Dynamic Monte Carlo Simulations for a Square-Lattice Ising Ferromagnet with a Phonon Heat Bath

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Abstract

We derive a direct connection between Monte Carlo time and physical time in terms of physical parameters, using a quantum Hamiltonian with a $d$-dimensional phonon heat bath interacting with a square-lattice Ising ferromagnet. Based on the calculated transition rates, we perform dynamic Monte Carlo simulations using absorbing Markov chains to measure the lifetimes of the metastable state at low temperatures. We also calculate the lifetimes analytically using absorbing Markov chains. The phonon dynamic gives field-dependent prefactors in the lifetimes at low temperatures, that are different from the piecewise field-independent prefactors obtained from the Glauber dynamic.

Key words: Phonon dynamic, Dynamic Monte Carlo: lifetimes, field-dependent, prefactor

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1. Introduction

Dynamics of classical Ising spin systems have been studied extensively using the Glauber dynamic [1]. The Glauber dynamic was later also derived by Martin [2] starting from a quantum Hamiltonian consisting of an exchange interaction and a coupling to a fermionic thermal heat bath attached to each spin. This derivation was performed in a weak-coupling limit in which the square of the coupling constant multiplied by a characteristic time becomes an arbitrary finite constant. In this limit, the time evolution of the system was proved to be Markovian.

A different dynamic would change the time evolution of the system, but not its equilibrium properties. Here we study the quantum nearest-neighbor Ising ferromagnet with an applied longitudinal magnetic field and a linear coupling between the Ising spins and a phonon (i.e. bosonic) heat bath. We calculated the transition rates from one configuration to another resulting from the spin-phonon coupling. We then applied these transition rates to dynamic Monte Carlo simulations and measured the average lifetimes $\langle \tau \rangle$ of the metastable state [3]. To measure $\langle \tau \rangle$, we set the initial configuration with all spins up and applied a magnetic field $H<0$. We define $\langle \tau \rangle$ as the num-
number of spin-flip attempts until the magnetization reaches zero. Exact predictions [4] of the lifetime \( \langle \tau \rangle \) as \( T \to 0 \) are given by

\[
T \ln(\tau) = \Gamma(H, J) = 8J \ell_c - 2|H| (\ell_c^2 - \ell_c + 1), \quad (1)
\]

where the linear critical droplet size is \( \ell_c = [2J/|H|] \), \([x]\) denotes the smallest integer not less than \( x \), and \( \Gamma \) is the energy cost of a critical droplet. The critical droplet is a cluster of overturned spins which is an \( \ell_c \times (\ell_c - 1) \) rectangle with one additional overturned spin on one of the long sides of the rectangle. This formula is valid for \( 2J/|H| \) not an integer and \( |H| < 4J \). Here we show that the specific dynamic crucially affects the time evolution of the system.

2. Dynamic Quantum Model

The total Hamiltonian we use is \( \mathcal{H} = \mathcal{H}_{\text{sp}} + \mathcal{H}_{\text{ph}} + \mathcal{H}_{\text{sp-ph}} \). The spin Hamiltonian \( \mathcal{H}_{\text{sp}} \) and phonon Hamiltonian \( \mathcal{H}_{\text{ph}} \) are given by

\[
\mathcal{H}_{\text{sp}} = -J \sum_{\langle i, j \rangle} \sigma_i^z \sigma_j^z - H_z \sum_i \sigma_i^z
\]

\[
\mathcal{H}_{\text{ph}} = \sum_q \hbar \omega_q c_q^\dagger c_q,
\]

where the first summation runs over nearest-neighbor sites only, \( J > 0 \) is the exchange coupling constant, \( \sigma_i^z \) are the \( z \) components of Pauli spin operators attached to lattice site \( i \), \( H_z \) is a longitudinal magnetic field, \( \vec{q} \) is the wave vector of a phonon mode, \( \omega_q \) is an angular frequency of the phonon mode with \( \vec{q} \), and \( c_q^\dagger \) and \( c_q \) are creation and annihilation operators of the phonon mode with \( \vec{q} \). For simplicity, we ignore the direction of \( \vec{q} \); so hereafter we drop the vector symbol on \( \vec{q} \). If we consider only linear coupling between spin operators \( V(\vec{q}) \) and strains caused by phonons, the general spin-phonon interaction for a single spin \( \vec{q} \) at the origin in real space is

\[
\sum_q \sqrt{\frac{\hbar}{2NM\omega_q}} (iq \sigma_i^z) (c_q^\dagger - c_q) e^{i\vec{q} \cdot \vec{R}_j}, \quad (4)
\]

where \( \lambda \) is the coupling strength between the spin system and the phonon heat bath.

With the given spin Hamiltonian, the dynamic is determined by the generalized master equation [6,7]:

\[
\frac{d\rho(t)}{dt} = i\hbar [\rho(t), \mathcal{H}_{\text{sp}}] + \delta_{m'm} \sum_{n \neq m} \rho(t)_{nm} W_{mn} - \gamma_{m'm} \rho(t)_{m'm},
\]

\[
\gamma_{m'm} = \frac{W_{m} + W_{m'}}{2}, \quad W_{m} = \sum_{k \neq m} W_{km}, \quad (5)
\]

where \( \rho(t) \) is the time dependent density matrix of the spin system, \( m', n, k, m \) are eigenstates of \( \mathcal{H}_{\text{sp}} \), \( \rho(t)_{m'm} = \langle m' | \rho(t) | m \rangle \), and \( W_{km} \) is a transition rate from the \( m \)-th to the \( k \)-th eigenstate. In our case, because there are no off-diagonal terms in \( \mathcal{H}_{\text{sp}} \), this generalized master equation becomes identical to the master equation which Glauber used in his paper [1], but with different \( W_{km} \). Assuming that the correlation time of the heat bath is much shorter than the times of interest, we integrate over all degrees of freedom of the heat bath in order to obtain the transition rates. The transition rate from the \( l \)-th to the \( k \)-th eigenstate of \( \mathcal{H}_{\text{sp}} \) becomes

\[
W_{k,l} = \frac{2\pi}{\hbar} \sum_{q,n_q} \langle n_q + 1, k | \mathcal{H}_{\text{sp-ph}} | n_q, l \rangle^2 \times \langle n_q | \rho_{\text{ph}} | n_q \rangle \delta(E_l - E_k - \hbar \omega_q), \quad (6)
\]

with the energy eigenvalues of \( \mathcal{H}_{\text{sp}} \) \( E_l > E_k \). Here \( n_q \) is the average occupation number of the phonon mode with \( q \), and \( \rho_{\text{ph}} \) is the density matrix of the phonon bath. We can calculate the transition rate when \( E_l < E_k \) similarly. Eventually we obtain

\[
W_{k,l} = \frac{\lambda^2}{\Theta_\eta \Omega_d^{d+1} c^{d+2}} \left( \frac{(E_k - E_l)^d}{\Theta_{\eta}} - 1 \right), \quad (7)
\]

where \( d \) is the dimension of the heat bath, \( \Theta = 2(2\pi) \) for \( d = 1, 2, 3 \), \( \eta \) is the mass density of a unit cell, \( c \) is the sound velocity, and \( \beta = 1/k_B T \). The two major differences from the Glauber dynamic
are the energy term in the numerator and the negative sign in the denominator. In the limit $T \to 0$, the transition rates vanish when $E_i = E_k$ (this can occur for $|H| = 2J, 4J$). The transition rates satisfy detailed balance.

3. Lifetimes of the Metastable State

We perform dynamic Monte Carlo simulations using Absorbing Markov Chains (MCAMC) \cite{3,8} at low temperatures with both the Glauber and $d$-dimensional phonon dynamics. For $2J < |H| < 4J$, the critical droplet consists of a single overturned spin, so the $n$-fold way algorithm \cite{9} ($s=1$ MCAMC) gives adequate speed-ups. However, when $|H|$ approaches 2 from below or above, the $s=2$ MCAMC algorithm is needed to prevent the system from fluctuating between the all-spins-up state and the state with all spins up except for one overturned spin. For $J < |H| < 2J$, the critical droplet has an L-shape formed by three overturned spins. This necessitates using $s=3$ MCAMC to prevent the system from fluctuating between the state with all spins up except for one overturned spin and the state with two overturned nearest neighbor spins. Periodic boundary conditions are used. For both dynamics, average lifetimes are measured over 2000 escapes with the system size $L=24$. The range of temperatures used is between $T/J = 0.04$ and $T/J = 0.2$. At very low temperatures for a given field, MPFUN \cite{10} is used for high-precision calculations. Since at low temperatures the lifetime is the inverse of the probability that the system escapes from the metastable well, the lifetime is written as

$$\langle \tau \rangle = A e^{\beta T},$$

where $A$ is a prefactor and $\Gamma$ is given in Eq.(1). In a given field, the prefactor $A$ and $\Gamma$ can be extrapolated to zero temperature from the measured lifetimes: $T \ln(\tau) = T \ln A + \Gamma$ (Figure 1).

The exact lifetimes can be analytically obtained from Absorbing Markov Chains (AMC) \cite{3,8} in principle. For $2J < |H| < 4J$, $\ell_c = 1$, two transient states are needed while for $J < |H| < 2J$, $\ell_c = 2$, seven transient states are needed. For fields lower than $J$, a large number of transient states are needed so practically it is not possible to compute the exact lifetimes from AMC. The Glauber and phonon dynamics provide the same energy barrier $\Gamma$. However, the prefactor $A$ in the lifetime resulting from the phonon dynamic is different from that from the Glauber dynamic. The Glauber prefactor is known to be $A = 5/4$ for $\ell_c = 1$, $A = 3/8$ for $\ell_c = 2$ \cite{8}, and $3/(8(\ell_c - 1))$ for $\ell_c \geq 2$ \cite{11}. The $d$-dimensional phonon dynamic gives a prefactor $A$ that has a non-constant derivative with respect to $|H|$ and that depends on the dimension of the heat bath. For $2J < |H| < 4J$,

$$A(|H|, d) = \frac{4(2|H| - 4J)^d + (8J - 2|H|)^d}{4(2|H| - 4J)^d(8J - 2|H|)^d}.$$  \hspace{1cm} (9)

In the limit that $d \to 0$, $A$ approaches the Glauber prefactor, 5/4. For an infinite-dimensional bath, $A \to \infty$ for $2J < |H| < 5J/2$ and $7J/2 < |H| < 4J$, $A \to 1/4$ for $|H| = 5J/2$, $A \to 0$ for $5J/2 < |H| < 7J/2$, and $A \to 1$ for $|H| = 7J/2$. For $J < |H| < 2J$,

$$A(|H|, d) = \frac{|H|^d + 2(2J - |H|)^d}{2^d+3|H|^d(2J - |H|)^d}.$$  \hspace{1cm} (10)

In the limit that $d \to 0$, $A$ approaches the Glauber prefactor, 3/8. For an infinite dimensional bath, $A \to 0$ for $J < |H| < 3J/2$, $A \to 1/8$ for $|H| = 3J/2$, and $A \to \infty$ for $3J/2 < |H| < 2J$. The expressions (9) and (10) for the prefactor are exact as $T \to 0$. 

![Figure 1](image)
At nonzero temperatures there are correction terms on the order of $e^{-\delta\beta}$ where $\delta$ depends on the field. Figure 2 shows the prefactor $A$ vs. $|H|$ for the phonon and Glauber dynamics. The prefactors for integer values of $2J/|H|$ are obtained from the MCAMC simulation data, while the prefactors in other magnetic fields are from Eqs. (9) and (10). We have confirmed that the measured prefactors agree with the calculated values for the $d$-dimensional phonon dynamic.

The prefactor from the phonon dynamic diverges as $|H| \to 2J$ or $4J$ because certain spin flips are not allowed. For $|H|=4J$, the probability to flip a spin in the all-spin-up state vanishes, while for $|H|=2J$ the probability to flip a spin in the configuration with three nearest-neighbor spins up and one down vanishes. At $|H|=2J$, the energy barrier is $2(8J-2|H|)$ for the phonon dynamic because the system reaches a critical droplet by creating two overturned 2nd-neighbor spins or two overturned 3rd-neighbor spins. Figure 1 shows $\Gamma=8J$ at $|H|=2J$. However, this behaviour does not occur at $|H|=J$, so the prefactor from the phonon dynamic is finite as $|H|$ approaches $J$. For bulk iron, the exchange coupling constant $J$ corresponds to about 300 T [12]. So $|H|=J$ is too high to achieve in a laboratory although the actual value of $J$ may vary with structure and surrounding environment of materials.

4. Conclusion

We derived a relationship between Monte Carlo time and physical time in terms of material parameters, starting from a quantum Hamiltonian with a phonon heat bath. We applied this dynamic to the square-lattice Ising ferromagnet and measured the lifetime of the metastable state. This dynamic gives a very different low-temperature prefactor from the Glauber dynamic.

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