Chaotic dynamics and spin correlation functions in a chain of nanomagnets

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We study a chain of coupled nanomagnets in a classical approximation. We show that the infinitely long chain of coupled nanomagnets can be equivalently mapped onto an effective one-dimensional Hamiltonian with a fictitious time-dependent perturbation. We establish a connection between the dynamical characteristics of the classical system and spin correlation time. The decay rate for the spin correlation functions turns out to depend logarithmically on the maximal Lyapunov exponent. Furthermore, we discuss the nontrivial role of the exchange anisotropy within the chain.

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I. INTRODUCTION

Nanoscale magnetic structures have promising applications as basic elements in future nanoelectronics devices and are frequently discussed in the context of quantum information processing. The principal challenge of quantum information technology is finding an efficient procedure for the generation and manipulation of the many-qubit entangled states. Those can be realized on the basis of, e.g., Rydberg atoms located in optical quantum cavities,[1–3] Josephson junctions,[4] or ion traps.[5] One very promising realization is based on single molecular nanomagnets (SMMs).[6–8] These are molecular structures with a large effective spin. A prototypical representative of this family of compounds is Mn_{12} acetate in which $S = 16$. Molecular nanomagnets show a number of interesting phenomena that have been the focus of theoretical and experimental research during the last two decades.[6–17] For instance, SMMs show a bistable behavior as a result of the strong uniaxial anisotropy,[6] as well as a tunneling of the magnetization.[7] An attractive feature for information storage is the large relaxation time of molecular nanomagnets.[11]

SMMs are usually modeled by spin-chain Hamiltonians augmented by different kinds of interaction terms responsible for different compounds. These interaction contributions are highly nontrivial and, in most cases, are anisotropic. This makes the analytical treatment very cumbersome, calling for efficient theoretical approaches. In this paper we investigate the properties of a classical spin chain coupled by anisotropic exchange interactions. This case is relevant not only for chains of exchange-coupled SMMs,[18] but also for several other realistic physical problems, including weakly coupled antiferromagnetic rings[19] and large spin multiples coupled by the Dzyaloshinskii-Moriya (DM) exchange interaction.[20] We will demonstrate that even for multidimensional complex physical systems, it is still possible to obtain analytical results using special mathematical techniques presented in Ref. 23. Its applicability to the SMMs is shown in Refs. 21 and 22. In the first step, one evaluates the Lyapunov exponents and the spin correlation functions for the system. One can then extract information on the properties of the system beyond the classical limit. For example, there is a deep connection between the classical Lyapunov exponents and the quantum Loschmidt echo,[24] which is a natural measure of the quantum stability and of the fidelity of quantum teleportation.[25] If the Lyapunov regime is reached for a quantum system, then the decay rate for the teleportation fidelity can be identified via the Lyapunov exponent. Formal criteria for the Lyapunov regime[26] in the case of a chain of SMMs can be estimated from the relation $\lambda < J^2/\Delta$, where λ is the Lyapunov exponent, Δ is the mean level spacing, and J is the exchange-interaction constant between SMM spins (which prohibits the integrability of the system leading thus to the chaotic dynamics). Furthermore, it can be shown that the spin correlation functions can be expressed through the Lyapunov exponent.

This paper is organized as follows. In Sec. II we give a brief exposition of our model and present the details of the principal investigation technique. In Sec. III we discuss the relation between the relevant spin correlation functions and their classical analogs. Section IV contains the treatment of the system in the chaotic domain. Finally, the conclusions section summarizes our findings. All necessary mathematical details are presented in the Appendices.

II. THEORETICAL FORMULATION

The prototype model Hamiltonian for the exchange-coupled SMM is

$$H = J\sum_n S_n^z S_{n+1}^z + g\sum_n \left(S_n^x S_{n+1}^x + S_n^y S_{n+1}^y\right) + \beta\sum_n \left(S_n^z\right)^2, \quad (1)$$

where J and g are exchange-interaction constants, and $\beta = -DS^2$ is the anisotropy barrier height of the system. For the prototypical Mn_{12} acetates,[6] $D \sim 0.7K$ sets the value of the barrier parameter,[22] and $S^{x,y,z}$ are spin projection operators of the SMM. Due to the large spin of the SMM (see Sec. I), an analytical quantum mechanical treatment of the model (1) is hardly accessible. To make progress, we choose the semiclassical parametrization as follows:

$$S_n^z = \cos\theta_n, \quad S_n^x = \sin\theta_n\cos\varphi_n, \quad S_n^y = \sin\theta_n\sin\varphi_n. \quad (2)$$

Then the Hamiltonian (1) can be rewritten in the more convenient form

$$H = J\sum_n \cos\theta_n \cos\theta_{n+1} + g\sum_n \sin\theta_n \sin\theta_{n+1} \times \cos(\varphi_{n+1} - \varphi_n) + \beta\sum_n \cos^2\theta_n. \quad (3)$$

Our aim is the evaluation of the correlation functions and the study of the spin dynamics governed by the Hamiltonian (3). Since this is a highly nonlinear problem, it cannot be done in a simple and direct way. However, one can rigorously show that there is a direct map between the chain of SMMs and a one-dimensional (1D) model Hamiltonian with a fictitious time-dependent external perturbation.

The equilibrium state for the model (3) satisfies the minimum condition of the infinite-dimensional functional $H[\theta,\varphi]$,

$$\frac{\partial H}{\partial \theta_n} = 0, \quad \frac{\partial H}{\partial \varphi_n} = 0, \quad n = 1,2,\ldots,\infty. \quad (4)$$

Considering the Hamiltonian (3), we retain only the first-order terms of the anisotropy parameter $\varepsilon = (J-g)/2g \ll 1$. Then, after straightforward but laborious calculations, we deduce from (4) that the following relations hold:

$$S_{n+1} = (-1)^m \{S_n - \beta\sin(2\theta_n)[1 - \varepsilon\cos(2\theta_n)]\}, \quad (5)$$

$$\theta_{n+1} = (-1)^m\theta_n + \pi\nu + (-1)^\nu \arcsin S_{n+1},$$
$$\varphi_{n+1} = \varphi_n + \pi m; \quad m = 0,1; \quad \nu = 0,1; \quad (6)$$

where $S_{n+1} = \sin(\theta_{n+1} - \theta_n)$. The index ν refers to the two possible solutions when inverting the trigonometric expression for S_{n+1}. Depending on the sign of the rescaled barrier height $\beta \to \mp\beta/g$, the index $m = 0,1$ defines the energy minimum condition. For convenience, we will use positively defined $\beta > 0$ and consequently $m = 0$ in our calculations. The above result is just a recurrence relation in the form of the explicit map $(S_{n+1},\theta_{n+1}) = \hat{T}(S_n,\theta_n)$. Our idea is to find a Hamiltonian model that is equivalent to (5). Let us consider the following perturbed 1D Hamiltonian system:

$$H = H_0(s) + \beta V(\theta) T \sum_{n=-\infty}^{+\infty} \delta(t - nT),$$
$$H_0(S) = \nu\pi S + (-1)^\nu (S\arcsin S + \sqrt{1 - S^2}), \quad (7)$$
$$V(\theta) = -\left(\cos^2 - \frac{\varepsilon}{4}\cos^2 2\theta\right).$$

The respective Hamiltonian equations read

$$\frac{dS}{dt} = -\frac{\partial H}{\partial \theta} = -\beta V'(\theta) T \sum_{n=-\infty}^{+\infty} \delta(t - nT),$$
$$\frac{d\theta}{dt} = \frac{\partial H}{\partial S} = \omega(S), \quad (8)$$
$$\omega_\nu(S) = \pi\nu + (-1)^\nu \arcsin s.$$

Their integration simplifies due to the presence of the δ function in the perturbation term because the evolution operator $(\bar{S};\bar{\theta}) = \hat{T}(S;\theta)$ splits into pulse-induced $\hat{T}_\delta$ and free-evolution $\hat{T}_R$ terms:

$$\hat{T} = \hat{T}_R \otimes \hat{T}_\delta,$$
$$\bar{S} \equiv S(t_0 + t - 0); \quad \bar{\theta} \equiv \theta(t_0 + T - 0), \quad (9)$$
$$S \equiv S(t_0 - 0); \quad \theta \equiv \theta(t_0 - 0).$$

For the operator of free evolution, we simply have

$$\hat{T}_R(S;\theta) = [S;\theta + \omega_\nu(S)T]. \quad (10)$$

The explicit form of the pulse-induced evolution operator $\hat{T}_\delta$ can be derived after an integration of the system (6) on the small time interval $(t_0 - 0, t_0 + 0)$ around t_0, where the pulse is applied, as

$$S(t_0 + 0) - S(t_0 - 0) = \int_{t_0-0}^{t_0+0} \dot{S} dt$$
$$= -\int_{t_0-0}^{t_0+0} \beta \frac{\partial V(\theta)}{\partial \theta} T \sum_{k=-\infty}^{+\infty} \delta(t - kT) = -\beta T \frac{\partial V(\theta)}{\partial \theta}, \quad (11)$$
$$\theta(t_0 + 0) - \theta(t_0 - 0) = \int_{t_0-0}^{t_0+0} \dot{\theta} dt = 0.$$

By taking into account Eq. (11), for the pulse-induced evolution operator, we obtain

$$\hat{T}_\delta = \left[-\beta\frac{\partial V(\theta)}{\partial\theta}, \theta\right]. \quad (12)$$

Combining Eqs. (10) and (12), the complete evolution picture can be expressed through the following map:

$$(\bar{S},\bar{\theta}) = \hat{T}(S,\theta) = \hat{T}_R \hat{T}_\delta(S,\theta) = \hat{T}_R\left[S - \beta T\frac{\partial V(S,\theta)}{\partial\theta}, \theta\right]$$
$$= \left[S - \beta\frac{\partial V(\theta)}{\partial\theta}; \theta + \omega_\nu(\bar{S})\right], \quad (13)$$

or in the explicit form

$$S_{n+1} = S_n - \beta\left(\sin 2\theta_n - \frac{\varepsilon}{2}\sin 4\theta_n\right),$$
$$\theta_{n+1} = \theta_n + \omega_\nu(S_{n+1}), \quad (14)$$
$$\omega_\nu(S_n) = \pi\nu + (-1)^\nu \arcsin S_n.$$

For the details of the derivation of Eq. (14), see Appendix A.

This result is obtained for the kicked Hamiltonian model with $T = 1$ and it matches exactly the recurrence relations in Eq. (5) obtained for the SMM chain. Such an analogy is quite important since the infinite-dimensional nonlinear system (3) is now equivalent to the 1D Hamiltonian model. We note that the discrete time in the perturbation term (7) is fictitious and corresponds to the number of the spins in the chain (1).

III. SPIN DYNAMICS AND CORRELATION FUNCTIONS

We will proceed with the equivalent 1D Hamiltonian model with fictitious time-dependent perturbation (7), which is more convenient than the multidimensional nonlinear model (3). Due to the nonlinearity of the model (7), we should expect a rich and complex dynamics. In particular, our purpose is to establish a connection between the chaotic dynamics and the decay rates of the spin correlation functions. As a first step, we construct the Jacobian matrix of the map (14),

$$\hat{M} = \begin{pmatrix} \frac{\partial \bar{S}}{\partial S} & \frac{\partial \bar{S}}{\partial \theta} \\ \frac{\partial \bar{\theta}}{\partial S} & \frac{\partial \bar{\theta}}{\partial \theta} \end{pmatrix} = \begin{pmatrix} 1 & -\beta V''(\theta) \\ \omega'(\bar{S}) & 1-\beta\omega'(\bar{S})V''(\theta) \end{pmatrix}. \quad (15)$$

The Lyapunov exponents can be evaluated as eigenvalues of this matrix, and are thus given by

$$\lambda_{1,2} = 1 + \frac{K}{2} \pm \sqrt{\left(1+\frac{1}{2}K\right)^2 - 1}, \quad (16)$$

where

$$K = -\beta\omega_\nu'(\bar{S})V''(\theta) \quad (17)$$

is the chaos parameter.[27] From Eqs. (16) and (17) for the chaos parameter K, we find the following simple relation:

$$K = -\frac{2\beta(\cos 2\theta - \varepsilon\cos 4\theta)}{\sqrt{1-S2}}. \quad (18)$$

The dynamics is expected to be chaotic if $K > 0$, $\lambda_1 > 1$ or $K < -4, \lambda_2 < -1$. Therefore, from Eq. (18), we obtain the relevant intervals for the angle variable,

$$\theta \in \left[\pi m + \frac{1}{2}\arccos\left(\frac{1}{2\varepsilon} - \sqrt{\frac{1}{4\varepsilon^2}+2}\right);\right.$$
$$\left.(m+1)\pi - \frac{1}{2}\arccos\left(\frac{1}{2\varepsilon} - \sqrt{\frac{1}{4\varepsilon^2}+2}\right)\right], \quad (19)$$

where $m = 0, \pm 1, \ldots$.

In the isotropic case $J \approx g$, $\varepsilon \to 0$, this leads to

$$\theta \in \left[\pi m + \frac{\pi}{4}; (m+1)\pi - \frac{\pi}{4}\right], \quad (20)$$

where $m = 0, \pm 1, \ldots$.

Equation (19) defines the width of the chaotic domain where the parameter of chaos (18) is larger than one, $K > 1$. Obviously, the width of the chaotic domain depends on the values of anisotropy, and it is easy to see that in the case of small anisotropy, the area of chaos is narrower than in the zero anisotropy case, $\Delta\theta(\varepsilon = 0) > \Delta\theta(\varepsilon \ll 1)$. Therefore we conclude that small anisotropy leads to the less chaotic regime.

From the parameter of the chaos (18) (also plotted in Fig. 1), we conclude that the phase space of the system consists of domains corresponding to a regular and a chaotic motion. Later we will use the random-phase approximation, which is valid precisely in the latter domain.[27]

In order to obtain explicit expressions for the spin correlation functions, we rewrite the recurrence relations in Eqs. (14) in the following form:

$$\begin{aligned}\theta_{n+1} &= \theta_n + \omega(s_{n+1}) = \theta_n + \omega_\nu[S_n - \beta V'(\theta)] \\ &= \theta_n + \omega_\nu(S_n) - \beta V'(\theta)\omega_\nu'(S_n) \\ &= \theta_n + \omega_\nu(S_n) - \beta\left(\sin 2\theta_n - \frac{\varepsilon}{2}\sin 4\theta_n\right). \end{aligned} \quad (21)$$

For the angular variable, we infer the self-consistent recurrence relation

$$\theta_{n+1} = \theta_n + \omega_\nu(S_n) - \beta\left(\sin 2\theta_n - \frac{\varepsilon}{2}\sin 4\theta_n\right). \quad (22)$$

The correlation function is given by

$$\begin{aligned}\langle S_{n+1}|S_j\rangle &= \frac{1}{2\pi}\int_0^{2\pi} d\theta_0 e^{i(\theta_n-\theta_0)} \\ &= \frac{1}{2\pi}\int_0^{2\pi} d\theta_0 e^{i[\theta_{n-1}+\omega_\nu(S_{n-1}) - K_0\sin 2\theta_{n-1} + \frac{K_0\varepsilon}{2}\sin 4\theta_{n-1}-\theta_0]}, \end{aligned} \quad (23)$$

and can be calculated using the above iterative procedure as well as the expression for the Bessel function, $\exp(iz\sin\varphi) = \sum_{m=-\infty}^{+\infty} J_m(z)e^{im\varphi}$. By taking into account that $\omega_\nu(S_n) = \omega \approx \text{const}$, and $K_0 = \beta\omega'(S_n) \approx \text{const}$, from Eq. (23), we deduce

$$\begin{aligned}\langle S_{j+n}|S_j\rangle &= \frac{1}{2\pi}\int_0^{2\pi} d\theta_0 e^{i(\theta_n-\theta_0)} = \frac{1}{2\pi}\int_0^{2\pi} d\theta_0 e^{i(\theta_{n-1}-\theta_0)} e^{-iK_0\sin 2\theta_{n-1}} e^{\frac{iK_0\varepsilon}{2}\sin 4\theta_{n-1}} \\ &= \frac{1}{2\pi}\int_0^{2\pi} d\theta_0 e^{i(\theta_{n-1}-\theta_0)} \sum_{m_1=-\infty}^{+\infty} J_{m_1}(K_0)e^{-2im_1\theta_{n-1}} \sum_{l_1=-\infty}^{+\infty} J_{l_1}\left(\frac{K_0\varepsilon}{2}\right)e^{4il_1\theta_{n-1}} \\ &= e^{in\omega}\sum_{m_1=-\infty}^{+\infty}\sum_{m_2=-\infty}^{+\infty}\cdots\sum_{m_n=-\infty}^{+\infty}\sum_{l_1=-\infty}^{+\infty}\sum_{l_2=-\infty}^{+\infty}\cdots\sum_{l_n=-\infty}^{+\infty}(-1)^{l_1+l_2+\cdots+l_n} \\ &\quad\times e^{-2i\omega m_1}e^{-2i\omega(m_1+m_2)}\cdots e^{-2i\omega(m_1+m_2+\cdots+m_{n-1})}e^{-2i\omega l_1}e^{-2i\omega(l_1+l_2)}\cdots e^{-2i\omega(l_1+l_2+\cdots+l_{n-1})} \\ &\quad\times J_{m_1}[K_0]J_{m_2}[(1-2m_1+4l_1)K_0]\cdots J_{m_n}\{[1-2(m_1+m_2+\cdots+m_{n-1}) \\ &\quad+4(l_1+l_2+\cdots+l_{n-1})]K_0\} \\ &\quad\times J_{l_1}\left[\frac{K_0\varepsilon}{2}\right]\cdots J_{l_n}\left[\frac{1-2(m_1+m_2+\cdots+m_{n-1})+4(l_1+l_2+\cdots+l_{n-1})K_0\varepsilon}{2}\right] \\ &\quad\times\delta_{1-2(m_1+m_2+\cdots+m_n)+4(l_1+l_2+\cdots+l_n);1}. \end{aligned} \quad (24)$$

For the details of the derivation of Eq. (24), see Appendix C.

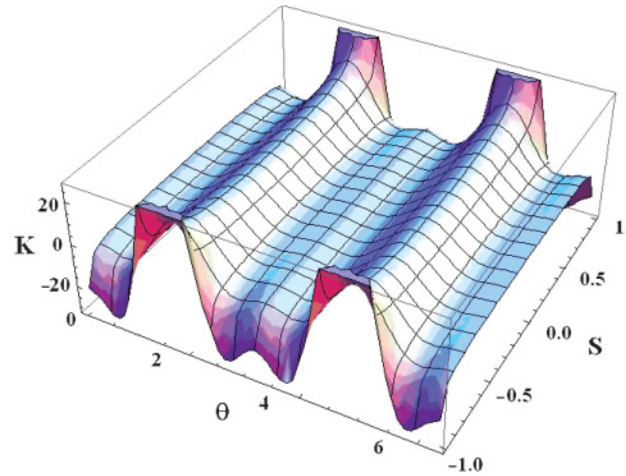

FIG. 1. (Color online) The parameter $K(\theta,S)$ signifying chaotic behavior, plotted according to Eq. (18) for the values of the parameters $\beta=3$, $\varepsilon=0.5$.

In the case of a large Lyapunov exponent $J_m(K_0)\sim(K_0)^{-1/2}$, where $K_0\gg 1$, we infer from (24)

$$\langle S_{j+n}|S_j\rangle\sim\frac{e^{in\omega}}{\left(K_0^2\varepsilon/2\right)^{n/2}}=\exp\left(-\frac{n}{\tau_c}\right)e^{in\omega},\qquad(25)$$

where $\tau_c=2/\ln(\frac{K_0^2\varepsilon}{2})$ is the correlation length. Since $K_0\sim\beta$, we have the following estimation:

$$\tau_c\sim\frac{2}{\ln\left(\frac{\beta^2\varepsilon}{2}\right)}.\qquad(26)$$

In the isotropic case $\varepsilon=0$, one can perform the same calculations [insertion of $\varepsilon=0$ into Eq. (26) gives a wrong result] and show that

$$\tau_c'\sim\frac{2}{\ln\beta}\qquad(27)$$

holds. Taking into account Eqs. (26) and (27), and expressions for the rescaled interaction constants $\varepsilon\to\frac{J-g}{2g},\beta\to\frac{\beta}{g}$, we conclude that the role of the anisotropy is not trivial. Namely, the strong anisotropy

$$J-g>\frac{4g^2}{\beta}\qquad(28)$$

suppresses the spin correlations, because then $\tau_c'>\tau_c$. However, the weak anisotropy

$$J-g<\frac{4g^2}{\beta}\qquad(29)$$

enhances the correlations $\tau_c'<\tau_c$.

It should be stressed that the reliability of the analytical estimates is limited. This is particularly apparent for the case where the numerical and the analytical predictions deviate from each other, due to the limited range of applicability of the analytical expressions derived after rough approximations.

The role of the anisotropy $\varepsilon=(J-g)/2g$ can be clarified numerically as well. In order to better understand the physical features of the model (1), we will study the phase portrait of the system. The results of the numerical evaluation of the recurrence relations (14) are presented in Figs. 2–5. As we see from Fig. 2, the phase space of the system consists of two topologically different domains separated from each other by a separatrix. Most of the phase space belongs to the domain of the regular motion and open-phase trajectories. The domain of closed-phase trajectories mainly corresponds to the irregular motion, and a small island of a regular motion is observed only in the center of the portrait. From this formal mathematical statement, one can extract interesting physical information. Closed trajectories belong to the oscillatory regime and open trajectories belong to the rotational one. Therefore, we expect that two types of motion can be realized for the model (1). The domain of the regular spin rotational motion is defined by the relation $0.2<|S_n|<1$. Therefore, if $|S_n|<0.2$, then the spin oscillation is chaotic and, only for very small amplitude, an island of regular oscillations is observed in the center. If the anisotropy parameter is zero, $\varepsilon=0$, then the island of the regular oscillatory motion disappears (see Fig. 3). This means that without the small anisotropy, the spin system is less correlated [see Eqs. (28) and (29)]. Such a geometrical interpretation can be extrapolated from the pair of the canonical variables (S_n,θ_n) to the real spin variables $S_n^z=\cos\theta_n$ using the parametrization (2) and a simple relation $S_n=\sin(\theta_n-\theta_{n-1})$.

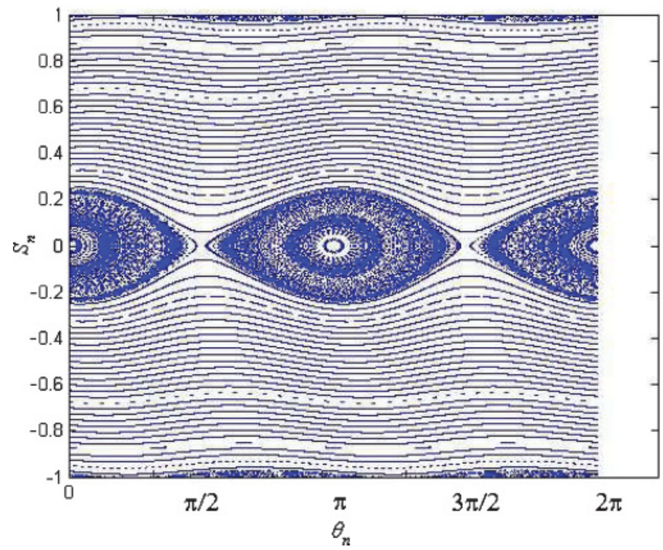

FIG. 2. (Color online) Results of the numerical calculations of the recurrence relations (14) on the phase plane (S_n,θ_n) for the following parameters: $\beta=0.05$, $\epsilon=0.005$. About a hundred trajectories are generated for the set of different initial conditions (S_0,θ_0).

IV. SPIN DIFFUSION AND KINETIC APPROACH

The dynamical picture does not apply in the chaotic regime for $K>0$ or $K<-4$. An adequate language in this case is the statistical approach. Instead of the dynamical variables, the key role is played by the probability distribution function, which is a solution of the Fokker-Planck equation. Its derivation is rather straightforward for chaotic dynamical models and is based on the Kolmogorov, Arnold, Moser (KAM) theory.[23] Interested readers can find all the technical details of the derivation for the spin-chain model in the recent work of

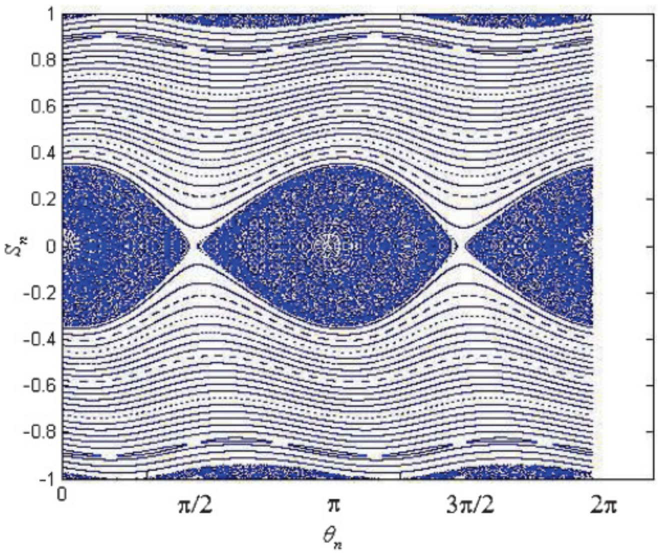

FIG. 3. (Color online) Results of the numerical calculations of the recurrence relations (14) on the phase plane (S_n,θ_n) for the following parameters: $\beta = 0.05$, $\epsilon = 0$. About a hundred trajectories are generated for the set of different initial conditions (S_0,θ_0).

Ref. 24. Here we are using the final result adapted to the SMM system. The probability distribution of the spin variable, $S_n = \sin(\theta_n - \theta_{n-1})$, is described by the following diffusion equation:

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial S^2}, \tag{30}$$

where $D(S) = \frac{\beta^2}{4}(1 + \frac{\varepsilon^2}{4})$ is the diffusion coefficient. For the details of the derivation of Eq. (30), see Appendix B. The fundamental solution of this equation is

$$f(S,t) = \frac{1}{2\sqrt{\pi Dt}} \exp\left(-\frac{S^2}{4Dt}\right), \tag{31}$$

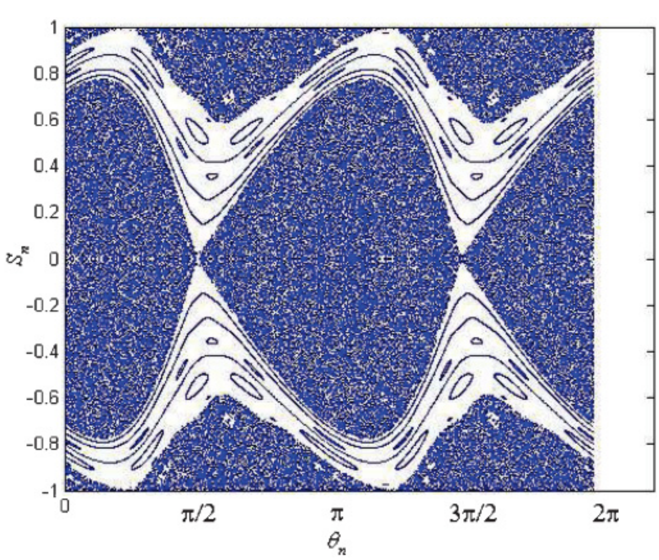

FIG. 4. (Color online) Results of the numerical calculations of the recurrence relations (14) on the phase plane (S_n,θ_n) for the following parameters: $\beta = 0.3$, $\epsilon = 0.15$. About a hundred trajectories are generated for the set of different initial conditions (S_0,θ_0).

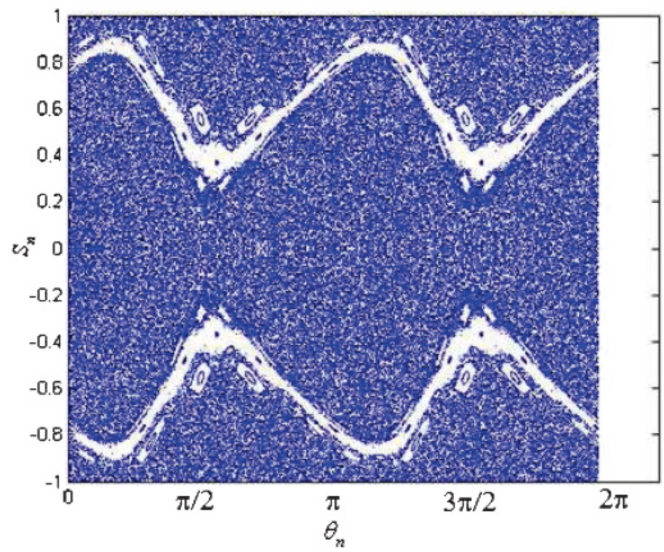

FIG. 5. (Color online) Results of the numerical calculations of the recurrence relations (14) on the phase plane (S_n,θ_n) for the following parameters: $\beta = 0.3$, $\epsilon = 0$. About a hundred trajectories are generated for the set of different initial conditions (S_0,θ_0). With the increase of the value of parameter β, the domain of the chaotic motion covers almost the whole phase space (see Figs. 4 and 5), because the chaos parameter K given by Eq. (18) is proportional to the constant β.

and can be found in many classical textbooks (see, e.g., Ref. 30). This solution (31) is defined on the interval $-\infty < S < \infty$, whereas we need one for the interval $-1 \leqslant S \leqslant 1$. In order to find a solution relevant to our problem, we will consider the following boundary and initial conditions for the diffusion equation (30):

$$f = W_0 \quad \text{for} \quad t = 0, \quad f = g_1(t) \quad \text{for} \quad S = -1, \\ f = g_2(t) \quad \text{for} \quad S = 1, \tag{32}$$

and we will look for the solution in the form

$$f(S,t) = 2\sum_{m=1}^{\infty} \sin(m\pi S)\exp(-Dm^2\pi^2 t)M_m(t), \tag{33}$$

where

$$M_m(t) = \int_0^1 f_0(\xi)\sin(n\pi\xi)\,d\xi + Dm\pi \int_0^1 \exp(Dm^2\pi^2\tau) \\ \times [g_1(\tau) - (-1)^m g_2(\tau)]d\tau. \tag{34}$$

In the simple case $g_1(t) = g_2(t) = 0$, we obtain from Eqs. (30)–(34)

$$f(S,t) = \frac{4W_0}{\pi}\sum_{m=0}^{\infty} \frac{1}{(2m+1)} \sin[(2m+1)\pi S] \\ \times \exp[-D(2m+1)\pi^2 t], \tag{35}$$

where the coefficient W_0 can be defined from the normalization condition $\int_{-1}^{+1}\int_0^{+\infty} f(S,t)dSdt = 1$, $W_0 = \frac{D\pi^4}{7\varsigma(3)}$. Here, $\varsigma(s) = \sum_{k=1}^{\infty} k^{-s}$ is the Riemann zeta function.[28] We note the direct correspondence between the fictitious time and the spin index $t \to nT$, $T = 1$ given by Eq. (7). For the averages of the

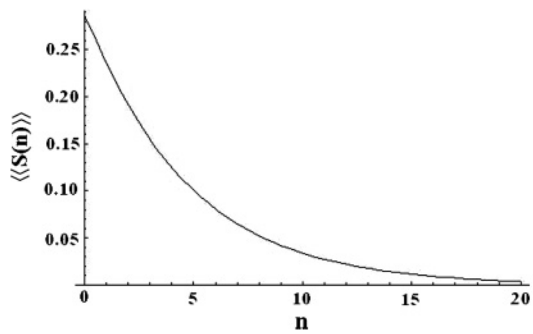

FIG. 6. Results of the numerical integration for the statistically averaged random alignment factor $\langle\langle\sin^2(\theta_n-\theta_{n-1})\rangle\rangle$ in the diffusive approximation (37) for $\beta=0.3$ and $\epsilon=0.15$.

discrete random variable $S\equiv S_n=\sin(\theta_n-\theta_{n-1})$, we follow the standard procedure [see Ref. 21, Eqs. (18)–(20)] and utilize the distribution function given by Eq. (35). The integration is performed over the interval $-1\leqslant S_n\leqslant 1$. As a result, we obtain

$$\langle\langle S_n^2\rangle\rangle=\langle\langle S^2\rangle\rangle=\langle\langle\sin^2(\theta_n-\theta_{n-1})\rangle\rangle=\int_{-1}^{+1}S^2 f(S,t)\,dS$$
$$=\frac{4W_0}{\pi}\sum_{m=0}^{\infty}\frac{1}{(2m+1)}\int_{-1}^{+1}S^2\sin[(2m+1)\pi|S|]dS$$
$$\times\exp[-D(2m+1)\pi^2 t]. \tag{36}$$

After an integration, we get

$$\langle\langle S^2\rangle\rangle=\langle\langle\sin^2(\theta_n-\theta_{n-1})\rangle\rangle$$
$$=\frac{4W_0}{\pi^2}e^{-D\pi^2 n}F\left(\left\{\frac{1}{2},\frac{1}{2},1\right\},\left\{\frac{3}{2},\frac{3}{2}\right\},e^{-2D\pi^2 n}\right)$$
$$-\frac{W_0}{\pi^4}e^{-D\pi^2 n}\Phi\left(e^{-2D\pi^2 n},4,\frac{1}{2}\right), \tag{37}$$

where $F(\{a_1,\ldots,a_p\};\{b_1,\ldots,b_q\};z)=\sum_{k=0}^{\infty}\frac{(a_1)_k,\ldots,(a_p)_k}{(b_1)_k,\ldots,(b_q)_k}\frac{z^k}{k!}$ is the generalized hypergeometric function and $\Phi(z,s,a)=\sum_{k=0}^{\infty}\frac{z^k}{(k+a)^s}$ is the generalized Riemann zeta function.[28] From Eq. (37), we immediately see that the statistically averaged random alignment factor $\langle\langle\sin^2(\theta_n-\theta_{n-1})\rangle\rangle$ is not uniform along the spin chain (see Fig. 6), but rather decays exponentially with n. This result is reasonable since the solution for the distribution function (35) is obtained via deterministic initial and boundary conditions (32). Therefore, a maximum correlation is expected for $n=0$. Since $t=nT$, $t=0$ and $n=0$ correspond to the boundary where the distribution function is defined precisely. This means that far away from the boundary for $n\gg 1$, randomness occurs and the correlation decays.

V. CONCLUSIONS

In this paper we considered an anisotropic nonlinear spin chain, which serves as a model for a chain of coupled nanomagnets. We have shown that there is a direct map between an infinite-dimensional spin-chain model and an equivalent effective 1D classical Hamiltonian with a discrete fictitious time-dependent perturbation. We have established a direct connection between the dynamical characteristics of the classical system and the spin correlation time of the original quantum chain. The decay rate for the spin correlation functions turns out to depend logarithmically on the maximal Lyapunov exponent. In addition, for anisotropic couplings, we found an interesting counterintuitive feature: the small anisotropy leads to the formation of small islands of the regular motion in a chaotic sea of the system's phase space. As a result, the spin correlations become stronger within the islands of regular motion. We argue that these results obtained within the classical approximation are interesting in other regimes. If the Lyapunov regime is reached for a quantum system, which takes place for the Lyapunov exponent $\lambda<J^2/\Delta$, where Δ is the mean level spacing and J is the exchange-interaction constant between spins, then the decay rate for the teleportation fidelity in a device based on such spin chains is directly related to λ.

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APPENDIX A: DERIVATION OF THE RECURRENCE RELATIONS

Let us consider the equilibrium state for the model (3):

$$\frac{\partial H}{\partial\varphi_n}=[\cos(\theta_n-\theta_{n+1})-\cos(\theta_n+\theta_{n+1})]\sin(\varphi_{n+1}-\varphi_n)$$
$$-[\cos(\theta_{n-1}-\theta_n)-\cos(\theta_{n-1}+\theta_n)]\sin(\varphi_{n+1}-\varphi_n), \tag{A1}$$

$$\frac{\partial H}{\partial\theta_n}=-\frac{J}{2}[\sin(\theta_n+\theta_{n+1})+\sin(\theta_{n-1}+\theta_n)+\sin(\theta_n-\theta_{n+1})$$
$$-\sin(\theta_{n-1}+\theta_n)]-\frac{g}{2}[\sin(\theta_n-\theta_{n+1})-\sin(\theta_{n-1}-\theta_n)$$
$$-\sin(\theta_n+\theta_{n+1})-\sin(\theta_{n-1}+\theta_n)]\cos(\varphi_{n+1}-\varphi_n)$$
$$+\beta\sin 2\theta_n=0. \tag{A2}$$

After the introduction of the notation $S_n=\sin(\theta_n-\theta_{n-1})$, from (A1) and (A2) we find

$$\left(\frac{J}{2}+\frac{g}{2}\right)S_{n+1}-\left(\frac{J}{2}+\frac{g}{2}\right)S_n-\left(\frac{J}{2}-\frac{g}{2}\right)\sin(\theta_n+\theta_{n+1})$$
$$-\left(\frac{J}{2}-\frac{g}{2}\right)\sin(\theta_{n-1}+\theta_n)+\beta\sin(2\theta_n)=0, \tag{A3}$$
$$\varphi_{n+1}=\varphi_n+\pi m;\quad m=0,1.$$

Let the asymmetry parameter be defined by $\varepsilon=|J-g|$, $\varepsilon<J,g$. Next we perform a rescaling of the interaction constants $\frac{\varepsilon}{2g}\to\varepsilon$, $\beta\to\mp\frac{\beta}{g}$. From (A3) we deduce

$$(S_{n+1}-S_n)-\varepsilon\sin(\theta_n+\theta_{n+1})\varepsilon-\sin(\theta_{n-1}+\theta_n)$$
$$+\beta\sin(2\theta_n)=0, \tag{A4}$$
$$\theta_{n+1}=\theta_n+\pi\nu+(-1)^\nu\arcsin[S_{n+1}];\quad\nu=0,1.$$

Depending on the sign of the rescaled barrier height $\beta \to \mp\frac{\beta}{g}$, the value of the index $m = 0,1$ defines the energy minimum condition. For convenience, we will use positively defined $\beta > 0$ and consequently $m = 0$. In the simplest case, $\nu = 0$, so that from (A4) we obtain

$$(S_{n+1} - S_n) - \varepsilon[\sin[2\theta_n]\sqrt{1 - S_{n+1}^2} + \cos(2\theta_n)S_{n+1} + \sin(2\theta_n)\sqrt{1 - S_n^2} - \cos(2\theta_n)S_{n+1}] + \beta\sin(2\theta_n) = 0. \tag{A5}$$

By retaining only the first-order terms with respect to the small parameter $\varepsilon = \frac{|J-g|}{2g}$, from (A5) we obtain the following recurrence relations (14):

$$S_{n+1} = S_n - \beta\left(\sin 2\theta_n - \frac{\varepsilon}{2}\sin 4\theta_n\right),$$
$$\theta_{n+1} = \theta_n + \omega_\nu(S_{n+1}), \tag{A6}$$
$$\omega_\nu(S_n) = \pi\nu + (-1)^\nu \arcsin S_n.$$

APPENDIX B: DERIVATION OF THE KINETIC EQUATION

The starting point for the derivation of the kinetic equation is the equivalent effective Hamiltonian (7),

$$\frac{dS}{dt} = -\frac{\partial H}{\partial\theta} = -\beta V'(\theta)T\sum_{n=-\infty}^{+\infty}\delta(t - nT),$$
$$\frac{d\theta}{dt} = \frac{\partial H}{\partial S} = \omega(S), \quad \omega_\nu(S) = \pi\nu + (-1)^\nu \arcsin s. \tag{B1}$$

Here the variable S plays the role of the adiabatic (slowly varying) action variable, while the angular variable θ is the fast variable. Due to the presence of the two different time scales in the system,

$$H = H_0(S) + \varepsilon V(S,\theta,t), \tag{B2}$$

for the derivation of the kinetic equation, we will follow the standard procedure.[29] The distribution function of the random variable $f(S,t)$ obeys the Liouvillian equation of motion:

$$i\frac{\partial f_0}{\partial t} = (\hat{L}_0 + \varepsilon\hat{L}_1)f_0, \quad \hat{L}_0 = i\omega(S)\frac{\partial}{\partial\theta},$$
$$\hat{L}_1 = -i\left(\frac{\partial V}{\partial S}\frac{\partial}{\partial\theta} - \frac{\partial V}{\partial S}\frac{\partial}{\partial\theta}\right). \tag{B3}$$

The formal solution of the Liouville equation with the accuracy of second-order terms in the small parameter ε reads

$$f_0(S,t) = f(S,0) - i\varepsilon \times \sum_m \int_0^t dt_1 \exp\left[\mathrm{im}\int_0^{t_1}\omega(t')dt'\right]\langle n|\hat{L}_1|m\rangle f_0(S,0) + (-i\varepsilon)^2\sum_m\int_0^t dt_1\int_0^{t_1}dt_2\exp\left[-\mathrm{im}\int_{t_1}^{t_2}\omega(t')dt'\right] \times \langle 0|\hat{L}_1(t_1)|m\rangle\langle m|\hat{L}_1(t_2)|0\rangle f_0(S,0). \tag{B4}$$

Here, $\langle n|\hat{L}_1|m\rangle\frac{1}{2\pi}\int_0^{2\pi}d\theta e^{-in\theta}\hat{L}_1 e^{im\theta}$ is the matrix element of the Liouville operator. After averaging over the initial phases $f(I,t) = \langle\langle f_0(I,t)\rangle\rangle$ and applying the random-phase approximation with respect to the fast chaotic variable $\Psi(t_2,t_1) = \int_{t_1}^{t_2}\omega(t')dt' = \theta(t_1) - \theta(t_2)$, we get

$$\langle\langle \exp im\Psi(t_2,t_1)\rangle\rangle \approx \exp[-(t_1 - t_2)/\tau_c]\exp[-im\omega(t_1 - t_2)]. \tag{B5}$$

From (B4), we obtain

$$\frac{\partial f}{\partial t} = -2\varepsilon^2\sum_{m>0}\sum_{p>0}\frac{(1/\tau_c)\langle 0|\hat{L}_{1p}|m\rangle\langle m|\hat{L}_{1-p}|0\rangle f}{(1/\tau_c)^2 + (m\omega - p\Omega)^2}, \tag{B6}$$

where

$$\langle 0|\hat{L}_{1p}|m\rangle\langle m|\hat{L}_{1-p}|0\rangle = \left(\frac{\Omega}{2\pi}\right)^2\frac{1}{(2\pi)^2}\int_{-T/2}^{T/2}dt_1\int_{-T/2}^{T/2}dt_2\int_0^{2\pi}d\theta'\int d\theta''\hat{L}_1 \times (t_1)e^{im(\theta'-\theta'')}\hat{L}_1(t_2)e^{-ip\Omega(t_1-t_2)}, \tag{B7}$$

and the following notation is used: $\tau_c = 2T/\ln K$, $T = \frac{2\pi}{\Omega}$. After calculating the integrals in (B7), in the limit $\frac{1}{\tau_{c\Omega}} \to 0$, $T = 1$ form (B6), we simply recover the diffusion equation (30)

$$\frac{\partial f(S,t)}{\partial t} = \frac{\partial}{\partial S}D(S)\frac{\partial f(S,t)}{\partial S}, \tag{B8}$$

$$D(S) = \frac{\beta^2}{4}\left(1 + \frac{\varepsilon^2}{4}\right). \tag{B9}$$

More details of the derivations can be found in Ref. 29.

APPENDIX C: CORRELATION FUNCTIONS

For the evaluation of the multiple series in Eq. (24), one should sum up the contributions from the main nonoscillatory terms. Due to the δ function $\delta_{1-2(m_1+m_2+\cdots+m_n)+4(l_1+l_2+\cdots+l_n),1}$ in Eq. (24), and the fast exponential factors $e^{i4\omega(l_1+l_2+\cdots+l_n)}$, $e^{-2i\omega(m_1+m_2+\cdots+m_n)}$, the relevant terms in Eq. (24) are those with

$$m_1 + m_2 + \cdots + m_n = 0, \quad l_1 + l_2 + \cdots + l_n = 0. \tag{C1}$$

Using the asymptotic expressions for Bessel functions,

$$J_m(K_0) \sim K_0^{-1/2} \quad \text{for} \quad K_0 \gg 1, \tag{C2}$$

and condition (C1), one can easily obtain (26) from (24).

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