

Magnetic field direction dependence of the spin liquid state in α -RuCl₃

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Numerous experiments have shown that α -RuCl₃ exhibits a spin liquid (SL) state near 7.1 T when an in-plane magnetic field is applied perpendicular to the Ru-Ru bond directions ([110]), while SL states are rarely observed under fields applied along the Ru-Ru bond ([100]). The underlying mechanism for this pronounced anisotropy remains elusive. In this work, we employ semiclassical spin dynamics simulations to investigate the magnetization evolution of α -RuCl₃ with lattice distortion under varying external magnetic fields. It is found that each [100] direction has its own dominant orientation, and each [110] orientation marks the boundary, where the two alignments compete with each other. The magnetizations are influenced by multiple interactions and perturbations from lattice distortions, leading to the occurrence of the SL state in the [110] direction. These results provide new insights into the field-induced phase transitions in α -RuCl₃ and the microscopic mechanisms underlying the emergence of spin liquid behavior.

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I. INTRODUCTION

Spin liquid (SL) states [1] refer to magnetically disordered phases in which strong frustration inhibits the establishment of conventional long-range magnetic order [2]. Characterized by long-range quantum entanglement [3], SLs offer a promising platform for fault-tolerant topological quantum computation [4,5]. Among various SL candidates, α -RuCl₃ has garnered significant interest for its simple chemical composition and layered honeycomb lattice structure [1,2,6], positioning it as a leading material for realizing the Kitaev quantum spin liquid (QSL) phase [7]. The Kitaev model predicts that the bond-dependent anisotropic interaction, known as the Kitaev interaction [8,9], can stabilize an SL state in a two-dimensional $S = 1/2$ honeycomb lattice. However, in α -RuCl₃, the presence of additional multibody interactions, such as the Heisenberg interaction (J) and the off-diagonal symmetric exchange interaction (Γ), breaks the ideal Kitaev conditions and instead stabilizes a zigzag antiferromagnetic ground state [10–13].

In recent years, experiments have revealed a clear directional dependence of the SL state's occurrence on the magnetic field [10,14–21]. When the magnetic field is applied perpendicular to the Ru-Ru bond (i.e., along the [110] direction) within the honeycomb plane, the antiferromagnetic zigzag order flips to a disordered state at a critical field of approximately 7.1 T [10,15,22,23]. The thermal Hall effect [24–28] and a continuous spin excitation spectrum

[27,29–31] for this disorder state are widely regarded as indicators of the occurrence of the SL state. In contrast, when the field is applied along the Ru-Ru bond (i.e., the [100] direction), these quantum disordered features are absent, and magnetic order persists up to 7.3 T or a higher critical field [17,22]. The origin of this field-directional dependence of the occurrence of the SL state needs to be explained. Villadiego [18] proposed that [100] direction crystal symmetry suppresses the emergence of SL states. He calculated quantum Hall states to find SL states by pseudospin U(1) theory and found that crystal symmetry in the [100] direction leads to pseudospin U(1) cancellation. Wagner *et al.* [19] argued that the spins along the [100] direction are subjected to symmetric interactions and that the field-induced inhomogeneity of the spin tilt in the [110] direction leads to the second zigzag state appearing only in the [110] direction. Tanaka *et al.* [20] suggested that the two gapped excited states in the [100] direction vanish due to symmetry breaking, resulting in changes to the system's topological properties and driving the Chern number to zero, leading to the disappearance of the SL state. The previous studies have primarily focused on the role of symmetry in suppressing or enabling SL states. We employ micromagnetic simulations to directly visualize the evolution of magnetic moments in real space under external perturbations. This method allows us to capture dynamic transitions and the competition between magnetic phases, offering insights that extend beyond static analyses or purely quantum theoretical frameworks.

In this work, we employ the micromagnetic method to examine the evolution of its magnetic states under external magnetic fields and analyze the total system energy to investigate the directional dependence of the field-induced disordered regime. Our results reveal the microscopic origin of the direction-dependent stability of this regime, explaining why spin-liquid-like behavior emerges only when the magnetic field is applied along the [110] direction. While our

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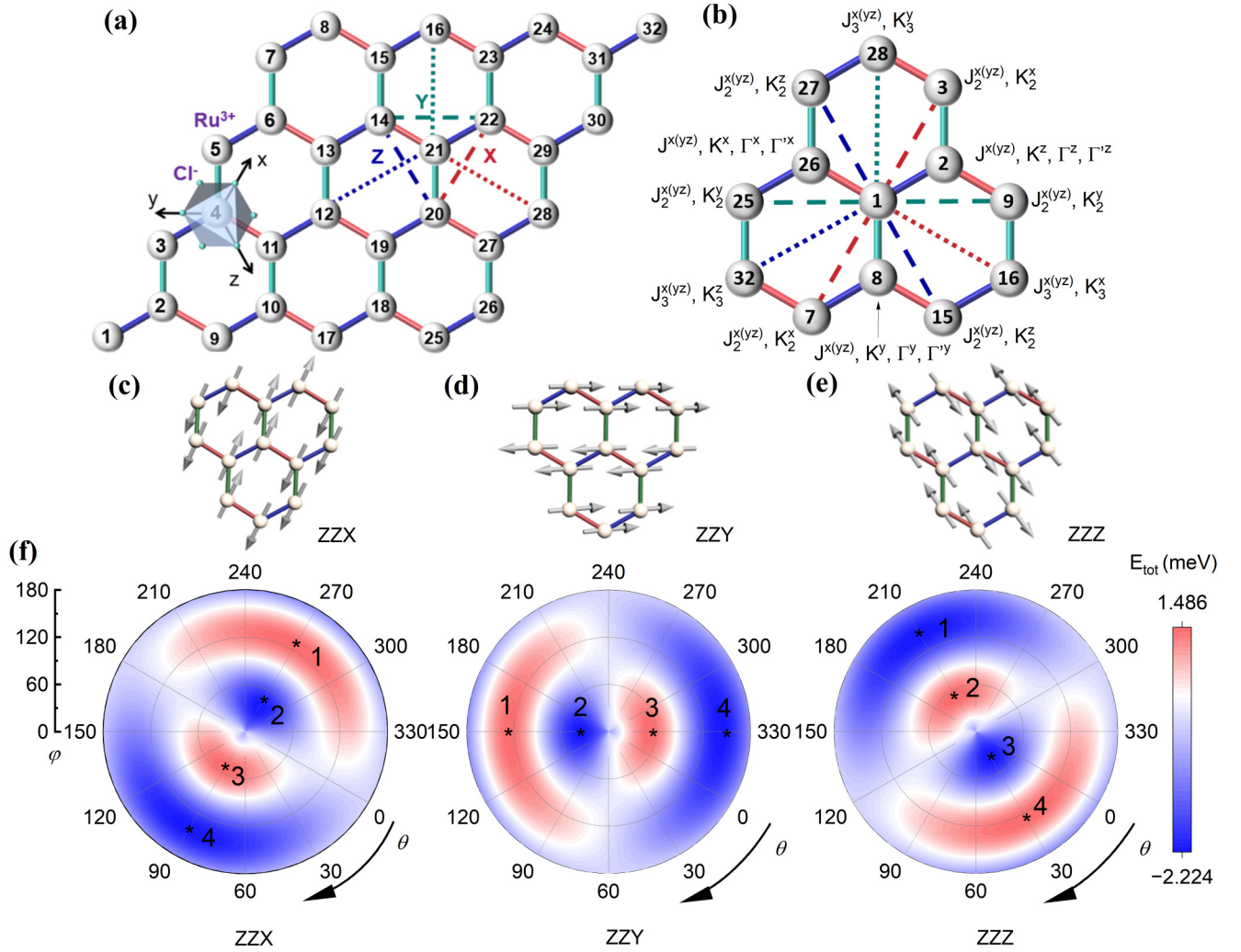


FIG. 1. Lattice model and three kinds of initial magnetic states. (a) The lattice structure of 32-site Ru^{3+} in $\alpha\text{-RuCl}_3$ is illustrated, where the coordinates (x, y, z) correspond to the cubic axes of local octahedra formed by Cl atoms. The X, Y, and Z bonds are represented by red, green, and blue colors, respectively. The honeycomb lattice is defined by first-, second-, and third-nearest-neighbor bonds, depicted by solid, dashed, and dotted lines, respectively. (b) Take the first point as an example to illustrate the exchange terms in each direction corresponding to the first-, second-, and third-nearest-neighbor relationship. (c)–(e) The arrangement of the initial magnetic moments ZZX , ZZY , and ZZZ . (f) The total energy landscape as a function of magnetic moment orientation. The radial coordinate ϕ denotes the magnetic moment angle from the honeycomb plane, while the azimuthal angle θ corresponds to the clockwise in-plane rotation of the magnetic moment, with 0° defined along the $X[100]$ direction. From left to right, the panels show the energy landscapes for initial configurations of ZZX , ZZY , and ZZZ , respectively. The points labeled 1–4 in each panel correspond to the local maxima and minima of the total energy. The specific angles and energy values for these points are listed in Table I.

semiclassical approach cannot capture genuine quantum entanglement, it provides a classical framework that reproduces the experimental signatures associated with the SL regime. This finding offers a new microscopic perspective on magnetic field control in $\alpha\text{-RuCl}_3$ and establishes a theoretical basis for designing orientation-sensitive quantum devices, such as topological qubits with tunable magnetic field directions.

II. MODEL AND METHOD

$\alpha\text{-RuCl}_3$ is a two-dimensional (2D) van der Waals (vdW) magnetic material with weak interlayer interactions mediated by vdW force [32]. The intralayer Ru^{3+} ions form a honeycomb lattice, with each Ru^{3+} ion surrounded by six Cl^- ions

in perfect octahedral coordination. Considering that the interlayer exchange interactions are significantly weaker than the intralayer exchange interactions, our simulations focus on a single layer of $\alpha\text{-RuCl}_3$. Since only Ru^{3+} ions carry magnetic moments, the micromagnetic simulations are confined to these ions. To capture the intrinsic disorder commonly associated with SL materials, we employed a model consisting of 32 periodically arranged Ru^{3+} sites [16] in Fig. 1(a). The colors in the figure represent the direction of the Ru-Ru bond, and the solid and dashed lines distinguish the bond distances. Blue, green, and red represent the X-, Y-, and Z-type bonds, respectively. Solid, dashed, and dotted lines denote first-, second-, and third-nearest-neighbor bonds, while the line styles also reflect variations in bond lengths. The edges of the local

TABLE I. Characterization of the degenerate energy minima corresponding to the three zigzag states in Fig. 1(f).

	ZZX		ZZY		ZZZ	
	(θ, ϕ)	E (meV)	(θ, ϕ)	E (meV)	(θ, ϕ)	E (meV)
1	(270°, 127°)	1.478	(150°, 127°)	1.478	(210°, 144°)	-2.224
2	(270°, 36°)	-2.224	(150°, 36°)	-2.224	(210°, 53°)	1.478
3	(90°, 53°)	1.478	(330°, 53°)	1.478	(30°, 36°)	-2.224
4	(90°, 144°)	-2.224	(330°, 144°)	-2.224	(30°, 127°)	1.478

octahedron formed by Cl^- ions are the coordinates ($\mathbf{x}, \mathbf{y}, \mathbf{z}$) of the system. X-, Y-, and Z-type bonds are perpendicular to the $\mathbf{x}$ -, $\mathbf{y}$ -, and $\mathbf{z}$ -axes, respectively. In our labeling system, the first-nearest-neighbor Ru-Ru bonds of the red, green, and blue solid lines are X[100], Y[100], and Z[100], respectively. The second-nearest-neighbor Ru-Ru bonds of the red, green, and blue dashed lines denote X[110], Y[110], and Z[110]. This definition of the directions is crucial for understanding the arrangement of magnetic moments. After evaluating several models, we found that the $\{J, K, \Gamma, \Gamma', J_3\}$ mode [16,33,34] is insufficient to reproduce the observed magnetization dynamics (see Tables SI and SII and Fig. S1 of the Supplemental Material [35–38]). To address this, we employ a more complete effective field model that includes interactions up to the third-nearest neighbors [11,39]. The Hamiltonian is written as

$$\begin{aligned}
H = & \sum_{(i,j) \in \gamma(\alpha\beta)} [J^\gamma \mathbf{m}_i \cdot \mathbf{m}_j + K^\gamma m_i^\gamma m_j^\gamma + \Gamma^\gamma (m_i^\alpha m_j^\beta + m_i^\beta m_j^\alpha) \\
& + \Gamma'^\gamma (m_i^\alpha m_j^\gamma + m_i^\beta m_j^\gamma + m_i^\gamma m_j^\alpha + m_i^\gamma m_j^\beta)] \\
& + \sum_{\langle(i,j)\rangle \in \gamma(\alpha\beta)} [J_2^\gamma \mathbf{m}_i \cdot \mathbf{m}_j + K_2^\gamma m_i^\gamma m_j^\gamma] \\
& + \sum_{\langle\langle(i,j)\rangle\rangle \in \gamma(\alpha\beta)} [J_3^\gamma \mathbf{m}_i \cdot \mathbf{m}_j + K_3^\gamma m_i^\gamma m_j^\gamma], \quad (1)
\end{aligned}$$

where $\langle i, j \rangle$, $\langle\langle i, j \rangle\rangle$, and $\langle\langle\langle i, j \rangle\rangle\rangle$ denote the first-, second-, and third-nearest-neighbor bonds, respectively. $\mathbf{m}_{i(j)}$ stands for the spin magnetic moment of the site $i(j)$ Ru^{3+} . α , β , and γ refer to the bond types, and the cycle corresponds to the three directions of the neighboring bonds, i.e., the X type, the Y type, and the Z type. The parameters J , J_2 , and J_3 denote the first-, second-, and third-nearest Heisenberg couplings, respectively. K , K_2 , and K_3 denote the first-, second-, and third-nearest Kitaev interactions, respectively. Γ and Γ' denote the first-nearest symmetric off-diagonal terms [40].

The effective field of the system is

$$\begin{aligned}
\mathbf{H}_{\text{eff}}^\gamma = & -\frac{1}{M_s} \sum_{(i,j) \in \gamma(\alpha\beta)} [J^\gamma \mathbf{m}_i + K^\gamma \mathbf{m}_j^\gamma + \Gamma^\gamma (\mathbf{m}_i^\alpha + \mathbf{m}_j^\beta) \\
& + \Gamma'^\gamma (\mathbf{m}_i^\alpha + \mathbf{m}_j^\beta + \mathbf{m}_j^\alpha + \mathbf{m}_i^\beta)] \\
& -\frac{1}{M_s} \sum_{\langle(i,j)\rangle \in \gamma(\alpha\beta)} [J_2^\gamma \mathbf{m}_i + K_2^\gamma \mathbf{m}_j^\gamma] \\
& -\frac{1}{M_s} \sum_{\langle\langle(i,j)\rangle\rangle \in \gamma(\alpha\beta)} [J_3^\gamma \mathbf{m}_i + K_3^\gamma \mathbf{m}_j^\gamma] + \mathbf{H}_i^\gamma, \quad (2)
\end{aligned}$$

where $\mathbf{H}_{\text{eff}}^\gamma$ is the fraction of the effective field in the γ bond direction, calculated for the three directions around each Ru^{3+} ion. $\mathbf{m}_{i(j)}^{\gamma(\alpha\beta)}$ denotes $\gamma(\alpha\beta)$ component of magnetization of site $i(j)$ Ru^{3+} . $\mathbf{H}_i^\gamma$ is γ component of the external magnetic field of site i Ru^{3+} . M_s is the saturation magnetization strength [41] with $M_s = 1.2\mu_B$. The magnetic parameters used in the calculations are as follows: $J = 0.24$ T, $J_2 = -0.90$ T, $J_3 = 0$ T, $K = -12.92$ T, $K_2 = 1.22$ T, $K_3 = 0.10$ T, $\Gamma = 10.88$ T, and $\Gamma' = -0.99$ T. This parameter set was tuned to match key experimental features, including resonance spectra [22], magnetization flip magnetic field [22,23], and zero-field stable magnetization angles [42]. We have compared this parameter set with a five-parameter model $\{J, K, \Gamma, \Gamma', J_3\}$, and it demonstrates a superior fit to the resonance spectrum. The second-neighbor interaction parameters J_2 and K_2 play a critical role in adjusting the relative weighting of high- and low-frequency components in the terahertz (THz) resonance spectrum (see Fig. S3 of the Supplemental Material [35]).

The magnetic dynamics of each Ru^{3+} ion are governed by the Landau-Lifshitz (LL) equation [43], which can be expressed as

$$\frac{d\mathbf{m}_i}{dt} = -\gamma_g (\mathbf{m}_i \times \mu_0 \mathbf{H}_{\text{eff}}^\gamma) - \alpha \frac{\gamma_g}{M_s} \mathbf{m}_i \times (\mathbf{m}_i \times \mu_0 \mathbf{H}_{\text{eff}}^\gamma), \quad (3)$$

where γ_g represents the gyromagnetic ratio [44] with $\gamma_g = 1.76 \times 10^{14}$ Hz T $^{-1}$, α is the Gilbert effective damping, and μ_0 denotes vacuum permeability. We calculate the kinetic equations to obtain a series of information about the steady state and oscillations of the magnetic moments, and discuss the specific progression of the magnetic moments in detail.

Each Ru^{3+} ion in $\alpha\text{-RuCl}_3$ is initialized with a specific magnetization direction to characterize the phase. The system then evolves under the influence of the effective magnetic field until it reaches a steady-state magnetization configuration. The total system energy corresponds to the sum of energies from all 32-site Ru^{3+} ions within the supercell. For dynamic analysis, we apply the fast Fourier transform (FFT) to the time-resolved magnetization data, which reveals the dominant oscillation frequencies during the system's evolution. This method is uniquely powerful for capturing dynamic transitions and the competition between magnetic phases, enabling us to identify an intermediate phase. By focusing on this classical precursor to a potential quantum spin liquid, we aim to unravel the microscopic mechanisms underlying the anisotropic field response.

III. RESULTS AND DISCUSSION

Extensive experiments and theoretical studies have confirmed that the ground state of α -RuCl₃ adopts a zigzag-type antiferromagnetic spin configuration [45–47], as illustrated in Figs. 1(c)–1(e). Our calculations reproduce this configuration, where each Ru³⁺ magnetization is tilted by approximately 36° from the honeycomb plane, with its in-plane projection directed along the second-nearest-neighbor Ru-Ru bond direction: X[110], Y[110], or Z[110]. Owing to the lattice symmetry, this results in three energetically degenerate zigzag states, termed ZZX, ZZY, and ZZZ. This is verified by calculating the total energy of a 32-site Ru³⁺ supercell with zigzag-type magnetization orientations across different directions [see Fig. 1(f)]. The radial coordinate ϕ represents the angle between the magnetic moment and the honeycomb plane, while the azimuthal angle θ corresponds to the in-plane rotation of the magnetic moment measured clockwise from the X[100] direction. The energy landscapes for ZZX, ZZY, and ZZZ configurations are shown from left to right, respectively. As can be seen from the left figure (ZZX) and Table I, two minimum-energy points 2 and 4 occur at $(\theta, \phi) = (270^\circ, 36^\circ)$ and $(90^\circ, 144^\circ)$, where the in-plane directions are orthogonal to the X[100] axis and the out-of-plane angles are complementary, indicating that the lowest-energy state corresponds to an antiparallel configuration. Similar results are also observed when the initial magnetizations are arrayed as ZZY and ZZZ states. As shown in Table I, the six minimum-energy points in Fig. 1(f) possess equal energy values, which further confirms that the three zigzag configurations are degenerate in the ground state. These results verify the degeneracy of the three zigzag states in the ideal crystal structure, and they agree with the findings of resonant elastic x-ray scattering (REXS) [48] and *ab initio* simulations [42].

Taking the ZZX state as the ground state, we investigated the magnetization response of the defect-free α -RuCl₃ lattice under an external magnetic field. Figures 2(a) and 2(b) show the magnetization curve under an external magnetic field applied in the X[100] and Y[110] directions, respectively. The Y[110] direction is selected because it forms the minimum angle ($\theta = 30^\circ$) with the X[100] direction, and subsequent calculations confirm that all [110] directions are equivalent. The red and blue lines represent the x components of the individual magnetic magnetization m_x , while the green line denotes the total magnetization m_{tot} amplitude of the 32-site Ru³⁺ system. The total magnetization m_{tot} refers to the projection of the total magnetization along the field direction. Starting from zero, the total magnetization increases as the external field destabilizes the antiparallel zigzag configuration. In Figs. 2(a) and 2(b), we present the real-space spin texture at representative magnetic field strengths. As the field increases, the spins undergo a gradual reorientation driven by the competition between Zeeman energy and exchange interactions. At low fields, the zigzag textures are preserved in an antiparallel configuration. Whereas at intermediate fields, the blue arrows ($\mathbf{m}_1$ represents $\mathbf{m}_1$ – $\mathbf{m}_8$ and $\mathbf{m}_{17}$ – $\mathbf{m}_{24}$) and the red arrows ($\mathbf{m}_9$ represents $\mathbf{m}_9$ – $\mathbf{m}_{16}$ and $\mathbf{m}_{25}$ – $\mathbf{m}_{32}$) both rotate toward the direction of the external magnetic field. As the system approaches the critical field, the spins increasingly align with the field direction, ultimately evolving into a nearly polarized

state. A field-induced phase transition occurs at 9 T when the field is applied along the X[100] direction [see Fig. 2(a)] and at 7.1 T along the Y[110] direction [see Fig. 2(b)]. This indicates a clear anisotropy in the system's magnetic response. Extensive experimental evidence has shown that an SL state emerges under an external magnetic field of 7.1 T applied along the [110] direction [15,22,23,49,50].

The second characteristic of the magnetization response is its $\varphi = 180^\circ$ periodicity with respect to the tilting angle as the external magnetic field rotates out of the honeycomb plane. In Fig. 2(c), the total magnetization strength m_{tot} varies with the out-of-plane magnetic field strength. The green curve and blue curve represent the rotation of the magnetic field direction from X[100] and Y[110] directions to the [111] direction, respectively. In both cases, the total magnetization shows a 180° angular period, consistent with experimental results reported by Kocsis *et al.* [51]. Some investigations have revealed that the total energy of α -RuCl₃ should exhibit sixfold symmetry variations due to the C_3 symmetry of its crystal structure [20,52–55]. We calculated the total energy of the system under an external magnetic field ($H = 1$ T) for the three magnetization arrangements. It was observed that, when the magnetic field is rotated within the honeycomb plane, the energy of the three magnetization states varies with a $\theta = 60^\circ$ period, consistent with the expected sixfold symmetry [see Fig. 2(d)]. This result supports the theoretical predictions made by Lampen-Kelley [56].

The calculations for the defect-free lattice above show that the 32-site Ru³⁺ ion model accurately captures the phase transition point and reflects the periodicity of this variation. However, the SL state is not observed, which contradicts the computational and experimental evidence. Several factors, such as static modulation of exchange couplings, lattice distortion, and temperature, were considered in the formation of the SL states. Our calculations show that the SL state emerges when the magnetic field is along the [110] direction if some perturbations are considered. To explain the direction-dependent emergence of SL states, we focus on lattice distortion [41], which is a common effect in real materials.

When the material lattice is distorted, the quenched distorted Ru³⁺ ion displacement ratio is $\eta = r/r_0$, where r_0 is the distance between Ru-Ru and r is the displaced Ru-Ru distance, as shown in Fig. 3(a). Lattice quenched distortion leads to changes in bond lengths that directly affect the exchange interaction parameters. For quantitative calculation of quenched distortion, the static modulation of the exchange interaction parameter due to the Ru³⁺ ion offset is denoted as η_X . For clarity, we adopt the linearized (differential) form appropriate for small bond length changes. For any exchange coupling $X \in \{J, K, \Gamma, \Gamma'\}$, we expand around the equilibrium bond length r_0 :

$$X(r_0 + \Delta r) \approx X(r_0) + \left. \frac{dX}{dr} \right|_{r_0} \Delta r = X(r_0)[1 + \lambda_X \varepsilon], \quad (4)$$

where $\varepsilon = \Delta r/r_0$ and $\lambda_X = d \ln X / d \ln r$ is the logarithmic sensitivity of X to bond length change. Thus, the modulation factor is $\eta_X = 1 + \lambda_X \varepsilon$. In subsequent calculations, the parameter modulation induced by lattice distortions is approximated as linear.

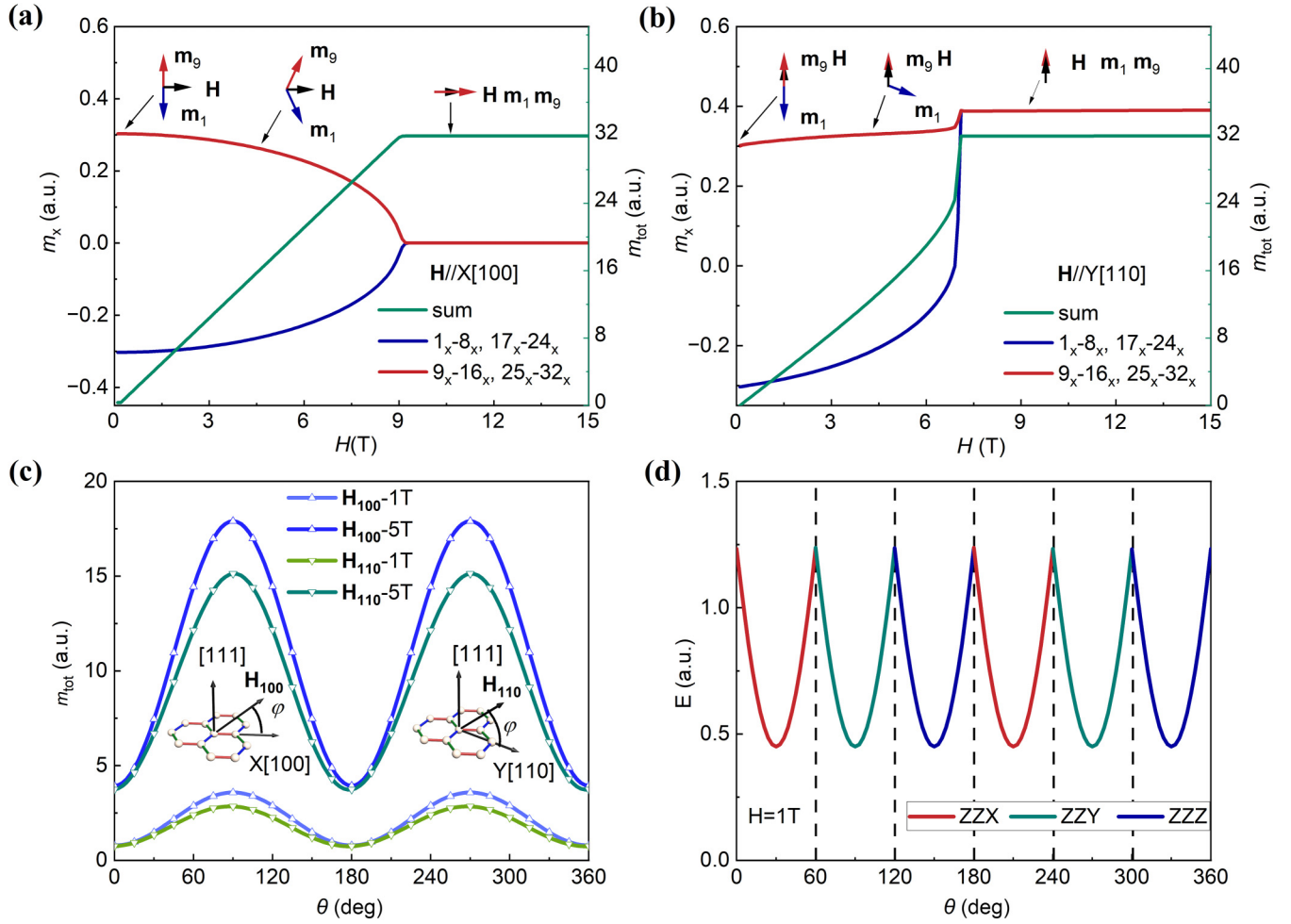


FIG. 2. Magnetization and energy of defect-free Lattice. Magnetization evolution of defect-free α -RuCl₃ under an external magnetic field along the (a) X[100] direction and (b) Y[110] direction. The red and blue lines represent the x components of the individual magnetic magnetization m_x , while the green line denotes the total magnetization m_{tot} along the external magnetic field. The blue, red, and black arrows represent $\mathbf{m}_1$, $\mathbf{m}_9$, and $\mathbf{H}$, respectively, illustrating the evolution of the real-space spin texture of the magnetic moments under an increasing external magnetic field. (c) Variation of total magnetization m_{tot} for 32-site Ru³⁺ ions under external field rotation out-of-plane ($H = 1$ T and 5 T) with ZZX initial configuration. Light blue and blue curves represent rotation outward from X[100], while light green and green represent rotation outward from Y[110]. (d) Total energy minimum variation as a function of in-plane magnetic field rotation at $H = 1$ T. The red, green, and blue curves correspond to the systems with ground states of ZZX, ZZY, and ZZZ, respectively.

In Fig. 3(a), when the site 1 Ru³⁺ ion is displaced by 1% in the Z¹⁻² direction toward site 2, the bond length of the Z¹⁻² bond is 0.99 times the original length, with $\eta = 0.99$. The bond lengths of the Y²⁻³ and X²⁻⁹ bonds are 1.00502 times their original lengths. We simulate the effect of bond length changes on SL states during lattice distortion. Based on the geometric rules of the honeycomb lattice, the ratios of bond length changes were calculated for 12 ions around a central ion, including the first-, second-, and third-nearest-neighbor spins. The lattice distortion parameters are given in Table SIII of the Supplemental Material [35]. Since the displacements are small (around 0.99), the relationship between parameter changes and distance changes can be approximated as linear. Using this setup, we quantified the lattice distortion and denoted the lattice distortion of the site 1 Ru³⁺ ion along the X[100], Y[100], and Z[100] directions as dX , dY , and dZ , respectively. All lattice distortions mentioned below

refer to the shift of the site 1 Ru³⁺ ion only. In the ideal honeycomb structure of α -RuCl₃, antisymmetric exchange interactions such as the Dzyaloshinskii-Moriya interaction (DMI) are symmetry-forbidden at the nearest-neighbor level. However, weak lattice distortions may allow small contributions from further-neighbor terms. In our case, the applied distortion corresponds to only about 1% of the lattice constant (~ 0.05 Å), which is considerably smaller than the ~ 0.2 Å distortion [57] reported in the literature as necessary to induce an appreciable DMI. Therefore, within our model, the contribution from antisymmetric exchange is negligible compared to the dominant symmetric interactions (K and Γ) [58].

After introducing the Z¹⁻² distortion into the material, we first calculated the magnetization response of the system under external magnetic fields along the X[100] and Y[110] directions, with initial magnetizations corresponding to the ZZX configuration. In Fig. 3(c), when the magnetic field is

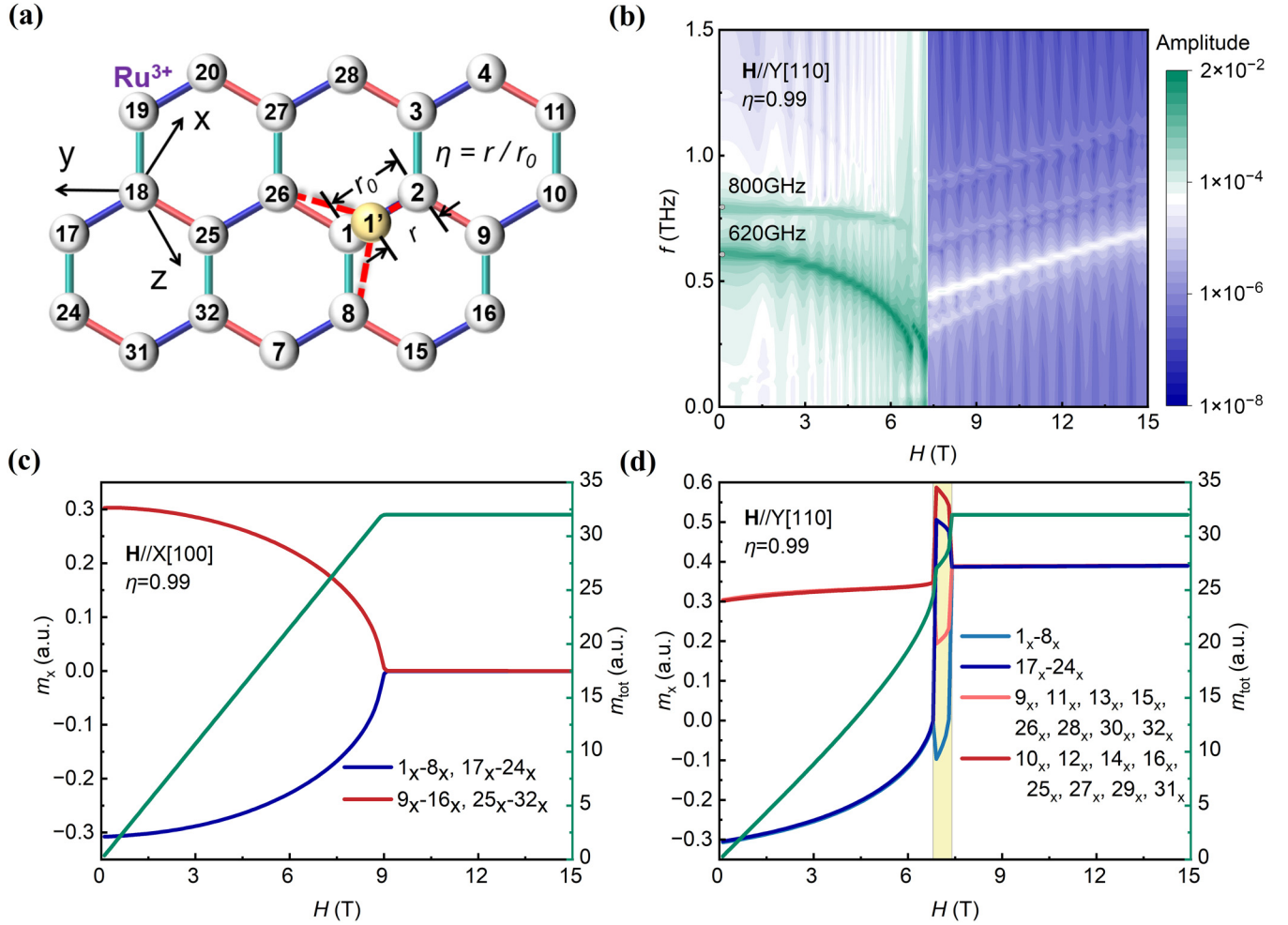


FIG. 3. Frequency excitation and magnetization of α - RuCl_3 with lattice distortion. (a) Schematic illustrating the Z-direction displacement of the Ru^{3+} ion at site 1 with a lattice distortion of $\eta = 0.99$. The primed notation (1') denotes the displaced ion, and red dashed lines show the resulting changes in interatomic distances. (b) Frequency excitation diagram of α - RuCl_3 with lattice distortion $\eta = 0.99$, under an external magnetic field applied along the $Y[110]$ direction. x component of magnetization m_x and total magnetization m_{tot} as functions of external magnetic field strength along the (c) $X[100]$ and (d) $Y[110]$ directions, for an initial ZZC configuration under distortion $\eta = 0.99$.

applied along the $X[100]$ direction, the response remains essentially identical to that of the defect-free lattice, indicating minimal influence from the distortion in this orientation. In contrast, as illustrated in Fig. 3(d), when the field is applied along the $Y[110]$ direction, four distinct magnetization states emerge within the highlighted yellow region. This behavior deviates from the conventional ZZC ordering and instead exhibits signatures consistent with an SL state.

To determine whether the magnetic configuration in this field region corresponds to an SL state, we calculated the resonance frequency of the system under an external magnetic field, as shown in Fig. 3(b). When the field is applied along the $Y[110]$ direction, the resonant frequencies at 0 T are 620 and 800 GHz, consistent with the excitation spectrum of the defect-free lattice (see Fig. S2 of the Supplemental Material [35]) up to 6.5 T. Near 7 T, two closely spaced phase transitions are observed at 6.5 and 7.1 T. In the intermediate region between these transitions, the system exhibits noticeable spectral broadening and the emergence of a few weak additional frequency components, which show a moderate deviation from the sharp modes observed in the defect-free

case. Similar excitation features were reported in the experiments by Sandilands *et al.* [31] and Ponomaryo *et al.* [22], where they were interpreted as possible signatures of the SL state. Based on this comparison, we identify the intermediate field region between the two transitions as an SL phase and highlight it in yellow in Fig. 3(d). We emphasize that while our semiclassical micromagnetic simulations reproduce key features of the experimentally identified SL regime, such as broadened excitation spectra and strong competition between nearly degenerate zigzag configurations, they do not capture genuine quantum entanglement or fractionalized excitations intrinsic to a true quantum spin liquid. Our results should therefore be understood as providing a classical mechanism that underpins the emergence of the experimentally observed SL regime, rather than a direct demonstration of a quantum spin liquid state.

Moreover, finite-temperature simulations (see Fig. S6 of the Supplemental Material [35]) indicate that the SL state around $H = 7.1$ T persists even when weak thermal fluctuations are present, confirming that this behavior is not restricted to $T = 0$. In addition, while our classical simulations

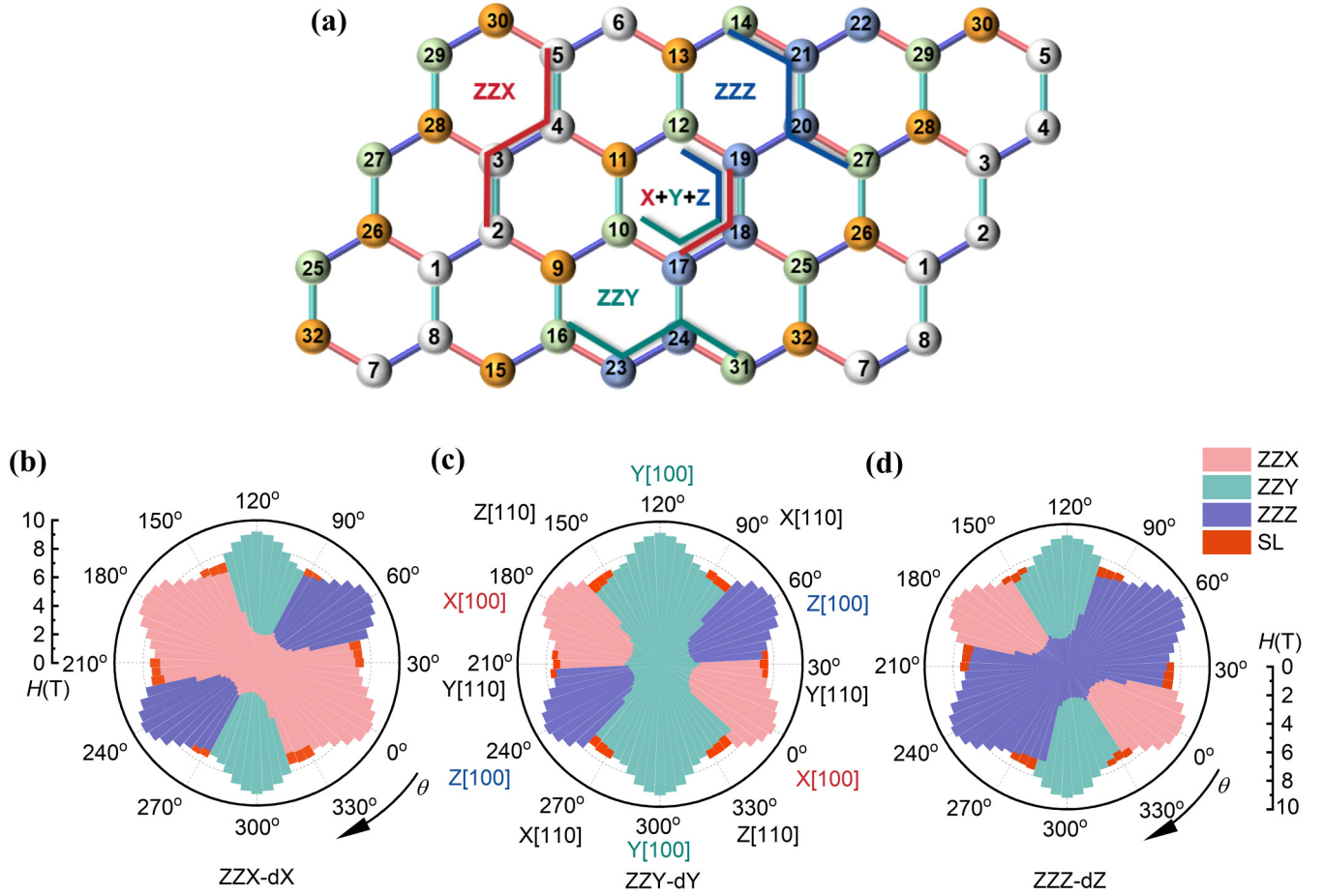


FIG. 4. Magnetic configurations of the SL phase and the magnetic phase diagram. (a) Schematic of magnetic configurations for Ru^{3+} ions within the SL region (highlighted in yellow) from Fig. 3(d). Colored spheres indicate four magnetization orientations, with red, blue, and green lines denoting ZZX, ZZY, and ZZZ orders, respectively. The state is characterized by the competition and coexistence of domains resembling the three zigzag orders. Magnetic phase diagram as a function of field strength and in-plane orientation θ for the initial configurations (b) ZZX-dX, (c) ZZY-dY, and (d) ZZZ-dZ. Pink, green, and blue regions indicate ZZX, ZZY, and ZZZ phases, while red regions denote the SL state. The blank zone represents a high-field quantum state of uncertain nature.

reproduce the low-field anisotropy of the spin-flip transitions, they predict a rapid saturation immediately after the transition. This contrasts with experimental observations of a gradual approach to saturation up to ~ 60 T, which we attribute to the inherently quantum nature of the high-field regime and consider that the occurrence of this phenomenon may be related to interlayer interactions and temperature effects. However, since our current structure is a monolayer, we are unable to reproduce the complex magnetic behaviors arising from interlayer interactions, making this a target for our future work.

To better illustrate the magnetization state of the detected SL phase, Fig. 4(a) shows a schematic of the magnetization state at 7 T, where white, yellow, green, and blue spheres are used to represent four distinct magnetization states. According to the spatial distribution patterns of these color spheres, the configuration can be interpreted as a state characterized by the competition and coexistence of domains resembling the three zigzag orders. Specifically, the distribution of white spheres ($\mathbf{m}_1-\mathbf{m}_8$) and blue spheres ($\mathbf{m}_{17}-\mathbf{m}_{24}$) corresponds to the ZZX configuration, while the arrangement of green and yellow spheres aligns with the ZZZ and ZZY configurations, respectively.

To clarify the conditions leading to the coexistence of three zigzag-type magnetic domains, we examine how the lattice distortion direction and the initial magnetization configurations affect the field-driven evolution of the system. Figures 4(b)–4(d) show the phase diagram of magnetization state as a function of the strength and direction of the external magnetic field, with the initial magnetization configurations set as ZZX, ZZY, and ZZZ. In these diagrams, the magnetic field is rotated within the honeycomb plane, while its magnitude varies from 0 to 10 T. The notation “ZZX-dX” indicates that the initial magnetization is in the ZZX state, and the lattice distortion direction is along the X[100] direction. Here, the $\theta = 0^\circ$ corresponds to the X[100] direction, and $\theta = 30^\circ$ corresponds to the Y[110] direction. Key angular directions and their respective crystallographic orientations are all indicated in Fig. 4(c). The pink, green, blue, and red regions correspond to ZZX, ZZY, ZZZ, and SL states, respectively. The region of high magnetic field blanked out in the figure is the high-field quantum state of uncertain nature. The corresponding total energy variation and magnetic increment as functions of magnetic field orientation, under lattice distortion, are shown in Fig. S4 of the Supplemental Material [35].

From Figs. 4(b)–4(d), the first thing worth noting is that the SL state appears near 7 T in the directions corresponding to each [110] direction. It appears within a narrow angular range of approximately 15° around the angle of the magnetic field tilted from X[100] equals $\theta = 30^\circ, 90^\circ, 150^\circ, 210^\circ, 270^\circ, 330^\circ$. The exact position may vary slightly, typically within 10° , depending on the initial magnetization state. Comparative analysis of the phase diagrams under three different conditions shows that the emergence of SL states is almost independent of the initial magnetization state and the direction of lattice distortion. These directions coincide with the junctions of individual zigzag phases, where ZZX, ZZY, and ZZZ have their respective boundaries. The SL state emerges at these boundary intersections, and we suggest that the strong energy competition at these junctions provides the necessary condition for the formation of SL states.

The second thing worth noting in Figs. 4(b)–4(d) is the angular dependence of different phase transitions. For example, in Fig. 4(b) ZZX state is set as the initial magnetization state, and the transition from ZZX to the FM state occupies the majority of the phase diagram when θ is between 320° – 40° and 140° – 220° . In these regions, only one spin flip occurrence, the ZZY and ZZZ states, is significantly suppressed by the dominant ZZX state. The critical field for spin flipping exhibits a periodic dependence on the angle of the external magnetic field, reaching a higher value of 9 T along the [100] direction and decreasing to approximately 7.1 T near the [110] direction. We also find other phase transitions in the phase diagram, the transition from ZZX to ZZY and ZZX to ZZZ, with the ZZY phase confined to the range of 95° to 135° and the ZZZ phase from 45° to 90° . Similar behavior is observed in Figs. 4(c) and 4(d): When the initial magnetization is set to ZZY, the ZZY state covers a larger range; likewise, when the initial magnetization is ZZZ, the ZZZ state becomes more prominent.

The flip magnetic field of the magnetization flip is also regular at these critical phase transition angles. We find that at $\theta = 35^\circ$, ZZX-dX remains in the ZZX state from 0 to 6.5 T, while ZZY-dY transitions from the ZZY to the ZZZ state at 2 T. It shows that, under different initial conditions, the system stays in distinct zigzag states at $\theta = 35^\circ$, with strong competition between these states. The first transition occurs near 2 T, where the system undergoes an energy hopping at a low magnetic field when the initial magnetic magnetization misaligns with the zigzag boundary. This transition aligns with the first phase transition at 1.6 T reported by Wagner *et al.* [19] in their magneto-optical coupling study of RuCl_3 . We confirm that this transition is a zigzag-to-zigzag reconfiguration rather than SL formation.

These findings illustrate the angular and magnetic field dependence of zigzag configurations and SL state emergence. To further elucidate the underlying mechanism, we turn to a detailed analysis of the energy landscape and its evolution under external fields.

Analyzing the system's energy illustrates the competition among the three zigzag configurations. In Fig. 5, when the external magnetic field is below 1 T, the energy exhibits a $\theta = 180^\circ$ periodicity. Although the three states share the same minimum energy, they are separated by substantial energy barriers, making transitions between them

energetically unfavorable. Thus, the system remains trapped in a given zigzag configuration. Specifically, ZZX is energetically favored along the X[110] direction, while ZZY minimizes energy along Y[110]. When the magnetic field is applied along X[110] and increased from zero, the magnetizations naturally align into the ZZX state. This provides a potential method for experimentally selecting magnetic configurations. As the external magnetic field increases, the angular periodicity of the system's energy gradually shifts from 180° to 60° . At 6.5 T, the energy period shifts to $\theta = 60^\circ$, signaling a transformation from twofold to sixfold symmetry [see Fig. 5(b)]. This marks the onset of SL behavior along the [110] directions. The energy barriers between the three zigzag states decrease with increasing field. At 6.6 T, the energy along the [110] direction rises sharply, allowing the system to transition more easily among states and creating the conditions for SL emergence. Near 7 T, the increased energy inhomogeneity suggests that the formation of SL states is probabilistic rather than deterministic, consistent with the original concept of SLs as lacking long-range magnetic order. By 7.4 T, the energy stabilizes along [110], suggesting a high-field polarized state.

Our simulations confirm that lattice distortions with $\eta = 0.99$ can induce SL states along the [110] direction. We further investigated how the emergence of SL states evolves with increasing distortion strength or defect density. The results indicate that enhancing the distortion, whether by lowering the distortion coefficient to $\eta = 0.97$ or introducing two to three distorted sites, does not shift the angular region near [110], where the SL state appears, but only modifies its field range (see Fig. S5 of the Supplemental Material [35]). For example, with $\eta = 0.97$, the SL state spans from 6.7 to 7.4 T. We also examined the effects of moderate parameter variations and temperature fluctuations (see Figs. S6 and S7 of the Supplemental Material [35]). A small increase in exchange parameters (e.g., within 1%) or temperature variation shows minimal impact on the SL region. Since perfect crystals are unrealistic in experiments, intrinsic defects, lattice distortions, or finite temperatures are likely present, which explains why SL states are observed in experiments but are absent in idealized simulations. We conclude that any perturbation, whether structural or thermal, can induce internal energy fluctuations that enhance competition among the three zigzag configurations. This competition leads to the emergence of SL states near the potential boundaries of each zigzag phase, i.e., along each [110] direction.

IV. CONCLUSIONS

We simulate the evolution of Ru^{3+} magnetizations in a monolayer honeycomb lattice of $\alpha\text{-RuCl}_3$ under an external magnetic field, focusing on three types of initial zigzag configurations and corresponding lattice distortions in relation to the emergence of SL states. SL state appears near 7 T in the directions corresponding to each [110] direction. Each [100] direction has its own dominant orientation, and the magnetization remains stable until the phase transition. Each [110] orientation marks the boundary of these dominant orientations, where the two alignments compete with each other. The magnetizations are influenced by multiple interac-

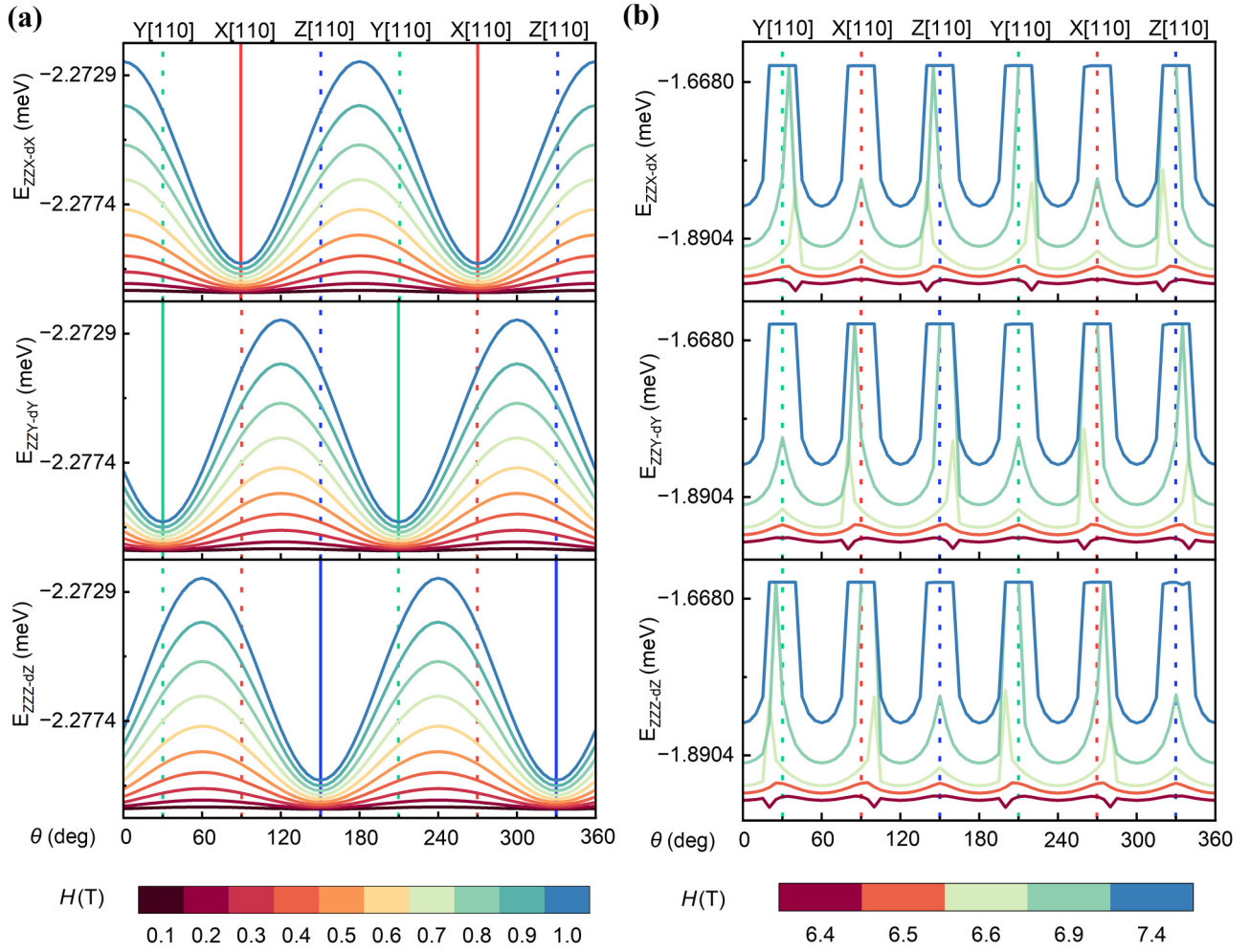


FIG. 5. Total energy analysis of α -RuCl₃ with lattice distortion. Total energy profiles as a function of in-plane magnetic field direction under (a) low-field conditions ($H < 1$ T) and (b) intermediate fields ($6.4 \text{ T} < H < 7.4 \text{ T}$) for initial configurations ZZX-dX, ZZY-dY, and ZZZ-dZ.

tions and perturbations from lattice distortions, leading to the emergence of SL states in the [110] direction. The SL state originates from energetic competition among different zigzag states, particularly along the [110] direction, and manifests as a well-defined magnetic magnetization configuration. This analysis clarifies why SL states are consistently observed in the [110] direction in numerous experiments, while no such states emerge along other crystallographic directions.

The datasets generated during the current study are available under the following publicly accessible repository (see Ref. [59]) or alternatively from the corresponding authors upon reasonable request.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [59].

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