^n$) and stored in the memory, instead of the actual form of the quantum state; this leads to a significant reduction of the memory requirement.

We investigated the validity of MPS truncation for a class of CETS (details in the appendix [12]); the result suggests that the truncation in MPS is efficient in the high-temperature limit. This is expected as there is no entanglement in the CETS in that limit. However, in the $T \to 0$ limit, due to the degeneracy of the ground state, the truncation would cause large errors.

On the other hand, the MPS representation of quantum states can lead to an alternative way to obtain the CETS.

[1] With belief propagation, for a chain of $d$-dimensional qubits, the partition function scales as $(N-1)d^2$.

This is because the CETS can in principle be mapped to the ground state of certain artificial Hamiltonians [21]; a DMRG procedure can therefore be implemented for the CETS, which results in a MPS representation. For example, to solve the ground-state problem, applying the phase estimation algorithm (PEA) to the MPS can result a projection to the *exact* ground state, with an efficiency depending on the fidelity of the MPS [2]. To this end, we elaborate this point more by including a discussion in the appendix [12] on how to modify our method to map any given MPS representation to the state of a register of qubits.

*Conclusion.* To summarize, we have developed an algorithm which identifies a class of classical spin problems that can be simulated efficiently with a quantum computer. In this class of problems, our method scales efficiently compared with MCMC methods [6,7,22], as it is independent of the gap of the Markov chain and temperature. On the other hand, we believe that the tools developed here could be useful for classifying the complexity classes of certain spin models. An avenue for further research is the complexity classification of spin systems by their $t$-renormalizability, which may suggest a deeper understanding of the connection between complexity theory and quantum simulation.

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