

Relaxation dynamics of a quantum spin coupled to a topological edge state

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(Received 19 February 2025; revised 12 May 2025; accepted 5 June 2025; published 30 June 2025)

A classical impurity spin coupled to the spinful Su-Schrieffer-Heeger (SSH) chain is known to exhibit complex switching dynamics with incomplete spin relaxation. Here, we study the corrections that result from a full quantum treatment of the impurity spin. We find that in the topologically trivial case, the quantum spin behaves similarly to the classical one due to the absence of the Kondo effect for the trivial insulator. In the topological case, the quantum spin is significantly less likely to relax: It can be stuck at a prerelaxation plateau with a sizable deviation from the expected relaxed value, and there is a large parameter regime where it does not relax at all but features an anomalously large Larmor frequency. Furthermore, we find an additional quantum effect where the prerelaxation plateau can be hyperpolarized, i.e., the spin is stuck at a polarization value larger than the ground-state expectation value. This is possible due to the (incomplete) Kondo screening of the quantum spin, which is absent in the classical case. Our results are obtained via the ground-state density-matrix renormalization group algorithm (DMRG) and the time-dependent variational principle (TDVP), where the charge-SU(2) symmetry of the problem was exploited. Furthermore, we introduce and benchmark a method to predict the dynamics from the given numerical data based on the sparse identification of nonlinear dynamics (SINDy). This allows us to prolong the simulation timescale by a factor of 2.5, up to a maximal time of 10^3 inverse hoppings.

DOI: [10.1103/5qp-v-b713](https://doi.org/10.1103/5qp-v-b713)

I. INTRODUCTION

A quantum spin is the basic building block of systems that can be turned into quantum devices. The spin can be manipulated by external fields, but interactions with an environment can lead to eventual decoherence and relaxation. The understanding of this dynamics is an essential prerequisite for the development of spintronics-based devices, where the spin is used as a carrier of information, but is also relevant for the rapid recent developments in quantum information theory. From a more fundamental point of view, it poses a case study of the physics of open quantum systems and lifts the analysis of quantum impurity models, which has an extensive history [1,2], into the nonequilibrium domain [3,4].

As with all time-dependent problems, the main technical challenge in understanding the spin dynamics is to access long propagation times. While the direct exchange interaction is on the scale of femtoseconds, nontrivial dynamics can occur over a wide range of time scales that can be several orders of magnitude larger. The study of impurity models in equilibrium has stimulated the development of novel techniques like the numerical renormalization group (NRG) [2], but accessing

the nonequilibrium dynamics of a quantum spin attached to an environment remains a difficult problem [5–7].

In addition to tailoring external fields, controlling the environment provides another route to manipulate the dynamics of the spin. In the following, we focus on the case of fermionic baths (substrates), where a particularly interesting case arises when the spin is coupled to the robust surface state of a topological insulator. One expects that the resulting spin dynamics should differ fundamentally compared to both metallic and topologically trivial substrates. The authors of Ref. [8] investigated magnetic impurities embedded in Bi_2Te_3 and Bi_2Se_3 using time-dependent density-functional theory and found a wide range of excitation lifetimes, reaching up to microseconds for Mn impurities. Using Mn adatoms on Bi_2Se_3 has also been proposed as a building block of a magnetic sensor device [9]. The effective interaction of several magnetic impurities mediated by topological edge states has been investigated using first-principle methods [10]. Analogous protection and engineered response have recently been demonstrated in photonic topological platforms, with robust polarization conversion in anisotropic metamaterial bilayers [11] and ultralow-frequency topological scattering resonances in magnetized core-shell plasmonic cylinders [12].

While the two- and three-dimensional cases are most interesting from an application point of view, the one-dimensional case is useful in elucidating the fundamental physics with few or even no additional approximations. One way to model a topological substrate is through the paradigmatic

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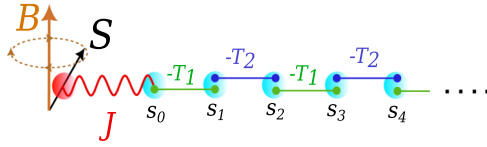


FIG. 1. Sketch of the system studied in this work. An impurity spin S is coupled via an exchange interaction J to the edge of a SSH chain whose hoppings are dimerized as $T_1 = T - \delta T$ and $T_2 = T + \delta T$. The spin is switched by an external field $B(t)$.

Su-Schrieffer-Heeger (SSH) model [13,14]. A recent study investigated this setup for a classical instead of a quantum spin, which results in an effective one-particle problem and makes long-time dynamics tractable [15]. By virtue of absorbing Lindblad boundaries, the authors were able to reach timescales which exceed the intrinsic electronic one (set by the inverse hopping amplitude) by a factor of 10^5 . It was observed that an in-gap edge state facilitates the spin relaxation in a wider parameter range of the dynamical phase diagram as compared to the topologically trivial case. However, the relaxation process generally remains incomplete and the spin is stuck at a few percent below its relaxed value for very long times.

In this work, we build on these results and investigate what happens when the spin is faithfully treated as a quantum object with $S = 1/2$. This is an interesting question because a quantum spin has the fundamental property that the substrate electrons can truly screen it via the Kondo effect, up to a total singlet in the metallic case, instead of just aligning themselves antiferromagnetically to it. In the metallic and topologically nontrivial cases, the competition of the Kondo effect and a local external field leads to deviation from the saturated magnetization value already in equilibrium. In this paper, we switch the direction of the magnetic field at time $t = 0$ and study the ensuing nonequilibrium dynamics. It turns out that the quantum spin is generally less likely to relax than a classical one and that it features hyperpolarization, i.e., its polarization can exceed the equilibrium value and remain stuck in this prerelaxed state.

We compute the ground state of the system at hand using the density-matrix renormalization group (DMRG) method and simulate the ensuing dynamics via the time-dependent variational principle (TDVP) [16]. By exploiting the charge-SU(2) symmetry of the problem, this allows us to reach timescales of ~ 400 inverse hoppings. We extend this timescale further by employing the sparse identification of nonlinear dynamics (SINDy) [17–20], which attempts to learn the subsequent dynamics from the data at earlier times. This allows us to gain an additional factor of 2.5, bringing the maximally achieved propagation time to 10^3 inverse hoppings.

II. MODEL

We investigate the following Hamiltonian (see Fig. 1):

$$H = - \sum_{j=0}^{L-2} \sum_{\sigma} [(T - (-1)^j \delta T) c_{j,\sigma}^{\dagger} c_{j+1,\sigma} + \text{H.c.}] + J s_0 \cdot S - B(t) \cdot S, \quad (1)$$

where $c_{j,\sigma}^{\dagger}$ creates an electron with spin projection $\sigma = \uparrow, \downarrow$ at site j , and $s_j = \frac{1}{2} \sum_{\sigma\sigma'} c_{j,\sigma}^{\dagger} \boldsymbol{\tau}_{\sigma\sigma'} c_{j,\sigma'}$ is its spin operator constructed using the vector of Pauli matrices $\boldsymbol{\tau}$. T is the nearest-neighbor hopping amplitude, which we set to $T = 1$ from now on. The uncoupled system ($J = 0$) is in a topologically nontrivial phase for $\delta T > 0$. Note that the bulk gap is given by $\Delta = 4|\delta T|$.

The impurity spin is described by the vector of spin operators $S = (S^x, S^y, S^z)$. It is coupled to the first site of the electronic substrate via the exchange interaction $J > 0$ and is manipulated by the external field $B(t) = [B^x(t), B^y(t), B^z(t)]$. We set $J = 1$.

In this work, we study switching dynamics, i.e., we prepare the system in the ground state with

$$B(t=0) = (B, 0, 0) \quad (2)$$

and simulate the ensuing time evolution with $B(t > 0) = (0, 0, B)$. Since the exchange interaction is isotropic, one expects that the system relaxes toward a state where the x and z components are exchanged, $\langle S^{x,z} \rangle_{\text{relax}} = \langle S^{z,x}(t=0) \rangle$.

We use finite chains of length $L = 401$. The switching puts additional energy into the system, which is transported away in the substrate with some finite speed. This wavefront is reflected at the opposite boundary and moves back to the impurity spin. The simulation should be stopped before the spin is influenced by this finite-size effect. This sets a maximal propagation time, which can be estimated from the dispersion relation, see Appendix A.

III. METHODS

A. DMRG, TDVP

We employ the DMRG algorithm to first compute the ground state of Eq. (1). The DMRG is a variational method within the class of variational matrix-product states (MPS) and is especially efficient in one dimension due to the area law of the entanglement entropy. The MPS ansatz is controlled by the bond dimension χ , which is related to the number of free parameters in the ansatz.

By exploiting symmetries, the MPS tensors get a block structure, so that a larger effective χ can be accessed. For our problem, the ground state features a spin-U(1) symmetry, but it is broken during the time evolution by the switching of the magnetic field. Another symmetry is particle number conservation, which is in fact part of an even larger charge-SU(2) symmetry [21,22]. The prerequisite for this is the bipartiteness of the lattice, which allows to define the phase factors $(-1)^j = \pm 1$ for the respective sublattices. The symmetry is generated by the pseudospin operators

$$\begin{aligned} T_j^+ &= (-1)^j c_{j,\downarrow} c_{j,\uparrow}, \\ T_j^- &= (-1)^j c_{j,\uparrow}^{\dagger} c_{j,\downarrow}^{\dagger}, \\ T_j^z &= \frac{1}{2} (1 - c_{j,\uparrow}^{\dagger} c_{j,\uparrow} - c_{j,\downarrow}^{\dagger} c_{j,\downarrow}), \end{aligned} \quad (3)$$

which fulfill the SU(2) relations $[T_j^+, T_j^-] = 2T_j^z$ and $[T_j^z, T_j^{\pm}] = \pm T_j^{\pm}$. The global operators $T_{\text{tot}}^x = \sum_j (T_j^+ + T_j^-)/2$, $T_{\text{tot}}^y = \sum_j (T_j^+ - T_j^-)/(2i)$, and $T_{\text{tot}}^z = \sum_j T_j^z$ all commute with the Hamiltonian. Using $\mathbf{T}_i = (T_i^x, T_i^y, T_i^z)$, the total

pseudospin is defined via

$$\langle \mathbf{T}_{\text{tot}}^2 \rangle = \sum_{ij} \langle \mathbf{T}_i \cdot \mathbf{T}_j \rangle = T_{\text{tot}}(T_{\text{tot}} + 1). \quad (4)$$

We always work at half filling $\langle T_{\text{tot}}^z \rangle = 0$, and the ground state is always in the sector $T_{\text{tot}} = 0$, which we have verified exemplarily. By exploiting the full charge-SU(2) symmetry [23], we can effectively increase the bond dimension by a factor of 2.5 compared to the case of charge-U(1) conservation alone (which corresponds to just the pseudospin projection T_{tot}^z).

We use a charge-SU(2) effective bond dimension $\chi_{\text{SU}(2)} = 150$ to compute the ground state using a mixture of the two-site DMRG algorithm and the one-site algorithm with perturbations [24]. The resulting energy variance per site $\text{var}(E)/L = |\langle H^2 \rangle - \langle H \rangle^2|/L$ is of the order of $\text{var}(E)/L \sim 10^{-5}$, indicating a well-converged ground state. For the time propagation, we employ an adaptive variant of the time-dependent variational principle [16], where we dynamically choose whether the two-site or the one-site algorithm should be performed on a given site. We use the two-site algorithm close to the impurity spin and around the moving wavefront, which we detect by the relative growth of the entanglement entropy. The two-site algorithm is able to dynamically increase the bond dimension in order to faithfully describe the evolving state. We use a local truncated weight threshold of 10^{-7} and a time step of $dt = 0.1$. A benchmark with different thresholds is shown in Appendix B. We observe that the dynamics of the Kondo spin does not lead to a substantial growth of the entanglement, and the bond dimension does not need to increase beyond $\chi_{\text{SU}(2)} = 150$ to faithfully capture the time evolution. In essence, one only needs to capture the outgoing wave packet and the rotation of the impurity spin. This motivates us to investigate whether the dynamics can be learned and captured by a cheaper method, which we describe in the following.

B. SINDy

In order to access larger timescales after the TDVP simulation has terminated, we employ the SINDy algorithm, which is a data-driven scheme to learn and predict the dynamics. It can be combined with any time evolution technique.

A physical motivation for the SINDy approach can be formulated as follows: A known classical differential equation with phenomenological parameters to describe spin dynamics is the Landau-Lifshitz-Gilbert (LLG) equation [25–27]. It is related to the microscopic Hamiltonian via a Redfield master equation requiring the weak-coupling, Markov, and classical-spin approximations, leading to the following form [28,29]:

$$\dot{\mathbf{S}}(t) = \mathbf{S}(t) \times \mathbf{B} - \alpha \mathbf{S}(t) \times \dot{\mathbf{S}}(t). \quad (5)$$

For the classical-spin case with fully included electronic degrees of freedom, its validity has been checked against the full time propagation [30].

In this work, we do not make the above assumptions but rather compute the exact dynamics using the TDVP up to a maximal time. We then assume that one can find an effective classical equation for the expectation value $\langle \mathbf{S}(t) \rangle$, which takes a more complex form than the LLG equation.

This equation can be found by the SINDy method [17–20], which determines a nonlinear function f that governs the time evolution of a set of m observables $\mathbf{A}_i(t)$ via

$$\frac{d}{dt} \mathbf{A}_i(t) = f(\{\mathbf{A}_j(t)\}). \quad (6)$$

In practice, one first performs a set of measurements of the system at times $t_1, t_2, \dots, t_n$ and then aggregates these data into an $n \times m$ matrix $\underline{X}$:

$$\underline{X} = \begin{bmatrix} \mathbf{A}_1(t_1) & \mathbf{A}_2(t_1) & \dots & \mathbf{A}_m(t_1) \\ \mathbf{A}_1(t_2) & \mathbf{A}_2(t_2) & \dots & \mathbf{A}_m(t_2) \\ \vdots & \vdots & & \vdots \\ \mathbf{A}_1(t_n) & \mathbf{A}_2(t_n) & \dots & \mathbf{A}_m(t_n) \end{bmatrix}. \quad (7)$$

Given $\underline{X}$, time derivatives can be approximated numerically using spline interpolation and reshaped into a matrix $\dot{\underline{X}}$. After this, a set of basis functions to form a library matrix $\underline{\Theta}(\underline{X})$ is chosen, such as polynomials up to order k :

$$\underline{\Theta}(\underline{X}) = [\underline{P}_0(\underline{X}) \quad \underline{P}_1(\underline{X}) \quad \underline{P}_2(\underline{X}) \quad \dots \quad \underline{P}_k(\underline{X})]. \quad (8)$$

For example, a term with $k = 2$ takes the form

$$\underline{P}_2(\underline{X}) = \begin{bmatrix} | & | & & | & | & & | \\ \mathbf{A}_1^2 & \mathbf{A}_1 \mathbf{A}_2 & \dots & \mathbf{A}_1 \mathbf{A}_m & \mathbf{A}_2^2 & \dots & \mathbf{A}_m^2 \\ | & | & & | & | & & | \end{bmatrix}. \quad (9)$$

Given $\dot{\underline{X}}$ and $\underline{\Theta}(\underline{X})$, one obtains a set of coefficients for the right-hand side of Eq. (6) with a matrix form $\underline{\Xi}$ by solving the following approximation problem:

$$\dot{\underline{X}} \approx \underline{\Theta}(\underline{X}) \underline{\Xi}. \quad (10)$$

Crucially, the set of coefficients is sparse, involving less functions than the full library.

The simplest way to apply the SINDy algorithm to our system is to set $\mathbf{A}(t) = \langle \mathbf{S}(t) \rangle$ and to learn an effective differential equation of the impurity spin. We find that this works rather well for the simple case of a metallic substrate, but fails for more complex dynamics. In the latter case, one needs to take more observables into account, which we discuss below.

IV. RESULTS

A. Ground state

Figure 2 shows the polarization of the impurity spin $\langle S^x(t=0) \rangle$ in the ground state as a function of the magnetic field B . The Kondo effect is not active for the trivial insulator ($\delta T < 0$), where the electrons are inert and the impurity spin is immediately fully polarized irrespective of the field strength B , resembling a classical spin. For the topological insulator ($\delta T > 0$), the edge state is able to screen the spin and a compromise state sets in, whereby the polarization is rather small even for weak fields.

B. Relaxation dynamics: Metal and trivial insulator

We now turn to the dynamics; we reiterate that the direction of the magnetic field is switched at time $t = 0$. We first look at the simple cases of a metal and a trivial insulator. There are three dynamical regimes, which are shown in Fig. 3 for $B = 1$. The metallic case ($\delta T = 0$) has been investigated before [31]

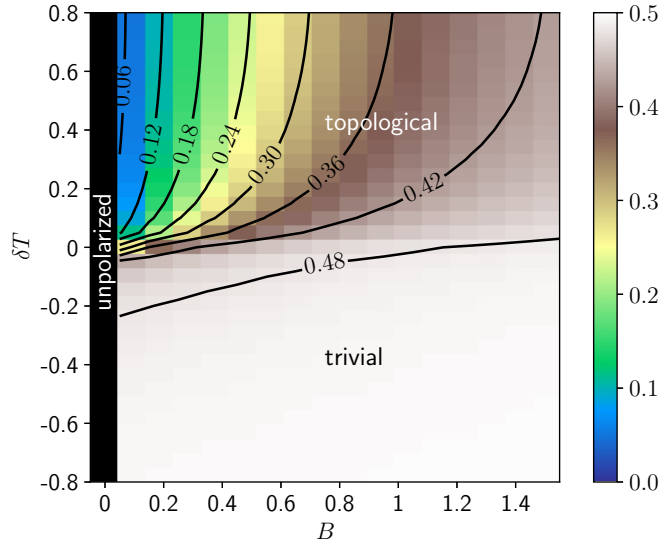


FIG. 2. Ground-state expectation value of the impurity spin $\langle S^x \rangle$ for $L = 401$, $T = J = 1$, and $\mathbf{B} = (B, 0, 0)$ computed using the DMRG at half filling.

and is reproduced here for completeness. One finds a precessional motion with a Larmor frequency of $\omega_L \approx B$, which is damped with a relaxation time of around $\tau \sim 20$ for the x component. For the trivial insulator, the Larmor frequency has to be compared with the gap size: For $\Delta = 4|\delta T| < \omega_L$, electrons can be excited across the gap and the behavior qualitatively resembles the metal, albeit with a longer relaxation time of around $\tau \sim 100$. For $\Delta = 4|\delta T| > \omega_L$, the gap cannot be surpassed and one finds precessional motion without any relaxation.

We now apply and benchmark the SINDy method. The dynamics in the metallic case can be learned readily from only $\mathbf{A}(t) = \langle \mathbf{S}(t) \rangle$. We vary the learning window (shaded gray area in Fig. 3) until the rest of the dynamics is satisfactorily reproduced; $t_{\text{learn}} \approx 13$, i.e., about half of the relaxation time, is enough to make an accurate prediction. For the insulating case, we find that the dynamics cannot be learned with $\langle \mathbf{S}(t) \rangle$ alone, one also needs to include the first substrate spin $\langle \mathbf{s}_0(t) \rangle$. We find $t_{\text{learn}} \approx 50$ to be sufficient, which is still about half of the relaxation time. Our interpretation is that in the insulating case, a strongly coupled two-spin system is formed at the edge, whereas in the metallic case, the substrate merely acts as an absorbing bath that can be effectively integrated out.

C. Relaxation process: Topological insulator

For the topological insulator, we can identify three distinct dynamic regimes. They are displayed in Fig. 4 as a full phase diagram, and exemplary TDVP data is shown at $B = 1$: (a) For a small value of $\delta T > 0$, the z component of the impurity spin surpasses the expected relaxation value $\langle S^z \rangle_{\text{relax}} = \langle S^x(t=0) \rangle$ and stays in this hyperpolarized state without any clear signature of relaxation in the given observation time. (b) For intermediate values of δT , the spin reaches a prerelaxation plateau below the expected relaxed value. This is similar to the case of a classical spin, but with a larger deviation from the

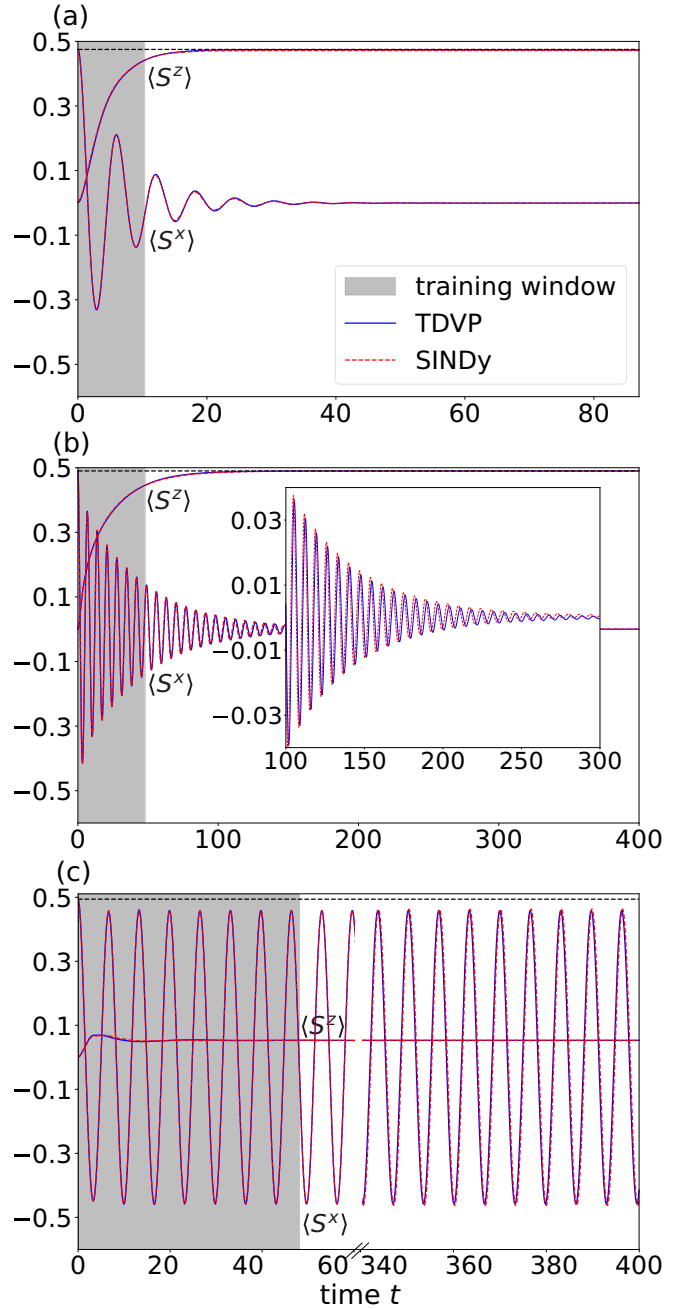


FIG. 3. Relaxation dynamics of the impurity spin for $B = 1$: (a) metallic case ($\delta T = 0$), (b) topologically trivial case with relaxation ($\delta T = -0.2 \Rightarrow \Delta = 0.8 < \omega_L \approx B$), (c) topologically trivial case without relaxation ($\delta T = -0.3 \Rightarrow \Delta = 1.2 > \omega_L \approx B$). The gray shading indicates the learning time window for the SINDy method. Note that in (b) and (c) larger time windows are considered than in (a).

relaxed value and an additional superimposed high-frequency oscillation. (c) For even larger δT , the gap is too large to overcome and strong oscillations without relaxation are found in all components. In the following, we discuss and analyze these results in more detail. We also illustrate how to quantify the above values in order to establish the phase diagram in Fig. 4.

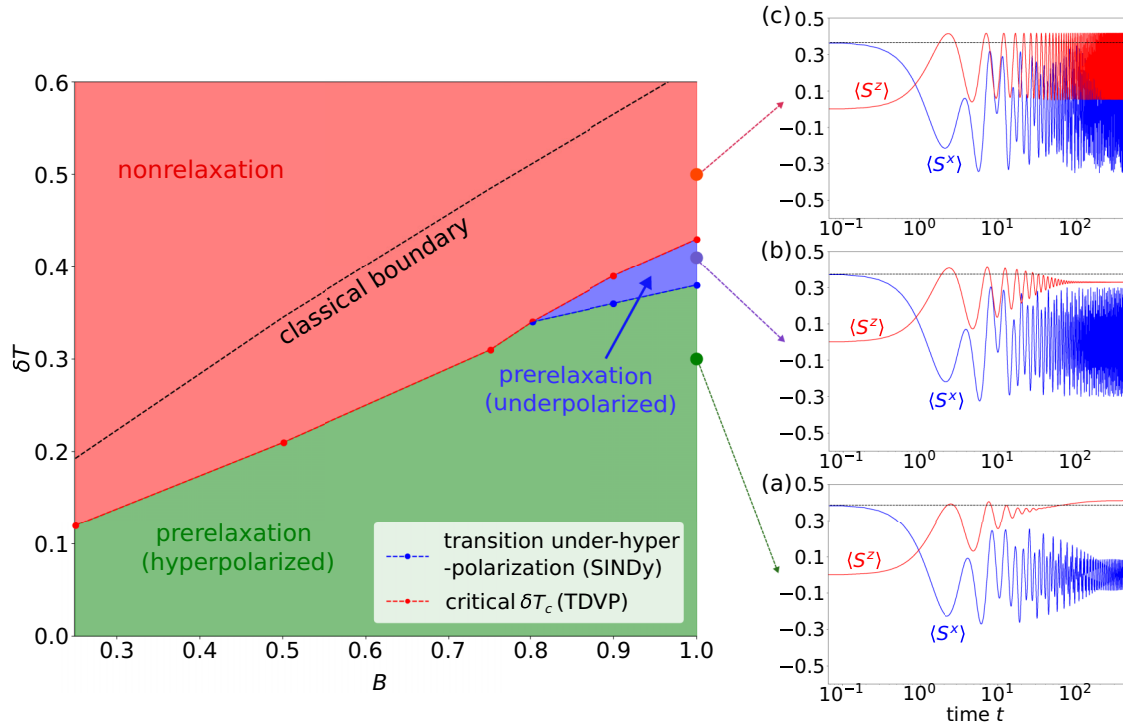


FIG. 4. Relaxation dynamics of the impurity spin in the topological case. Left: Schematic dynamical phase diagram as a function of B and δT . We find three distinct regimes; exemplary TDVP data for the time evolution at $B = 1$ is shown on the right. (a) prerelaxation and hyperpolarization (green, $\delta T = 0.3$), (b) prerelaxation and underpolarization (blue, $\delta T = 0.41$), and (c) nonrelaxation (red, $\delta T = 0.5$). The dotted horizontal lines indicate the expected relaxation value $\langle S^z \rangle_{\text{relax}} = \langle S^x \rangle(t = 0)$. For a classical spin, nonrelaxation occurs above the black dashed line.

In order to quantitatively discern the nonrelaxation regime (c) from the prerelaxation regimes (a) and (b), we compare the amplitude of the oscillations of $\langle S^z(t) \rangle$ at late and early times. We define the early-time oscillation as the full period immediately following the first maximum of $\langle S^z(t) \rangle$, and the late-time oscillation as the last complete period before the longest simulation time achievable via TDVP. The phase boundary δT_c in Fig. 4 (red dashed line) shows the parameters for which their ratio is $1/20$. Note that the nonrelaxation regime is larger than in the case of a classical spin (see the black dotted line in Fig. 4).

Next, we carry out a Fourier analysis of the TDVP data for $\langle S^x(t) \rangle$ at $B = 1$ and not too large δT and find two main frequencies, see Fig. 5. From the equation of motion for the impurity spin,

$$\langle \dot{S} \rangle = -i\langle [S, H] \rangle = -B \times \langle S \rangle + J \langle s_0 \times S \rangle, \quad (11)$$

we see that the influence of the substrate now enters via the torque term $\langle s_0 \times S \rangle$, which cannot be decoupled for the quantum spin without additional approximations, but must give origin to the double-frequency response.

By varying δT , we observe that the higher-frequency ω_L is continuously connected to the Larmor frequency $\omega_L \approx B$ at $\delta T = 0$, see Fig. 6(b). In Fig. 6(a), we study the damping of the ω_L oscillation for various values of δT , and observe that within the accessible time window the damping ceases around $\delta T \approx 0.39$. If one employs the same criterion for relaxation as in the topologically trivial case $\omega_L = \Delta = 4|\delta T|$, one similarly finds $\delta T \approx 0.39$ just

by inserting the larger ω_L from the topological case, see Fig. 6(b).

In order to discern the prerelaxation regime with hyperpolarization from the one with underpolarization, we analyze

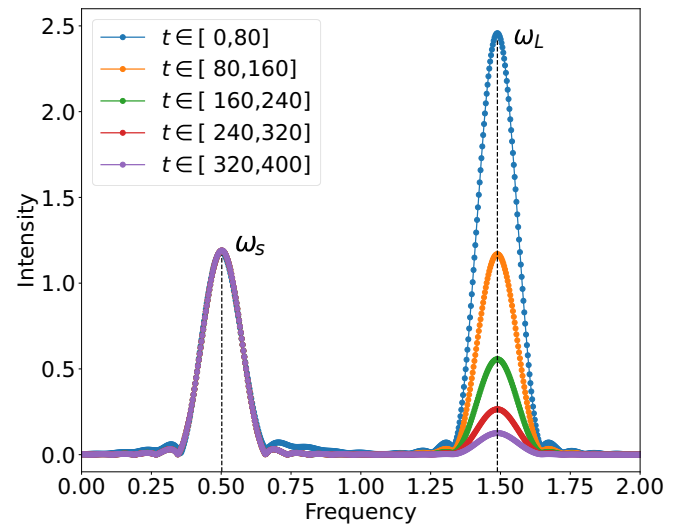


FIG. 5. Fourier analysis of the TDVP data for $\langle S^x(t) \rangle$ in the topologically nontrivial case $\delta T = 0.3$ at $B = 1$. The higher and lower frequencies are labeled ω_L and ω_S , respectively. By varying the time window used for the analysis, one can estimate the damping of the corresponding oscillations.

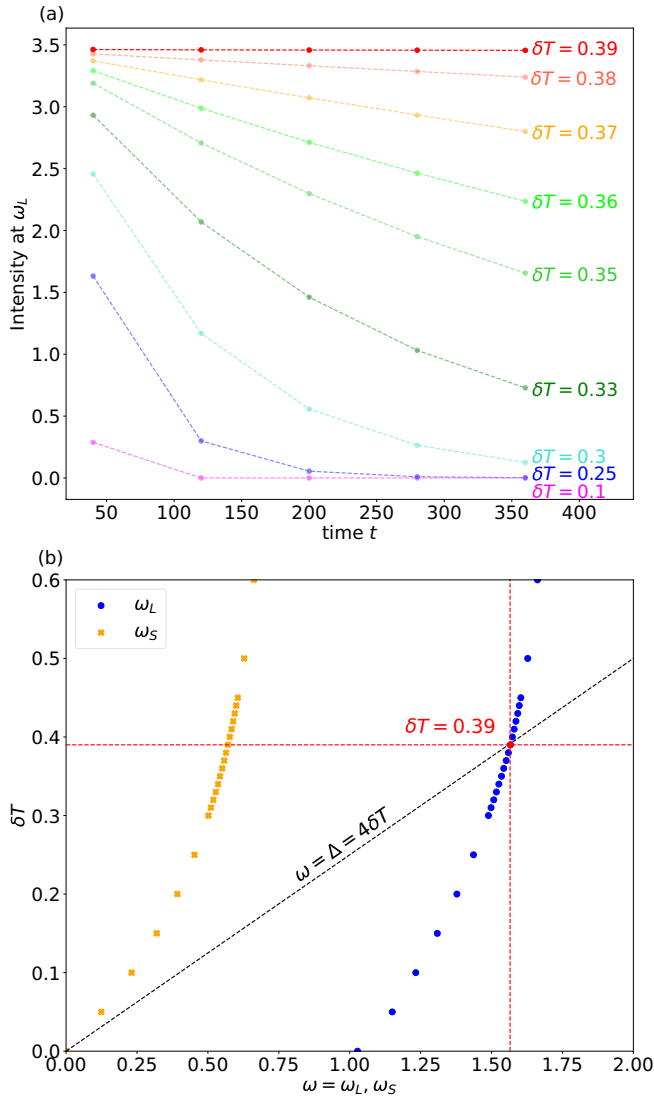


FIG. 6. (a) Intensity of the peak at the higher frequency ω_L at $B = 1$ for different δT and varying time windows (see Fig. 5). (b) Dependence of two main frequencies $\omega_{L,S}$ on δT . The black dashed line shows $\omega = \Delta = 4|\delta T|$.

$\langle S^z(t) \rangle - \langle S^z \rangle_{\text{relax}}$ at the maximum time $t_{\text{max}} = 400$ reached in the TDVP simulation. Figure 7 shows this quantity as a function of δT at $B = 1$, indicating a transition around $\delta T \sim 0.35$. One can obtain a better estimate for the boundary between the regimes of hyperpolarization and underpolarization by employing the SINDy method. We find that in the topologically nontrivial case, more observables are required than in the trivial case, and selecting these is not straightforward. To select them, we go back to the equation of motion for the impurity spin Eq. (11). We find that adding the torque term $\mathbf{T}(t) = \langle \mathbf{s}_0 \times \mathbf{S} \rangle$ as an additional observable to the list $\mathbf{A}(t)$ improves the quality of the SINDy prediction. Moreover, we find that it is beneficial to also include the first N_{sub} substrate spins $\langle \mathbf{s}_i \rangle$. Hence, the matrix $\underline{\Theta}$ is now given by

$$\underline{\Theta}(\mathbf{X}) = \begin{bmatrix} | & | & | & \dots & | \\ \langle \mathbf{S} \rangle & \langle \mathbf{T} \rangle & \langle \mathbf{s}_0 \rangle & \dots & \langle \mathbf{s}_{N_{\text{sub}}-1} \rangle \\ | & | & | & & | \end{bmatrix}, \quad (12)$$

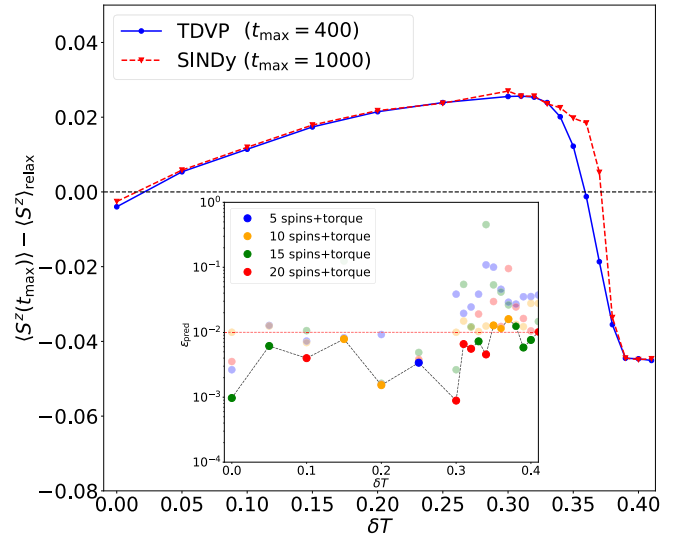


FIG. 7. Deviation of $\langle S^z(t_{\text{max}}) \rangle$ from the expected relaxed value $\langle S^z \rangle_{\text{relax}}$ as a function of δT at $B = 1$. A transition from hyperpolarization to underpolarization occurs around $\delta T \sim 0.35$. Inset: Average error Eq. (17) when taking a different number of $N_{\text{sub}} = 5, 10, 15, 20$ substrate spins into account within the SINDy approach. The black dashed line marks the minimal error.

$$\langle \mathbf{S} \rangle = \begin{bmatrix} | & | & | \\ \langle S^x \rangle & \langle S^y \rangle & \langle S^z \rangle \\ | & | & | \end{bmatrix}, \quad (13)$$

$$\langle \mathbf{T} \rangle = \begin{bmatrix} | & | & | \\ \langle T^x \rangle & \langle T^y \rangle & \langle T^z \rangle \\ | & | & | \end{bmatrix}, \quad (14)$$

$$\langle \mathbf{s}_j \rangle = \begin{bmatrix} | & | & | \\ \langle s_j^x \rangle & \langle s_j^y \rangle & \langle s_j^z \rangle \\ | & | & | \end{bmatrix}. \quad (15)$$

We find that using $t_{\text{learn}} = 100$, i.e., 1/4 of the maximum TDVP simulation time, as the learning window allows us predict the remaining 3/4 of the data with good accuracy, which is exemplified in Fig. 8. In order to quantify how many substrate spins should be included in the SINDy approach, we introduce the relative prediction error at a given time step as

$$\epsilon_{\text{pred}}(t_n) = \left| \frac{\langle \mathbf{S}_{\text{simul}}(t_n) \rangle - \langle \mathbf{S}_{\text{pred}}(t_n) \rangle}{\langle \mathbf{S}_{\text{simul}}(t_n) \rangle} \right|, \quad (16)$$

where the subscripts “simul” and “pred” refer to the TDVP data and the SINDy prediction, respectively. The total error is given by

$$\epsilon_{\text{pred}} = \frac{1}{N} \sum_{n=0}^N \epsilon_{\text{pred}}(t_{\text{learn}} + ndt). \quad (17)$$

In the inset to Fig. 7, we plot ϵ_{pred} as a function of δT at $B = 1$. In most cases, using $N_{\text{sub}} = 20$ spins yields the smallest error. From now on, the value of $N_{\text{sub}} \leq 20$ is always chosen such that the error becomes minimal.

We now use the entire TDVP data up to $t_{\text{max}} = 400$ to learn the dynamics and extract a prediction up to $t_{\text{max}} = 1000$.

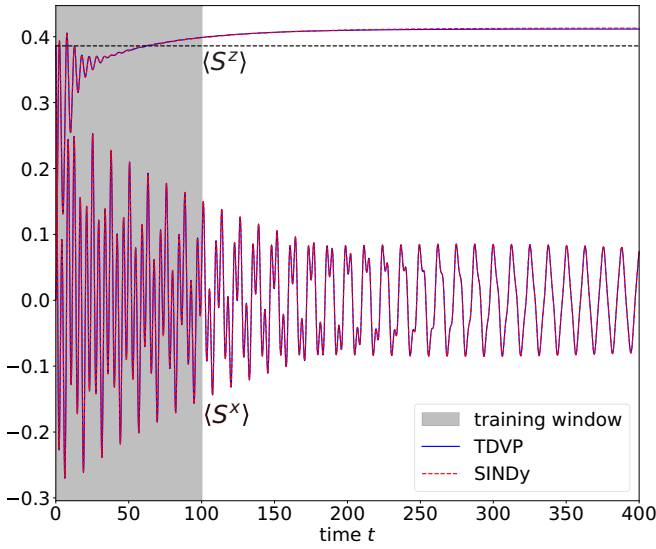


FIG. 8. Benchmark of the SINDy method for the topologically nontrivial case $\delta T = 0.3$ at $B = 1$. The impurity spin dynamics is learned from the TDVP results up to $t = 100$ and is then used to predict the data up to $t = 400$. We have included the expectation values of the impurity spin, the torque, and the first $N_{\text{sub}} = 20$ substrate spins into the learning data.

We repeat the previous analysis to determine the crossover between regimes of under- and hyperpolarization. The larger timescale accessible using the SINDy approach allows us to estimate the transition point more accurately, see Fig. 7. The corresponding results are shown as the blue dashed line in Fig. 4. We note that if one wanted to extend the timescale of the TDVP simulation to $t_{\text{max}} = 1000$, one would have to employ a system size of $L \sim 1000$, which would increase the numerical effort by at least a factor of $(2.5)^2 \sim 6$. This illustrates the potential of the SINDy method.

In the topologically nontrivial case, the counterintuitive regime of hyperpolarization cannot manifest for a classical spin. In the quantum case, the Kondo effect leads to a partial screening of the spin in the initial state, which hence allows for hyperpolarization. This can be compared to the phenomenon of “quantum distillation,” where a low-entropy state with large double occupancy is dynamically created upon lifting a trapping potential for interacting fermions [32], which could be regarded as hyperpolarization of the double occupancy.

V. DISCUSSION AND CONCLUSION

We have studied the relaxation process of a quantum spin coupled to a fermionic substrate, which we modeled as a one-dimensional SSH chain with a dimerization δT . The system was prepared in the ground state governed by a local magnetic field whose direction was switched at time $t = 0$.

In the topologically trivial case, the quantum spin behaves similarly to a classical one; it relaxes if the Larmor frequency $\omega_L \approx B$ is larger than the single-particle gap $\Delta = 4|\delta T|$ and does not relax otherwise.

In the topologically nontrivial case, we find three distinct regimes. For large δT , the spin does not relax; the corresponding region of the phase diagram is much larger

than in the case of a classical spin. For small-to-intermediate δT , we find two distinct prerelaxation regimes: for small (intermediate) δT , the spin relaxes toward a value that is larger (smaller) than the expected ground-state value. We find that the transition between both regimes is fairly sharp. The Kondo effect leads to a polarization of the quantum spin below the maximally polarized state, opening the possibility of overshooting the relaxed value and approaching it from above. Our results can hence be viewed as a dynamical overcoming of the Kondo effect. It remains an open question if and how full relaxation occurs at very long timescales.

We find that the relaxation process is governed by two different frequencies. The larger frequency ω_L is adiabatically connected to the Larmor frequency at $\delta T = 0$ but becomes anomalously large with increasing δT . The oscillation with ω_L is damped for parameters $\Delta = 4\delta T < \omega_L$, which lies in between the regimes of hyperpolarization and nonrelaxation. Nonrelaxation itself can be attributed to an anomalously high Larmor frequency. While the origin of this large Larmor frequency still needs to be clarified, it entails a well-defined energy scale, and some of the system behavior can be understood by just comparing it to the band gap. We also note that an anomalously high Larmor frequency was observed before in the case of adiabatic dynamics for spins $S > 1/2$ [33].

Our results were obtained using charge-SU(2) symmetric tensor network algorithms, specifically the ground-state DMRG as well as the time-dependent variational principle. We subsequently employed the SINDy method to predict the impurity-spin dynamics from an initial learning window. This method can be combined with any propagation algorithm and is also applicable to general system-bath models. We find that the simple damping dynamics of the metallic case $\delta T = 0$ is easily learnable; we can obtain an effective classical differential equation involving only $\langle \mathbf{S}(t) \rangle$, which can be regarded as a generalized Landau-Lifshitz-Gilbert equation. For a topologically nontrivial bath, no such simple equation can be found, and including system-bath correlations as well as bath-only expectation values becomes important. In this case, adding some domain knowledge of the physical problem is necessary in order to select the useful observables. One such guideline is to use the terms in the equation of motion for the system observables (in our case, the torque term). The SINDy approach allowed us to determine the crossover between the regimes of hyper- and underpolarization more accurately.

ACKNOWLEDGMENTS

Discussions with Michael Potthoff are gratefully acknowledged. This work was supported by the Deutsche Forschungsgemeinschaft through Grant No. KA 3360/4-1 (Project No. 508440990).

DATA AVAILABILITY

The data that support the findings of this article are not publicly available. The data are available from the authors upon reasonable request.

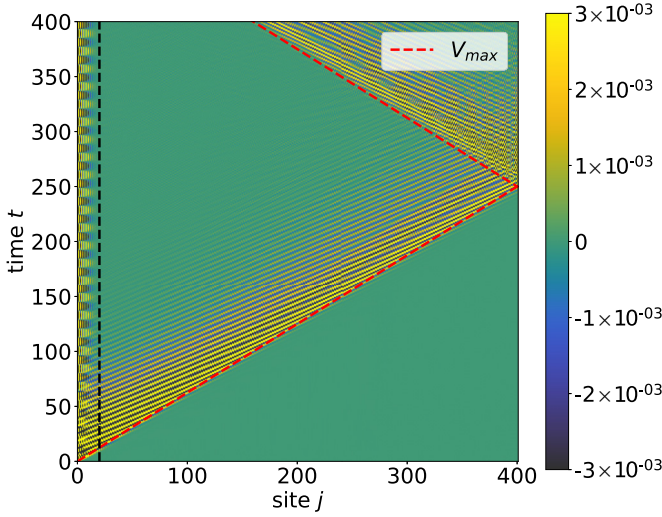


FIG. 9. Spin density $\langle s_j^z(t) \rangle$ in the substrate for $\delta T = 0.3$ and $B = 1$. The maximum wavefront speed calculated via Eq. (A1) is shown as the red dashed line.

APPENDIX A: WAVEFRONT AND MAXIMAL PROPAGATION TIME

In Fig. 9, we show the spin density in the substrate $\langle s_j^z(t) \rangle$ as a function of the time and position. Excess energy that is put into the system by the field switching is transported away. The wavefront has a maximal velocity $v_{\max}$, which can be estimated from

$$\begin{aligned} v_{\max} &= \max_k v(k) = \max_k \frac{\partial \epsilon(k)}{\partial k} \\ &= \max_k \frac{\partial}{\partial k} \sqrt{T_1^2 + T_2^2 + 2T_1 T_2 \cos(2k)} \\ &= \max_k \frac{2T_1 T_2 \sin(2k)}{\sqrt{T_1^2 + T_2^2 + 2T_1 T_2 \cos(2k)}}, \end{aligned} \quad (\text{A1})$$

where we used the dispersion relation of the free system $\epsilon(k)$, and $T_{1/2} = T \mp \delta T$. Figure 9 shows that this describes the wavefront obtained in the numerics rather well. The wavefront is reflected at the opposite boundary of the chain. To ensure that the impurity spin and substrate spins within L_{loc} sites next

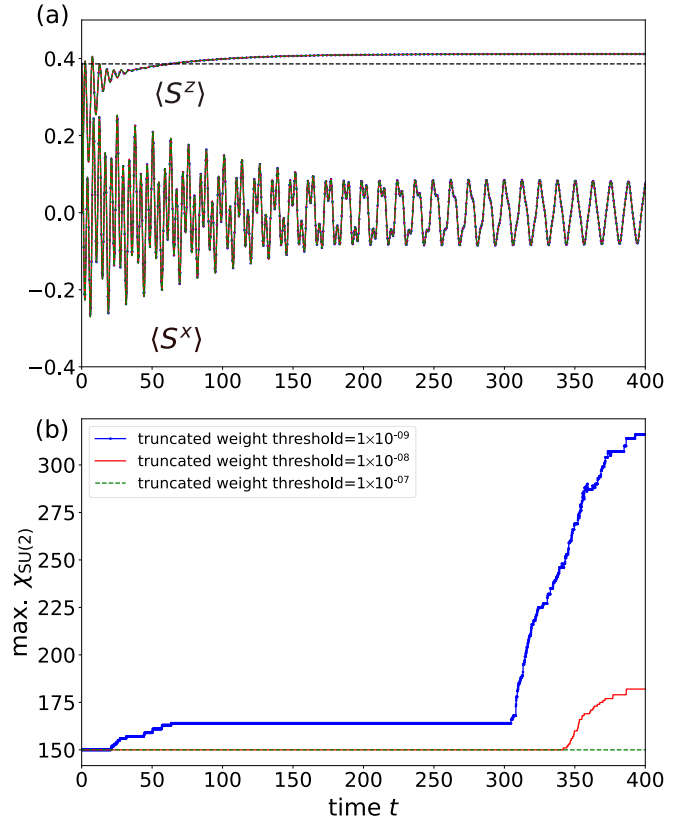


FIG. 10. TDVP time evolution for the topologically nontrivial case $\delta T = 0.3$ at $B = 1$ for three different values of the truncated weight. (a) Observables $\langle S^{x,z} \rangle$. (b) Maximum value of the effective bond dimensions $\chi_{\text{SU}(2)}$.

to it are unperturbed by this reflection, we are at most allowed to propagate until the maximal time given by

$$t_{\max}(L, T_1, T_2) = \frac{2L - L_{\text{loc}}}{v_{\max}(T_1, T_2)}. \quad (\text{A2})$$

APPENDIX B: CONVERGENCE TEST

We briefly demonstrate that our TDVP data is converged with respect to the choice of the truncated weight. To this end, Fig. 10 shows the observables $\langle S^{x,z} \rangle$ as well as the bond dimension during a time evolution for some typical parameters.

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