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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 identify 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 2D 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 Δ of the transition matrix is non-vanishing; 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 Δ 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, e.g. one-dimensional spin chains. This property will be exploited in this letter, 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.
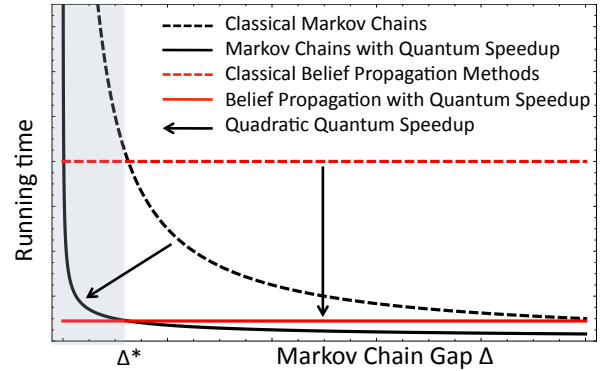

FIG. 1: (color online) The running time $\tau \sim O(1/\Delta)$ of Markov chain methods is limited by the gap Δ of the Markov matrix. A quantum quadratic speedup $\tau \sim O(1/\sqrt{\Delta})$ (black solid line) relative to classical Markov chains (black dashed line) can be achieved by a quantum computer. 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, become more efficient. Combined with amplitude amplification, a further quantum speedup is possible (red solid line).

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

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

where $s = \{0,1\}^N$, $\beta = 1/k_B T$ is the inverse temperature, $H(s)$ is the eigen-energy 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 $\rho = e^{-\beta H}/\text{Tr}(e^{-\beta H})$ by including a set of N ancilla qubits, performing bit-by-bit CNOTs such that $|s\rangle \otimes |0 \cdots 0\rangle_A \rightarrow |s\rangle \otimes |s\rangle_A$ 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.

Below we present a method for preparing the CETS of a classical Hamiltonian from the initial state $|0\cdots0\rangle$ by a sequence of locally-controlled rotations. Zalka's approach [10], as applied to discrete cases [12], 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

$$|s_1\cdots s_k\rangle|0\rangle \rightarrow |s_1\cdots s_k\rangle(\cos\theta_s|0\rangle + \sin\theta_s|1\rangle), \quad (2)$$

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 [13]. 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. More precsiely, we take into account the *structure* of the geometry of the physical systems and use the idea of the renormalization approach to obtain the rotation angles.

Real-space renormalization — This method is also related to the renormalization group method [14], which idea is to integrate out some degrees of freedom (coarse-graining) in the partition function Z, and describe the sub-system with a similar system with modified (renormalized) couplings. As an example, consider a linear chain of three spins (Fig 2a). The partition function after eliminating spin 3 (cf. Eq.(13)),

$$Z = \Lambda(\beta)\sum_{s_1,s_2} e^{B(\beta)s_1 s_2} \quad (3)$$

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. 2b), which also changes the effective interaction of spins 1 and 2.

Below, we define a sequential method for preparing a CETS for a generalized Ising Hamiltonian of N classical spins which has multiple spin-spin coupling constants:

$$H_s = \sum_j A_j s_j + \sum_{ij} B_{ij} s_i s_j + \sum_{ijk} C_{ijk} s_i s_j s_k + \ldots \quad (4)$$

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. (4), and an additional qubit initialized in the state $|0\rangle$ that will become spin $k+1$ of
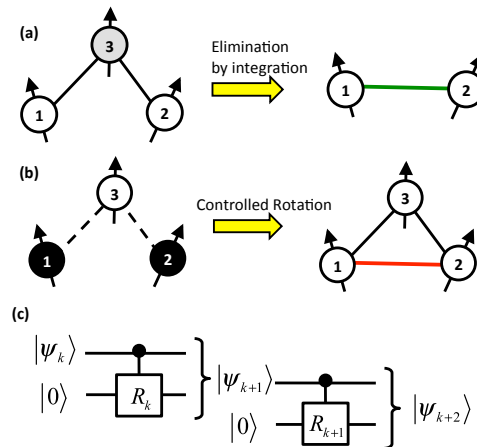

FIG. 2: (color online) Real space renormalization approach for preparing the coherent encoding of a thermal state (CETS). (a) Spin 3 is eliminated by integration, inducing an effective interaction (blue bond) between spin 1 and spin 2. (b) A controlled rotation is performed on spin 3, inducing an effective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

our CETS. Let us define the rotation angle, θ_s, by

$$\cos\theta_s \equiv \sqrt{e^{-\beta m_s}/W_s}, \quad (5)$$

where $W_s \equiv e^{-\beta m_s} + e^{\beta m_s} = 2\cosh(\beta m_s)$, and $m_s \equiv m(s_1,\ldots,s_k)$ is a function of the spin variables of the first k spins. After performing a controlled rotation (2) on spin $k+1$, with angles given by Eq. (5), we obtain a CETS $|\psi_{k+1}\rangle$ of a new $(k+1)$-spin Hamiltonian

$$H_{k+1} = \tilde{H}_k + m_s \cdot s_{k+1}. \quad (6)$$

To justify this statement, rewrite W in Eq. (5) as

$$W_s = e^{-\beta m_s} + e^{\beta m_s} = \Lambda_k e^{-\beta(H_k - \tilde{H}_k)}, \quad (7)$$

for some constant Λ_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 (5) is $\sum_s \sqrt{F(s)}|s\rangle$ with $F(s) \equiv F(s_1, s_2, \ldots, s_n)$ given by

$$F(s) = \frac{e^{-\beta H_k}}{Z_k} \times \frac{e^{-\beta m_s \cdot s_{k+1}}}{W_s} = \frac{e^{-\beta(\tilde{H}_k + m_s \cdot s_{k+1})}}{Z_k \Lambda_k} \quad (8)$$

i.e. a CETS for the Hamiltonian (6). Moreover, the new normalization constant is the same as the partition function Z_{k+1} for the system with Hamiltonian (6) and can be obtained simply by $Z_{k+1} = \Lambda_k Z_k$. The term $\tilde{H}_k$ in (6) is an Ising Hamiltonian of the form (4) 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 Λ_n can be shown to be the geometric mean of the LHS of (7)

$$\Lambda_k = 2 \prod_{m_s} [\cosh{(2\beta m_s)}]^{1/2^k} . \qquad (9)$$

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. 2c, 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. From now on, we will restrict ourselves to 2-renormalizable operations, which for example, includes local magnetic fields and two-spin interactions. Next, we will consider a general construction of a CETS for systems with finite range interaction, followed by some specific examples for further illustration.

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

$$H = H_s + H_t + H_{st}, \qquad (10)$$

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 $M^{-1/2} \sum_s \sqrt{e^{-\beta H_s} \cdot \gamma_s} |s\rangle$, where M is a normalization constant, and γ_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 (2),

$$|s\rangle |0 \ldots 0\rangle \to |s\rangle \sum_t \sqrt{e^{-\beta(H_t + H_{st})} \cdot (\gamma_t/\gamma_s)} |t\rangle , \quad (11)$$

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

$$\gamma_s = \sum_t \gamma_t e^{-\beta(H_t + H_{st})}, \qquad (12)$$

which is a recursion relation typically encountered in belief propagation[8] problems. For a group of z spins, and a given set of γ_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 [15] calculated with some ancilla qubits.

We can apply this approach to an $N \times N$ square lattice of Ising spins with non-uniform 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 [18] 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 2D Ising model without magnetic fields, an efficient t-renormalizable approach might exist, as classical polynomial algorithms exist for this problem [16].

In the following, we illustrate our method by explicitly giving several examples of physical interest.

Building blocks for frustrated magnets and spin ice — As the first 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. 2b), for the Hamiltonian $H_3 = Js_1 s_2 + Js_1 s_3 + Js_2 s_3$. Let us start with two qubits initialized as: $M^{-\frac{1}{2}} \sum_{s_1, s_2 = \{0,1\}} \sqrt{\gamma_{s_1 s_2} e^{-\beta J s_1 s_2}} |s_1 s_2\rangle$, 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 (5) depending on the values of the first two qubits. When we choose $m_s = J(s_1 + s_2)$ for some constant J, we can use the well-known result in renormalizing the 1D Ising chain [14], and write

$$W_s = e^{-\beta J(s_1 + s_2)} + e^{\beta J(s_1 + s_2)} = \Lambda e^{\beta B s_1 s_2}, \qquad (13)$$

where the coefficients Λ and B are

$$\begin{aligned} \Lambda &= 2\sqrt{\cosh{(2\beta J)}}, \qquad (14) \\ B &= (1/2\beta) \ln \cosh{(2\beta J)} . \end{aligned}$$

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 3-spin Ising cycle H_3.

Furthermore, we can build on top of this triangular lattice to prepare a CETS of the basic tetrahedral unit of spin ice [17] (see Fig. 3(a)). Let's add a fourth qubit to the system, and perform a rotation controlled by the first three qubits:

$$|s_1 s_2 s_3\rangle |0\rangle \to |s_1 s_2 s_3\rangle (\cos \theta_s |0\rangle + \sin \theta_s |1\rangle) , \qquad (15)$$
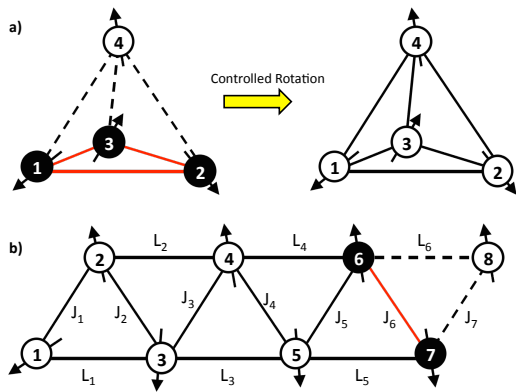
FIG. 3: (color online) Examples of thermal state generation for the basic units of Ising spin cycles and spin ice (a) A rotation on spin 4, controlled by spin 1,2, and 3, results a thermal state of the tetrahedral spin ice. (b). A next-nearest-neighbor spin chain is created by consecutive application of two-qubit controlled rotations.

where $\cos\theta_s$ is given in (5) with $m_s = J(s_1 + s_2 + s_3)$. In this case, we have,

$$
\begin{aligned}
W_s &= \Lambda e^{K(s_1 s_2 + s_2 s_3 + s_1 s_3)}, \\
\Lambda &= 2\left(\cosh^3(J)\cosh(3J)\right)^{1/4}, \\
K &= (1/4)\ln\left(\cosh(3J)/\cosh(J)\right).
\end{aligned}
\tag{16}
$$

This suggests that to compensate for the renormalization effect of adding the fourth spin, we can replace J with $J - K$ in (13) and (14) when preparing the CETS of the base triangle of the spin-ice tetrahedron that is indicated as red bonds in Fig. 3(a).

Ising spin chains with next-nearest-neighbor interactions and local magnetic fields — As another application of our renormalization method, we consider the application to spin chain with next-nearest-neighbor interaction, which generalizes the work done in [9]. Given a chain of n spins with nearest-neighbor interactions J_i, next-nearest-neighbor interactions L_i, and local fields h_i, the Hamiltonian is,

$$
H = \sum_{i=1}^{n-1} J_i s_i s_{i+1} + \sum_{i=1}^{n-2} L_i s_i s_{i+2} + \sum_{i=1}^{n} h_i s_i.
\tag{17}
$$

For $i \geq 3$, we define a 2-renormalizable controlled-rotation on the i-th qubit:

$$
|s_{i-2} s_{i-1}\rangle |0\rangle \to |s_{i-2} s_{i-1}\rangle (\cos\theta_i |0\rangle + \sin\theta_i |1\rangle), \tag{18}
$$

with $m_s = L_{i-2} s_{i-2} + J_{i-1} s_{i-1} + h_i s_i$ in (5) determining the rotation angles. Using

$$
g_i^{\pm\pm} \equiv 2\cosh(h_i \pm J_{i-1} \pm L_{i-2}), \tag{19}
$$

and following the procedure in (7), we can rewrite

$$
e^{-\beta m_s} + e^{\beta m_s} = \Lambda_i e^{\beta B_i s_{i-2} s_{i-1}} e^{\beta C_i s_{i-1}} e^{\beta D_i s_{i-2}}. \tag{20}
$$

This equality is satisfied for the following choices

$$
\begin{aligned}
\Lambda_i &= \left(g_i^{++} g_i^{+-} g_i^{-+} g_i^{--}\right)^{1/4}, \\
B_i &= (1/4\beta)\ln(g_i^{++} g_i^{--}/g_i^{-+} g_i^{+-}), \\
C_i &= (1/4\beta)\ln(g_i^{+-} g_i^{++}/g_i^{--} g_i^{-+}), \\
D_i &= (1/4\beta)\ln\left(g_i^{-+} g_i^{++}/g_i^{--} g_i^{+-}\right).
\end{aligned}
\tag{21}
$$

After the controlled rotation on the i-th qubit, the spin-spin coupling between the spins $i-2, i-1$ is thus renormalized as $J_{i-2} \to J_{i-2} + B_i$. Also, the local magnetic fields for these spins are renormalized as $h_{i-1} \to h_{i-1} + C_i$ and $h_{i-2} \to h_{i-2} + D_i$. Note that the next-nearest-neighbor coupling L_{i-2} term remains unchanged.

Our goal is a CETS of the Hamiltonian (17). We can eliminate the unwanted renormalization effects with the following procedure: (i) for $\mathtt{i} = \mathtt{1}..\mathtt{n}$, initialize $\mathtt{h[i]} = h_i$, $\mathtt{J[i]} = J_i$ and $\mathtt{L[i]} = L_i$; (ii) compute B_i, C_i and D_i from (21) using the values stored in $(\mathtt{h[i]}, \mathtt{J[i]}, \mathtt{L[i]})$; put $\mathtt{h[i-1]} = \mathtt{h[i-1]} - C_i$, $\mathtt{h[i-2]} = \mathtt{h[i-2]} - D_i$ and $\mathtt{J[i-2]} = \mathtt{J[i-2]} - B_i$; let $\mathtt{i} = \mathtt{i} - \mathtt{1}$. (iii) Repeat step (ii) until $\mathtt{i} = \mathtt{3}$. The desired CETS can then be obtained by a sequence of 2-locally controlled rotations using the stored values in $(\mathtt{h[i]}, \mathtt{J[i]}, \mathtt{L[i]})$ instead of the original h_i, J_i and L_i.

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, 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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