A single-chain magnet (SCM) can be considered to be a spin super-chain consisting of single-molecule magnets coupled with spin exchange interactions. We use a hybrid dynamical Monte-Carlo (DMC) method to study temperature-dependent dynamical magnetization behaviors of SCM systems with strong magnetic anisotropy. This method, with both thermal activations and Landau-Zener (LZ) quantum spin tunnelings taken into account, can capture main magnetization dynamics of such spin systems. For Mn$_2$Ni SCM system as an example, our DMC simulated magnetization curves are in agreement with experimental results under typical temperatures and sweeping rates and our simulated coercive fields as functions of temperature are also consistent with experimental curves. Our analysis indicates that the magnetization reversal is determined by both thermal-activated effects and LZ quantum spin tunnelings. At high temperature, the nucleation for the reversal starts mainly at the chain ends thanks to thermal hurdling effect of single spins and further growth of the reversed spin domains accomplishes the magnetization reversal, which is consistent with Glauber dynamics with finite size effect. When temperature decreases, the rates of the nucleation and the growth decrease and quantum spin tunneling increases so that at intermediate temperature both thermal and quantum effects play roles in the nucleation, which is consistent with recent experimental observation of quantum nucleation. At extra-low temperature the thermal effect cannot make the reversed domains grow, but the LZ effect can realize the magnetization reversal through reversing all the spins in the whole chain. These make a unified theory beyond Glauber dynamics, including both classical and quantum effects, for the temperature-dependent spin reversal modes and dynamical magnetization behaviors of SCM systems with strong anisotropy. This theory can help explore basic properties and applications of such important magnetic systems.

I. INTRODUCTION

Recently, nanoscale spin chains have been attracting great attention because of their important properties and potential applications in information science and technology. The single-chain magnet (SCM) is a new member of such nanoscale spin chains, and its basic spin unit come from some transition-metal or rare-earth ions combined with appropriate organic molecules, and thus can be considered to be a single-molecule magnet (SMM). A well known example of SCM is the [Mn$_2$Ni] system, with $C_{62}H_{64}N_{10}O_{16}Cl_2Mn_2Ni$ and $C_{66}H_{60}N_{12}O_{14}Cl_2Mn_2Ni$ as two typical formula units with spin $S = 3$. The basic spin unit of a SCM usually has a large spin with strong uniaxial magnetic anisotropy, and there are some spin exchange couplings between near spin units. Therefore, when addressing its spin properties, we can consider a SCM to be an anisotropic spin super-chain consisting of SMMs interacting with some spin exchanges.

Usually, a SMM has a large spin value ($S$) and strong magnetic anisotropy. The strong uniaxial anisotropy makes an energy barrier that hinders reversal of its spin. This leads to well-known Arrhenius law for its spin relaxation at high enough temperature. On the other hand, at low enough temperature, the SMM spin can be reversed through quantum Landau-Zener (LZ) spin tunneling. Various methods are used to study such phenomena. At intermediate temperatures, the thermal barrier-hurdling and quantum LZ effects both play important roles, and in addition there are some thermally-added LZ spin tunneling. There are always some step structures in experimental magnetization curves. These spin dynamical behaviors due to the classical and quantum effects, from low to high temperature, can be well simulated with a dynamical Monte Carlo (DMC) method. As for SCM systems, inter-spin exchange interactions play important roles and thermal effects can cause Glauber spin dynamics, which was originally proposed for one-dimensional Ising spin model. Furthermore, a systematical experimental study shows that quantum nucleation can become important to reverse single spins, create domains of reversed spins, and reverse the whole SCM. Therefore, there are at least two modes for the magnetization dynamics of SCM systems.

In this paper, we develop the hybrid DMC method and thereby investigate the [Mn$_2$Ni] SCM system as a typical example of SCMs, taking both classical and quantum effects into account. Our simulated magnetization curves for typical temperatures and sweeping rates are consistent with corresponding experimental curves. Our simulated coercive fields as functions of temperature, that is $B_c$-$T$ curves, are also in good agreement with experiment. It is very interesting that we can satisfactorily fit the simulated and experimental $B_c$-$T$ curves by one...
simple function. These means that the DMC method and simulated results are both reasonable and reliable for such SCM systems. Furthermore, we explore magnetization reversal modes for different temperatures on the basis of our simulated results and analyses. Consequently, we can unify the observed Glauber dynamics and quantum nucleation mechanism in terms of a unified theory. More detailed results will be presented in the following.

The rest of this paper is organized as follows. In section II, we describe our model treatment and dynamical Monte Carlo (DMC) simulation method. In section III, we present our main DMC simulated results: temperature-dependent magnetization curves and coercive fields for typical sweeping rates. In section IV, we investigate the magnetization dynamics and elucidate the magnetization reversal mechanism by analyzing our simulated results. In section V we make some further discussions. Finally, we shall present our conclusion in section VI.

II. MODEL AND METHODS

A. Model treatment

The single-chain magnet can be considered a one-dimensional composite spin lattice whose spins can be constructed by repeating a basic unit of [Mn$_2$Ni]: Mn-Ni-Mn (or Mn$^{3+}$-Ni$^{2+}$-Mn$^{3+}$). There are two kinds of spin exchange interactions: antiferromagnetic Ni-Mn and ferromagnetic Mn-Mn. The antiferromagnetic Ni-Mn interaction is much stronger than the ferromagnetic Mn-Mn one so that the low-temperatures physics of this spin chain can be modelled by an effective ferromagnetic chain of the units of [Mn$_2$Ni] ($S = 3$) with spin interaction only between the nearest units.$^{3,4,6,22}$

From now on, for brevity we use a site to describe a Mn$_2$Ni unit, and the spin chain consists of identical spins with $S = 3$ on identical lattice sites. The ferromagnetic spin Hamiltonian without magnetic field and inter-site interactions can be expressed as$^{7,9,14}$

$$\hat{H}_0 = \sum_{i=1}^{N} \left\{ -D(\hat{S}^z_i)^2 - E[(\hat{S}^x_i)^2 - (\hat{S}^y_i)^2] \right\}$$

(1)

where $D$ and $E$ are the anisotropic parameters, and $\hat{S}_i = \{\hat{S}^x_i, \hat{S}^y_i, \hat{S}^z_i\}$ is the spin vector operator for the $i$-th Mn$_2$Ni unit. Considering the unit-spin exchange interaction and applying a magnetic field, we obtain the following total Hamiltonian:$^{7,9,14}$

$$\hat{H} = \hat{H}_0 - \sum_{i=1}^{N-1} J \hat{S}_i \cdot \hat{S}_{i+1} - \sum_{i=1}^{N} g \mu_B B z \hat{S}^z_i,$$

(2)

where $g$ is the Lande $g$ factor ($g = 2$ is used), $\mu_B$ the Bohr magneton, and $J$ ($> 0$) the ferromagnetic exchange constant.

B. Simulation methods

We use a dynamical Monte Carlo method to simulate the spin dynamics of the interacting spin system under sweeping magnetic field.$^{32,36,37}$ We divide the time $t$ into small time steps with a step length $\Delta t$ and describe the Monte Carlo time points with $t(n)$, where $n$ takes 0, 1, 2, 3,..., At a special time point $t(n)$, the spin value $S^z_i$ (for each $i$) is assumed to be either $-S$ or $S$, which is reasonable due to the strong anisotropy. The spin can be reversed within a Monte Carlo step (MCS) through the three reversal mechanisms.

Without considering the $J$-term in the Hamiltonian$^{22}$, the spins in the chain are independent of each other. For each spin, there are 7 possible spin values for the $z$ component $S^z$: -3, -2, -1, 0, 1, 2, and 3. We have $S^z = -3$ when the magnetic field $B_z$ is $-B_0$, where $B_0$ is very large. In this case, we have a very deep potential well at the side of $S^z = -3$. When $B_z$ increases from $-B_0$, the depth of the potential well decreases. When $B_z$ approaches 0, there appears some probability of transiting from the spin state of $S^z = -3$. As shown in Fig. 1, there are usually three different mechanisms for the spin to transit from $S^z = -3$: (1) thermally activated spin reversal, (2) direct Landau-Zener spin tunnelling, and (3) thermally assisted Landau-Zener spin tunnelling. We always consider all the three mechanisms of spin reversal, although some of them play minor roles under some conditions. After the $J$-term is taken into account, the spins are coupled and we need to make some approximations. When we calculate the reversal probability of the $i$-th spin, we use an approximation $\hat{S}^z_i = \{0,0,S^z_i\}$ for all the spins at the neighboring $j$ sites, but keep all the three quantum spin operators at the site $i$ for calculating the LZ transition probabilities.

FIG. 1: A schematic of the three spin reversal mechanisms: Thermal-activated barrier hurdling (a), direct and thermal-assisted LZ tunnelings (b). The horizontal solid line with arrow means that the two energy levels satisfy the resonance conditions. The probabilities, energy levels, barrier, and other symbols are defined in the text.
To calculate the reversal probability of classical thermal activation, we temporarily neglect the energy term and consider $S^z$ as a continuous variable between -3 and +3. Thus, there is a potential barrier $\Delta E_i$ of the $i$-th spin between $S^z_i = -3$ and $S^z_i = 3$, as shown in Fig. 1. It can be expressed as the difference between the energy at the top and that at $S^z_i = -3$. The transition rate is equivalent to

$$R_i = R_0 \exp(-\frac{\Delta E_i}{k_B T}),$$

where $k_B$ is the Boltzmann constant, $T$ temperature, and $R_0$ the characteristic frequency for the spin system ($3 \times 10^8 \text{s}^{-1}$). As a result, we can obtain the following probability $P_{th}$ that the spin transits from $S^z = -3$ to $S^z = 3$ within the time decrement $\Delta t$.

$$P_{th} = 1 - \exp(-R_i \Delta t)$$

There is a necessary condition for a LZ tunnelling of a spin to occur: one of the spin energy levels on the side of $S^z = -3$ must be equivalent to another on the side of $S^z = 3$, for example, $E_m(t) = E_{m'}(t)$, as shown in Fig. 1. This is the resonant condition of the energy levels dependent on the magnetic field. The resonant levels can be shown with the crossing points in Fig. 2. With the neighboring spins taken into account, such conditions are satisfied at the following magnetic fields:\cite{21,22}

$$B_{mm'}^{i} = -\frac{J(S^z_{i-1} + S^z_{i+1}) + D(m + m')}{g \mu_B}$$

The corresponding LZ transition probability is given by

$$P_{LZ}^{m,m'} = 1 - \exp \left[ -\frac{\pi(\Delta_{m,m'})^2}{2\hbar g \mu_B |m - m'| \nu} \right]$$

where the tunnelling splitting $\Delta_{m,m'}$ is the energy gap at the avoided crossing of states $m$ and $m'$, and $\nu$ denotes the sweeping rate of the magnetic field. At a given time, there are at most three such pairs of $m$ and $m'$. When $m$ equals to $S = -3$ and $m'$ is $S'$, we obtain a direct LZ tunnelling with the probability $P_{LZ}^{m,m'} = |P_{LZ}^{S',S}|^2$. For other possible LZ tunnelling to happen, the spin at first must be excited from $S^z = -3$ to the $m$ values through some thermal activations, as shown in Fig. 1. The thermal probability $P_{th}^{S,m}$ from $S$ to $m$ can be obtained by using the expressions (3) and (4) with the pair of $S$ and $m$ on the same side of $S^z = -3$. After the spin transits to the side of $S^z = 3$, it will changes to 3 soon. Therefore, the probability of spin reversal in this channel, $P_{LZ}^{m}$, is given by $P_{LZ}^{m} = P_{th}^{S,m} \cdot P_{LZ}^{S,m'}$. All the three spin-reversal channels are combined to give the total probability for a spin reversal:\cite{22}

$$P^{\text{tot}} = 1 - (1 - P_{th}) \cdot (1 - P_{LZ}^{m}) \cdot \prod_{m} (1 - P_{LZ}^{m'})$$

III. MAIN SIMULATED RESULTS AND ANALYSIS

A. Model and simulation parameters

As for the parameters of the spin interaction and on-site anisotropy, we use $J/k_B = 1.56\text{K}$ and $D/k_B = 2.5\text{K}$ from thermodynamical measurements:\cite{7,8,11}. The transverse anisotropic parameter $E$ is much smaller, but necessary to realize the Landau-Zener spin tunnelling. We take $E/k_B = 0.1\text{K}$ by comparing our simulated results with experimental ones.

At the beginning, we set all of the spins at the state $S^z = -3$. The magnetic field starts from $-B_0$ and increases by an increment of $\Delta t \cdot \nu$ until $B_0$. In our simulations, we take $\Delta t = 0.1\text{ms}$ and use 100 units of Mn$_2$Ni with free boundary condition. The magnetization is calculated by averaging $S^z$ over the 100 spin sites. Each
data point is calculated by averaging 10000 independent runs to reduce possible errors. The value of $B_0$ is made large enough to obtain complete hysteresis loops with the help of a symmetrization treatment.

B. Magnetization hysteresis loops

Presented in Fig. 3 are our typical simulated magnetization curves for five different field sweeping rates $\nu$ (0.001, 0.004, 0.017, 0.07, and 0.28 tesla/s) at three different temperatures $T$: 2.5, 1.5, and 0.5 K. The simulated results show that the hysteresis loops are strongly dependent on both temperature $T$ and field sweeping rate $\nu$. Our simulation shows that there is no hysteresis loop for all the field sweeping rates when temperature reaches 3 K, and at 2.5 K, the thermal effects are dominant and spins can be easily reversed, which results in very small hysteresis loops. Our data analysis indicates that when the temperature further decreases, the thermal-activated spin exchange interaction in the $J$-term becomes less important and the thermal-assisted LZ spin tunnelling already takes place frequently. At 1.5 K, another typical temperature, these two channels are available for the spin being reversed, but the total reversal probability is less than that of 2.5 K, and hence the coercive fields is substantially larger than that of 2.5 K. When the temperature becomes very low, for example down to 0.5 K, our probability analysis reveals that the thermal activation is almost frozen and the spin reversal can be realized only through the direct LZ spin tunnelling, and as a result, the coercive fields are large because the transverse parameter $E$ is very small. Even at this low temperature, there is no clear step structure in the magnetization curves, which should be attributed to the strong spin exchange interaction in the $J$-term. This is in contrast to those in the cases of Mn$_{12}$ and Fe$_8$ systems\textsuperscript{36,37}. Our simulated magnetization curves also show that the larger the field sweeping rate, the larger the hysteresis loop. This trend can be explained by considering that larger sweeping rate means shorter time for spins to try towards reversal, as shown in classical nanoscale spin systems\textsuperscript{36,37}.

C. $T$-dependent coercive fields

Presented in Fig. 4 we present our systematical results on the coercive fields $B_c$ as functions of temperature $T$ for three sweeping rates $\nu$: 0.004, 0.035, and 0.14 tesla/s. The curves are well fitted with Eq. (8) using the set of parameters $(A, T_1, T_2)$ presented in Table I.

\begin{equation}
B_c = \frac{A}{1 + \exp\left(\frac{T}{T_1} - \frac{T_2}{T}\right)} \quad (8)
\end{equation}

For the three $B_c$-$T$ curves in Fig. 4, the fitting parameters $(A, T_1, T_2)$ are summarized in Table I. When the temperature is high, the $B_c$-$T$ curves are dominated by the $T_1$ term in the exponential, $B_c \sim A \exp\left(-\frac{T}{T_1}\right)$, which should be naturally attributed to thermal activations. When the temperature is below 1 K, the coercive fields substantially deviate from classical behavior. Especially when the temperature decreases below 0.5 K, the coercive fields tend to saturate, $B_c \sim A$. This means that the low-temperature saturation behavior is consistent with quantum LZ effect, in contrast with Glauber dynamics\textsuperscript{36,37}.

It is very surprising that the simple function (8) can satisfactorily describe the experimental $B_c$-$T$ curves for such sweeping rates, too. Our fitted parameters for the experimental curves are summarized in Table II. Clearly, our theoretical parameters are in good agreement with those from experimental data. These show that not only our simulated results are reasonable but also our model and methods are reliable for such real spin systems.

| $\nu$ (tesla/s) | $A$ (tesla) | $T_1$ (K) | $T_2$ (K) |
|----------------|------------|----------|----------|
| 0.004          | 3.22       | 0.62     | 2.54     |
| 0.035          | 3.27       | 0.65     | 3.27     |
| 0.14           | 3.31       | 0.67     | 3.63     |
The field sweeping rate \( \nu \) is 0.004 tesla/s. Here, the time is described with the sweeping field \( B \) in unit of tesla (T), and for brevity, only the right-most part of the spin chain is presented. The time evolution of the spin configurations under three typical temperatures: 2.5 K (a), 1.5 K (b), and 0.5 K (c). For the whole chain as shown in Fig. 5b, and the reversed spin domain begins from the end of the spin chain at -0.8 tesla for both of the figures, the field sweeping rate is \( \nu=0.004 \text{ tesla/s} \). In order to elucidate the dynamical magnetization in the single-chain magnet, it is useful to investigate the time evolution of the spin configurations of the whole spin chain over the time. Most important is when the magnetization changes abruptly from -3 to 3. Because the time is a linear function of the magnetic field, we use the field to describe the time in the following. Here we present the evolution of a single-chain magnet from the beginning to the finishing of its spin reversals for three temperatures: 2.5, 1.5, and 0.5 K. The spin configuration evolution of the right-most part of the chain is presented in Fig. 5, and the magnetization evolutions of the whole spin chain are demonstrated in Fig. 6. For both of the figures, the field sweeping rate is \( \nu=0.004 \text{ tesla/s} \). At the high temperature 2.5 K, it is clear that the spin reversal begins from the end of the spin chain at -0.8 tesla for the whole chain as shown in Fig. 6a (-0.53 tesla for the run shown in Fig. 5a) and the reversed spin domain grows by the leftward movement of the domain wall (the boundary between the two spin domains). At 0.97 tesla,
all the spins shown in Fig. 5a are already reversed, and then the whole chain are completely reversed at about 1.3 tesla. It should be pointed out that effective values of the magnetic field should vary to some extent from one run to another, maybe being a little different from those shown in Fig. 5. Under this temperature, our analysis shows that the probability of the nucleation of the reversed spin domain at the end of the chain is approximately equivalent to $1.3 \times 10^{-5}$ per MCS, gigantically larger than that at other (in-chain) sites of the spin chain, $1.6 \times 10^{-5} \sim 3.7 \times 10^{-7}$ per MCS; and the probability of the reversed spin domain to grow ranges from 0.02 to 0.34 per MCS. Noticeably, all of these are made by the classical thermal effects, because the LZ quantum effects are effectively tiny at this temperature.

At the intermediate temperature 1.5 K, the situation seems more complex. Our analysis indicates that the probability of the classical end nucleation reduces to $1.8 \times 10^{-9}$ per MCS and classical nucleation probability at in-chain sites is usually equivalent to $3.4 \times 10^{-11}$ per MCS, but the nucleation probability from LZ quantum spin tunneling at a site ranges $1.1 \times 10^{-7} \sim 1.1 \times 10^{-5}$ per MCS. It is clear that both thermal and quantum effects play roles in the nucleation, but the quantum nucleation is dominant over the classical nucleation. Further analysis shows that the quantum nucleation is realized through thermal-assisted LZ quantum spin tunneling, between 0.2 and 1.6 tesla for the whole chain as shown in Fig. 6b (0.66 and 1.58 tesla for the run in Fig. 5b). As for the growth probability of the reversed spin domain, it ranges from $2.1 \times 10^{-4}$ to $9.1 \times 10^{-3}$ per MCS, due to thermal-activated movement of domain walls. These imply that the quantum effects play no role in making the domain walls move. Therefore, our simulated results lead to quantum-dominant many-site nucleation and classical wall-moving growth of reversed spin domains for the magnetization dynamics at this temperature.

At extra-low temperature 0.5 K, our data show that classical nucleation due to thermal activation is frozen, but quantum nucleation due to direct LZ quantum effect goes into action, with the probability being up to $0.001 \sim 0.31$ per MCS from 2.8 to 3.3 tesla, as shown in Fig. 6c (2.89 to 3.2 for the run in Fig. 5c). At this temperature, our data indicate that the growth probability of a reversed domain is approximately $3.4 \times 10^{-9}$ per MCS, due to classical effects. Because the probability of quantum nucleation is larger than that of domain wall growth by six orders of magnitude and others are effectively zero, the spins are reversed randomly one by one through the direct LZ quantum effect at such extra-low temperature, with the classical effects being almost frozen.

### B. Unified mechanism

In Table III summarized are the probability values of classical end nucleation ($P_{ce}^n$), classical in-chain nucleation ($P_{ci}^n$), quantum nucleation ($P_q^m$), and classical growth (domain wall movement) of reversed spin domains ($P_g^r$) for the three typical temperatures ($T$).

| $T$ (K) | 2.5 | 1.5 | 0.5 |
|---------|-----|-----|-----|
| $P_{ce}^n$ | $1.3 \times 10^{-5}$ | $1.8 \times 10^{-9}$ | $< 10^{-15}$ |
| $P_{ci}^n$ | $(0.2 \sim 37.) \times 10^{-8}$ | $< 3.4 \times 10^{-11}$ | $< 10^{-15}$ |
| $P_q^m$ | $< 10^{-12}$ | $(0.11 \sim 1.1) \times 10^{-6}$ | $0.001 \sim 0.31$ |
| $P_g^r$ | $0.02 \sim 0.34$ | $(0.2 \sim 9.1) \times 10^{-3}$ | $3.4 \times 10^{-9}$ |

### V. FURTHER DISCUSSIONS

#### A. More about probabilities: $T$ trend

The probability values for classical processes, such as $P_{ce}^n$, $P_{ci}^n$, and $P_g^r$ for the two classical nucleations and the classical wall-moving growth, have a giant reduction when temperature decreases from high temperature (such as 2.5 K) to low temperature (such as 0.5 K), because the temperature is mainly in the exponential of the probability expressions, as shown in Eqs. (3) and (4). It, however, is nontrivial to understand the temperature trend of the probability of quantum nucleation ($P_q^m$). The quantum nucleation probability ranges from $0.001$ to $0.31$ per MCS at ultra-low temperature such as 0.5 K, but it decreases exponentially when temperature increases from 0.5 to 2.5 K. At first sight, it should be weakly dependent on temperature. Essentially, it depends on magnetic field because of three factors. First, the underlying spin tunneling can occurs only at some special values of magnetic field where resonant condition energy levels is satisfied, as shown in Figs. 1 and 2 and Eq. (5). Second, the tunneling splitting $\Delta_{mm'}$ decreases very quickly with...
increasing the order of perturbation in the sense of perturbation theory. Actually, the first order of perturbation appears approximately at 7.0 tesla, the second one at 3.24 tesla, and the third one at 0 tesla, as shown in Fig. 2. Importantly, $\Delta_{m0'}$ squared enters in the exponential of the probability expression for the quantum tunneling as shown in Eq. (6), and as a result, spin tunneling probability increases exponentially with magnetic field (for the sweeping of increasing field). Third, at high temperatures, the thermal effects are huge compared to the quantum effects and the whole chain is already reversed when the quantum effects have not yet occurred. At ultra-low temperature, because the thermal effects are frozen, the spins are waiting for so long time (large $B$) that spins can be reversed through the low-order quantum effects with large spin tunneling probability. Therefore, the quantum nucleation probability appears to exponentially increase with temperature.

B. Effects of chain length

The above pictures are based on our chain consisting of 100 sites. These should belong to short-chain regime. Now we address effects of chain length by analyzing the probabilities. Of course, it depends on temperature. At high temperature (such as 2.5K), for short chains such as our chain, there should be classical end nucleations at both of the ends and it is also likely for several classical in-chain nucleations to happen before the whole chain is reversed. This is because the high temperature reduces the effect of the energy difference between the end and in-chain sites. For short-enough chains, there should be only one domain of reversed spins. For much longer chain consisting of more than 10000 sites, there should be many domains of reversed spins with a characteristic length of every hundreds of sites (estimated in terms of $P_{c0}/P_{c1}$) and every domain grows independently. This is consistent with Glauber spin dynamics. At intermediate temperature, there are always two or more domains of reversed spins growing through classical wall-moving effect during the magnetization reversal. At low temperature such as 0.5 K, because the classical processes are almost frozen, the magnetization reversal is realized by reversing every spin in the chains through quantum spin tunneling effect. As usual, the longer the chain is, the more domains of reversed spins appears during the magnetization reversal.

C. Comparison with experiment

Our model parameters are from experimental observations. In addition, we consider a three-dimensional spin system by introducing a very weak inter-chain spin exchange coupling. Our Monte Carlo simulation indicates that its sublattice magnetization as a function of temperature is consistent with experimental results concerned. Our simulated magnetization curves shown Fig. 3 and $B_{c}-T$ curves in Fig. 4 are both in good agreement with experimental curves. These show that our model treatment and simulation methods are reliable and our simulated results, with parameters from experiment, are reasonable.

As for spin dynamics in SCM systems, Glauber behavior, usually with some modifications due to finite size effects, is frequently observed. On the other hand, there are convincing evidences that quantum nucleation plays some important roles in the magnetization dynamics. Consequently, our theory gives a unified description for both of these two dynamical phenomena on the basis of a unified mechanism.

VI. CONCLUSION

We have developed the hybrid DMC method to make it suitable to the spin chains with strong magnetic anisotropy, and used it to investigate temperature-dependent dynamical magnetization behaviors of [Mn$_2$Ni] SCM system as a typical example of SCMs. Our DMC simulated magnetization curves are in agreement with experimental results under typical temperatures and sweeping rates. We have also calculated the coercive fields as functions of temperature and plotted $B_{c}-T$ curves for typical sweeping rates. It is very interesting that our simulated $B_{c}-T$ curves are consistent with experimental ones and both of the simulated and experimental curves can be well fitted with a simple function. These means that our theory and simulated results are reasonable and reliable to such spin systems.

Furthermore, our analysis indicates that the magnetization reversal is determined by both thermal-activated effects and LZ quantum spin tunneings. At high temperature, the reversed spin domain can nucleate from one of the ends of chain and then grows due to the domain-wall movement thanks to thermal hurdles effect of single spins, which is consistent with Glauber dynamics with finite size effect. When temperature decreases, the rates of the classical nucleation and growth decrease exponentially and quantum spin tunneling increases exponentially, so that at intermediate temperature both thermal and quantum effects play substantial roles in the nucleation, which is consistent with recent experimental observation of quantum nucleation. At extra-low temperature the thermal effects are frozen and the LZ effect can realize the magnetization reversal through reversing all the spins in the whole chain. Therefore, the three typical regions can be understood under one unified theory.

In summary, these make a unified theory beyond Glauber dynamics, including both classical and quantum effects, for the dynamical magnetization behaviors and temperature-dependent spin reversal modes of SCM systems with strong anisotropy. This theory can be useful to explore basic properties and applications of such spin systems.
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