

Strain-controlled magnetic phase diagrams of the anisotropic three-dimensional Hubbard model

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Epitaxial strain provides a powerful, nonchemical route to tune the properties of functional materials by modifying the coupling between spin, charge, and lattice degrees of freedom. We investigate strain-controlled magnetic transitions within an anisotropic half-filled one-band Hubbard model in three dimensions. In this framework, strain is introduced through anisotropic hopping processes between nearest- and next-nearest-neighbor sites. Using a semiclassical Monte Carlo (s-MC) approach, we construct ground-state phase diagrams in the nonperturbative regime, which show how uniaxial hopping anisotropy stabilizes distinct magnetic ground states: Compressive strain drives a transition from a G-type to a C-type antiferromagnetic (AF) insulator, whereas tensile strain suppresses the C-type AF order, favoring an A-type AF phase. Furthermore, we examine the effect of the on-site Hubbard interaction strength (U) on these phase diagrams, revealing systematic evolution of the competing magnetic phases. Overall, our s-MC calculations emphasize that directional electronic anisotropy is a powerful tuning parameter for controlling competing magnetic orders in correlated systems, offering valuable insights for the design of strain-controlled materials.

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I. INTRODUCTION

Competing spin interactions are central to the unusual properties of correlated materials in physics [1–4]. The interplay between these interactions often leads to novel and intriguing phenomena [5–7]. Interestingly, when the strengths of these interactions are nearly balanced, the system becomes extremely sensitive to small perturbations like temperature, pressure, or strain, resulting in complex, rich phase diagrams where minor changes can trigger transitions between different magnetic phases [8,9]. This sensitivity is mostly due to the strong correspondence that exists between spin interactions and the crystal lattice. Since magnetic properties are intrinsically linked to the underlying structure, lattice distortions significantly influence magnetic behavior, directly altering exchange interactions and spin configurations [10,11]. Therefore, alterations to the crystal structure can directly impact the magnetic ground state. Understanding these coupled structural and

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magnetic transitions is crucial for advancing condensed matter physics and exploring applications in new technologies.

Materials exhibiting magnetostructural transitions, in which magnetic and lattice degrees of freedom are strongly coupled, are of considerable interest from both fundamental and applied viewpoints [12,13]. On the fundamental side, such transitions offer a well-defined framework to investigate how lattice symmetry breaking influences the magnetic ordering, electronic correlations, and exchange interactions, thereby providing valuable insights into the physics of correlated electron systems. From an applied perspective, this strong coupling enables external control of the magnetic states through strain, pressure, or temperature. This tunability is particularly promising for spintronic and memory applications, where switching between distinct magnetic states via structural modulation can enable energy-efficient, nonvolatile device operation [14]. A detailed understanding of these coupled magnetic and structural transitions is therefore crucial for advancing both fundamental condensed matter physics and functional material design.

The close connection between the lattice structure and the magnetism is clearly apparent in perovskite oxides, where chemical substitution typically causes simultaneous structural and magnetic transformations [15–17]. When a few of the ions are replaced by others of differing size or charge, the resulting chemical pressure introduces internal strain, distorting the crystal structure to accommodate the modified bonding [18,19]. These lattice distortions consequently alter interatomic distances and bond angles, directly tuning the superexchange pathways that govern magnetic ordering. A key example is $\text{Sr}_{1-x}\text{Ba}_x\text{MnO}_3$, where substituting Ba for Sr causes a progressive tetragonal distortion that strongly impacts the magnetic ground state [20,21]. At low Ba content, the nearly cubic phase exhibits a G-type antiferromagnetic (AF) order. However, as the Ba concentration rises, the increasing tetragonal distortion drives the system away from pure G-type AF order, initially resulting in a mixed antiferromagnetic-ferromagnetic phase before finally stabilizing a pure ferromagnetic (FM) order. Another significant illustration is $\text{La}_{0.2}\text{Sr}_{0.8}\text{MnO}_3$ [22–25]. This material has a nominally cubic perovskite structure and is paramagnetic (PM) above room temperature; however, local MnO_6 octahedral distortions are already present. Upon cooling, it undergoes a dramatic magnetostructural transition into a tetragonally distorted phase, which is intimately associated with the emergence of C-type AF ordering.

The same underlying principle, that lattice distortions induced by ionic-size mismatch can dictate magnetic ordering, is also evident in other Mn-based perovskites such as CaMnO_3 and CdMnO_3 . Differences in the ionic radii of Ca and Cd lead to distinct lattice symmetries and, consequently, different magnetic ground states: CaMnO_3 crystallizes in an orthorhombic perovskite structure and exhibits G-type AF ordering with $T_N \approx 123$ K [26,27], whereas CdMnO_3 , which incorporates the smaller Cd ion, is stabilized in a tetragonal perovskite lattice and displays a C-type AF ground state with a reduced $T_N \approx 86$ K [28].

Electronic instabilities, such as the Jahn-Teller effect, provide another route to structural distortion [29–31]. This effect, originating from the lifting of orbital degeneracies in transition-metal ions with partially filled d orbitals, drives spontaneous lattice distortions that lower the electronic energy. In perovskites, these distortions typically manifest as elongations or compressions of the metal-oxygen octahedra, directly coupling orbital, lattice, and spin degrees of freedom. A notable example is LaMnO_3 , where cooperative Jahn-Teller distortions of Mn^{3+} ions stabilize an orthorhombic structure at room temperature, strongly influencing its A-type AF order [32]. The principle of electronic instability driving structural change is also evident in materials like LaCoO_3 , which undergoes a phase transition from a rhombohedral structure to a cubic lattice at temperatures above approximately 1200 K, a transition often linked to spin-state changes [33].

While structural changes are naturally induced by intrinsic factors like ionic-size mismatch and electronic instabilities (e.g., the Jahn-Teller effect), epitaxial strain is one of the most commonly used extrinsic tools to modify and control material properties by driving structural phase transitions, modifying electronic bandwidth, or affecting magnetic ordering [34–40]. Specifically, when a material is grown epitaxially on a substrate with a different lattice constant, the resulting lattice mismatch generates strain that distorts the unit cell and perturbs the orbital overlap and exchange interactions

[41–43]. Hence, resulting strain can compress or elongate bond lengths and change bond angles, thereby tuning the strength and geometry of exchange interactions [44–51]. This directly affects key electronic parameters such as the hopping amplitudes and superexchange pathways, which are essential in determining the magnetic ground state [52,53].

The power of epitaxial strain in modifying bond lengths and angles, thus tuning electronic and magnetic behavior, is demonstrated across various material systems. An example of strain-controlled magnetism is found in the iridate Sr_2IrO_4 . While the bulk material shows a canted G-type AF order with Néel temperature $T_N \approx 240$ K [54], tensile strain enhances T_N , whereas compressive strain suppresses it [50,55,56]. This modulation of T_N is a direct result of strain-induced changes in the Ir–O–Ir bond angles. Similarly, EuTiO_3 , which in bulk crystallizes in a cubic perovskite structure and exhibits G-type AF ordering at low temperatures with $T_N \approx 5.6$ K [57–59], provides a demonstration of strain-driven transition. Under epitaxial strain, it undergoes a cubic-to-tetragonal distortion that weakens the AF superexchange and stabilizes a ferromagnetic order [60].

BiFeO_3 is another extensively studied example of a strain-induced magnetic transition; in this multiferroic material, strain can drive a transition between G-type and C-type AF orders [61–65]. First-principles density functional theory (DFT) studies on BiFeO_3 have explicitly demonstrated the strain-induced transition between C-type and G-type AF ordering, as well as its impact on band dispersion and optical properties [66–71]. Experimentally, these strain-driven magnetic transitions in BiFeO_3 have been realized in epitaxial thin films grown on different single-crystal substrates, where the substrate-induced lattice mismatch controls the magnitude of the strain. For example, growth on an LaAlO_3 substrate generates a large in-plane compressive strain [$\epsilon \approx -4.5\%$, with $c/a > 1$, where $\epsilon = (a_s - a_{\text{bulk}})/a_{\text{bulk}}$, a_s is the substrate (or imposed in-plane) lattice constant, and a_{bulk} is the bulk lattice constant of BiFeO_3], stabilizing a C-type AF state [72,73]. Instead, films grown on SrTiO_3 and NdScO_3 , which impose weak compressive ($\epsilon \approx -1.4\%$) and tensile ($\epsilon \approx +0.9\%$) strains, respectively, retain the bulklike G-type AF ground state, consistent with the relatively weak strain-induced exchange anisotropy in these systems [72,74,75].

Similar strain-controlled transitions have been reported in related perovskites, including BiCoO_3 [66,68] and BiCrO_3 [69,70], underscoring the broader role of strain in tuning magnetic phases. Even more intricate strain-driven phase behavior has been predicted in double perovskites: For instance, $\text{Ca}_2\text{FeOsO}_6$ transitions from a G-type ferrimagnetic phase to a C-type AF phase under compression, and further to an E-type AF phase under tensile strain [76], while $\text{Sr}_2\text{FeOsO}_6$ undergoes a C-type AF to G-type ferrimagnetic transition under epitaxial strain [77].

Such strain-induced symmetry lowering has profound consequences for both electronic and magnetic properties. It lifts degeneracies in the electronic band structure, alters the Fermi surface, and significantly influences transport behavior [39,78]. Simultaneously, lattice distortions modify interatomic distances and bond angles (particularly those involving magnetic and nonmagnetic ions such as oxygen), thereby tuning the superexchange interactions. Thus, these structural changes directly affect the strength and geometry of magnetic exchange, including both nearest-neighbor (NN) and next-nearest-neighbor (NNN) couplings [67,68]. This control over symmetry and exchange interactions is highly versatile: The specific structural transition (like a cubic-to-tetragonal distortion) can itself be triggered not only by epitaxial strain but also by other external or internal factors such as temperature, magnetic field, or chemical doping.

Despite DFT and experimental investigations, a comprehensive understanding of strain-driven magnetic phase competition across the full strain and finite-temperature regime remains incomplete. Most existing investigations have focused on specific strain windows and material realizations, leaving open important questions regarding the possible stabilization of additional magnetic phases, such as the A-type AF state under tensile strain. Moreover, the finite-temperature magnetic and transport phase behavior associated with these strain-driven transitions remains comparatively unexplored. Addressing these issues requires a microscopic theoretical framework capable of systematically capturing the interplay among electronic itinerancy, magnetic frustration, and electronic correlations over a broad range of strain, interaction strengths, and temperatures. Such a framework

is particularly relevant to correlated transition-metal oxides, where structural distortions can modify electronic hopping and magnetic exchange.

We utilize a half-filled one-band Hubbard model [79–84] as a minimal microscopic framework to investigate strain-driven magnetic phase transitions on a simple cubic lattice. Unlike conventional DFT approaches, which primarily probe ground-state properties, this model Hamiltonian framework enables a systematic investigation of finite-temperature magnetic ordering associated with strain-driven phase evolution. In our model, strain is incorporated through anisotropic NN (t_x , t_y , and t_z) and NNN (t'_{xy} , t'_{yz} , and t'_{xz}) hopping amplitudes. These direction-dependent hopping processes modify the electronic bandwidth and exchange anisotropy, thereby driving competition among multiple magnetic phases. To explore the resulting phase behavior, we systematically vary the hopping parameters and employ the semiclassical Monte Carlo (s-MC) technique [85–91] to map the finite-temperature magnetic and transport phase diagrams. In particular, we determine the evolution of the magnetic and metal-insulator transition temperatures under compressive and tensile strain. Our focus is on the nonperturbative regime, where the on-site Hubbard interaction (U) is comparable to the bare noninteracting electronic bandwidth ($W = 12$ for isotropic simple cubic lattice with $t = 1$ and $t' = 0$). Note that we use $U = 12$ throughout most of this work. Furthermore, by systematically varying U , we examine the robustness of the strain-driven magnetic phase transition and the evolution of the corresponding finite-temperature transport response.

Note that in this work, we consider an SU(2) symmetric one-band Hubbard model at half filling to study the specific role of spatial hopping anisotropy (t_z/t_x , t'_{xy} , and $t'_\perp$) in driving magnetic phase competition. While spin-orbit coupling, Dzyaloshinskii-Moriya interactions, and single-ion anisotropy can induce noncollinear spin textures in specific transition-metal oxides, we focus here on the spatially isotropic limit ($t_x = t_y = t_z$) as our base model to systematically analyze the primary role of the hopping anisotropy. Within this framework, the low-energy phase space is primarily driven by the dominant collinear ordering vectors $\mathbf{q} \in \{(\pi, \pi, \pi), (\pi, \pi, 0), (0, 0, \pi)\}$, corresponding to G-type, C-type, and A-type antiferromagnetic orders, respectively.

This paper is organized to first introduce the theoretical framework before discussing the results. We begin in Sec. II by defining the anisotropic one-band Hubbard Hamiltonian and outline the s-MC framework used to study strain-driven magnetic and transport phenomena. Details regarding the derivation of the effective Hamiltonian and the numerical procedures for computing magnetotransport observables are provided in Appendixes A and B, respectively. The results are then analyzed systematically: In Sec. III, we examine the effect of compressive strain on magnetic ordering, while Sec. IV extends the analysis to the tensile strain regime and reveals the associated reorganization of competing AF phases. In Sec. V, we further investigate the robustness of the strain-driven magnetic phase competition against variation of the on-site Hubbard interaction strength U . Finally, the key results are summarized in Sec. VI.

II. MODEL HAMILTONIAN AND COMPUTATIONAL METHOD

In order to investigate the strain-driven magnetotransport properties, we consider the following form of the one-band half-filled Hubbard Hamiltonian on a simple cubic lattice with periodic boundary conditions [82,85,92,93]:

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu \sum_i n_i = H_0 + H_I. \quad (1)$$

Here, t and t' represent the NN and NNN hopping amplitudes, respectively. $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (annihilates) an electron at site i with spin σ and $n_i (= \sum_\sigma c_{i,\sigma}^\dagger c_{i,\sigma})$ is the total number operator at site i . Furthermore, U (>0) is the on-site repulsive Hubbard interaction strength and μ is the chemical potential controlling the overall carrier density of the system. Finally, the Hamiltonian is formally split into a noninteracting quadratic part H_0 and an interaction quartic term H_I .

To make the model tractable, we decouple the H_I part using the Hubbard-Stratonovich (HS) transformation, which introduces auxiliary fields $\mathbf{m}_i$ and ϕ_i at each site. The vector field $\mathbf{m}_i$ and the scalar field ϕ_i are associated with spin and charge degrees of freedom, respectively. Next, we assume that the HS auxiliary fields are static in imaginary time and treat them as classical variables. At the saddle-point approximation, we relate the scalar auxiliary field ϕ_i to the local charge density n_i by imposing $i\phi_i = \frac{U}{2}\langle n_i \rangle$, effectively making ϕ_i proportional to the average charge density ($\langle n_i \rangle$). However, the auxiliary fields remain spatially nonuniform and experience thermal fluctuations, which are crucial for capturing finite-temperature magnetotransport phases. It is worth emphasizing that the HS transformation operates locally at each lattice site, enabling the decoupling of the on-site interaction term. Using these approximations (for details, see Appendix A), we obtain the following effective spin-fermion Hamiltonian [85–91]:

$$H_{\text{eff}} = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + \frac{U}{2} \sum_i (\langle n_i \rangle n_i - \mathbf{m}_i \cdot \boldsymbol{\sigma}_i) + \frac{U}{4} \sum_i (\mathbf{m}_i^2 - \langle n_i \rangle^2) - \mu \sum_i n_i, \quad (2)$$

where $\boldsymbol{\sigma}_i$ is the vector of Pauli matrices.

To solve the effective model, we employ the well-studied s-MC method. For any given configuration of auxiliary fields $\{\mathbf{m}_i\}$ and average charge densities $\{\langle n_i \rangle\}$, the effective Hamiltonian is initially diagonalized. The system is then simulated at a fixed temperature, where each lattice site is sequentially updated using the Metropolis algorithm to anneal the auxiliary spin fields $\{\mathbf{m}_i\}$. The system undergoes 2000 Monte Carlo sweeps (MCS) per temperature step: the first 1000 for thermal equilibration and the remaining 1000 for measuring observables. To ensure the system maintains the half-filled condition ($n = 1$), the charge densities $\{\langle n_i \rangle\}$ and the chemical potential μ are updated self-consistently every ten MCS. Physical observables are computed from 100 statistically independent equilibrium configurations, with measurements taken from every tenth configuration to reduce autocorrelation. We further average over ten independent Monte Carlo calculations starting from different initial auxiliary-field configurations. To ensure thorough equilibration, the temperature is decreased gradually from high temperatures. Furthermore, we implement the traveling-cluster approximation (TCA) [87–91, 94] using an $L_{\text{TCA}}^3 = 4^3$ update cluster that allows us to perform simulations on large system sizes, specifically $L^3 = 10^3$, which significantly helps to mitigate finite-size effects.

While the above procedure outlines the computational implementation, it is important to clarify the physical scope and limitations of the s-MC approach [85–91]. In this method, the auxiliary Hubbard-Stratonovich fields are treated as thermally fluctuating classical variables, while the fermionic sector is solved quantum mechanically through diagonalization at each Monte Carlo step. This hybrid formulation allows the method to retain the essential interplay between itinerant electrons and magnetic correlations while remaining computationally tractable for relatively large system sizes. Consequently, s-MC is particularly well suited for investigating finite-temperature magnetic ordering, transport behavior, metal-insulator transitions, and competition among multiple ordered phases in strongly correlated systems [85, 91].

The treatment of the auxiliary fields as static classical variables, while computationally advantageous, also introduces certain physical limitations. Since the auxiliary fields are treated as static classical variables without imaginary-time dynamics, quantum fluctuations of these fields are neglected [85]. As a result, the method cannot fully capture quantum coherence effects, low-temperature entanglement physics, or intrinsically quantum-disordered phases such as spin liquids. The absence of auxiliary-field quantum fluctuations may also lead to quantitative deviations at very low temperatures, including small shifts of phase boundaries and a tendency to overestimate the stability of ordered phases. Similarly, the method is not expected to accurately describe regimes

dominated by quantum critical fluctuations or excitation spectra requiring full dynamical correlations.

Compared to quantum Monte Carlo [82,95–97], which becomes severely restricted in frustrated systems due to the fermion sign problem, the s-MC approach remains sign-problem-free and can be efficiently applied to large three-dimensional lattices. Contrary to dynamical mean-field theory [93,98–100], which captures local dynamical correlations accurately but neglects nonlocal spatial fluctuations, s-MC explicitly incorporates real-space thermal fluctuations and short-range correlations. Furthermore, although methods based on tensor network [101–104] and density matrix renormalization group [105–108] provide highly accurate descriptions of low-dimensional quantum ground states, their extension to large three-dimensional systems and finite temperatures remains computationally demanding. Within this context, s-MC offers a favorable balance between computational efficiency and physical realism for studying finite-temperature phase competition in frustrated Hubbard models.

The present work focuses primarily on the strong-coupling regime at finite temperatures, where local moments are well developed and thermal fluctuations dominate over quantum fluctuations. In this regime, previous studies have demonstrated that the s-MC approach successfully reproduces several key features of the Hubbard model, including the formation of local moments, the non-monotonic evolution of T_N with interaction strength, and characteristic thermodynamic signatures observed in more computationally intensive approaches [85,87,89–91]. Therefore, although the precise numerical values of phase boundaries may be somewhat renormalized, the qualitative hierarchy of magnetic phases and the microscopic mechanism underlying strain-driven magnetic competition are expected to remain robust within the present framework.

With this computational framework in place, we next introduce the strain-dependent anisotropic hopping parameters that form the basis of our analysis. We incorporate direction-dependent hopping terms in the Hubbard model to account for the anisotropy arising from the strain in the materials, as discussed in the previous section. We subgroup the three NN hopping parameters, t_x , t_y , and t_z , corresponding to hopping along the x , y , and z directions, respectively, into two distinct groups: $t_x = t_y$ and t_z . Additionally, we include NNN hopping parameters, t'_{xy} , t'_{yz} , and t'_{xz} , corresponding to hopping in the xy , yz , and xz planes, and define $t'_\perp = t'_{yz} = t'_{xz}$. To maintain consistency across our s-MC simulations, we set $t_x = t_y = 1$ and express all other hopping parameters relative to t_x . For analyzing the effects of compressive and tensile epitaxial strain, we tune the values of t_z , t'_{xy} , and $t'_\perp$. We vary $0 \leq t_z \leq 2$, where $t_z < 1$ ($t_z > 1$) represents compressive (tensile) strain in the xy plane. For the NNN hopping terms, we consider $0 \leq t'_{xy} \leq 1$ and $0 \leq t'_\perp \leq 2$. Furthermore, the on-site repulsive Hubbard interaction strength (U), the noninteracting bandwidth (W), and the temperature (T) are measured relative to the hopping amplitude t_x . This ensures that the energy scales of the interaction and thermal effects are consistently defined relative to the hopping processes. While the anisotropic hopping parameters are motivated by strain-induced modifications of the electronic structure and magnetic exchange in correlated transition-metal oxides, the present study is not intended to provide a one-to-one material-specific description. Instead, we employ the anisotropic Hubbard model as a generic microscopic framework to systematically explore a broad parameter space and elucidate how strain-influenced anisotropic hopping drives these magnetic transitions.

To gain deeper insight into the magnetotransport properties of the system, we evaluate a range of physical observables. The magnetic behavior is characterized by calculating the local magnetic moments M and the spin structure factor $S(\mathbf{q})$, which captures quantum spin correlations. Representative magnetic spin configurations on a simple cubic lattice, characterized by distinct ordering vectors $\mathbf{q}$, are shown in Fig. 1. We also examine the temperature dependence of the specific heat C_v , looking for low-temperature peaks that signal the magnetic ordering phenomena. Transport characteristics are analyzed through the resistivity along the z direction ρ_z , defined as the inverse of the dc limit of the optical conductivity, along with the electronic density of states (DOS). A detailed description of these observables and their computational implementation is provided in Appendix B.

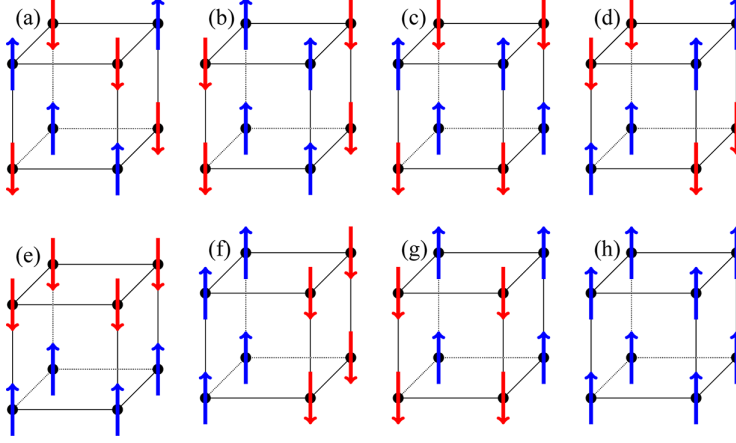


FIG. 1. Representative magnetic spin configurations on a simple cubic lattice, characterized by distinct ordering vectors $\mathbf{q}$. (a) G-type AF: Spins alternate along all three spatial directions, $\mathbf{q} = (\pi, \pi, \pi)$. (b) C-type AF($\pi, \pi, 0$): AF order in the xy planes with ferromagnetic stacking along z , $\mathbf{q} = (\pi, \pi, 0)$. (c) C-type AF($\pi, 0, \pi$): AF alignment in xz planes with ferromagnetic coupling along y , $\mathbf{q} = (\pi, 0, \pi)$. (d) C-type AF($0, \pi, \pi$): AF alignment in yz planes with ferromagnetic stacking along x , $\mathbf{q} = (0, \pi, \pi)$. (e) A-type AF($0, 0, \pi$): Spins align ferromagnetically within each xy plane, with neighboring planes stacked antiferromagnetically along the z axis; $\mathbf{q} = (0, 0, \pi)$. (f) A-type AF($0, \pi, 0$): Ferromagnetic alignment in the xz plane, with alternating spin orientation along the y axis; $\mathbf{q} = (0, \pi, 0)$. (g) A-type AF($\pi, 0, 0$): Ferromagnetic layers lie in the yz plane, coupled antiferromagnetically along the x direction; $\mathbf{q} = (\pi, 0, 0)$. (h) FM: Uniform spin alignment across the lattice, $\mathbf{q} = (0, 0, 0)$.

Before presenting the results, we explicitly verify whether the MCS performed for thermal equilibration in our s-MC simulations are sufficient to accurately calculate the physical observables. To assess the equilibration, we systematically increase the total number of MCS and examine the stability of both magnetic and thermodynamic observables for a fixed system size ($L^3 = 10^3$) and TCA cluster size ($L_{\text{TCA}}^3 = 4^3$). For each simulation, the first half of the MCS is used to ensure thermalization, while the remaining sweeps are utilized for data measurement as mentioned earlier. As shown in Fig. 2(a), the temperature dependence of the magnetic structure factor $S(\pi, \pi, \pi)$ remains consistent across different MCS values. The corresponding specific heat C_v [see the inset of Fig. 2(a)] plots also show excellent agreement with each other. Further confirmation of equilibration is provided in Fig. 2(b), where we plot the evolution of $S(\pi, \pi, \pi)$ as a function of MCS at a fixed low temperature $T = 0.05$ ($< T_N$). After an initial equilibration window of 1000 MCS, we measured average $S(\pi, \pi, \pi)$ in successive intervals (e.g., 1000–2000 MCS, then 2000–3000 MCS) using 100 statistically independent equilibrium configurations for each data point in the graph. The absence of any drift in the $S(\pi, \pi, \pi)$ value indicates that 2000 MCS (with the first 1000 for equilibration and the remaining 1000 for measurement) is sufficient for our case. Consequently, unless otherwise specified, all results presented in this work are obtained using 2000 MCS.

To ensure our conclusions are not influenced by finite-size effects, we also examine the dependence of our results on system size and TCA cluster size. By systematically varying the system size (L^3) and the TCA cluster size (L_{TCA}^3), we assess whether the extracted magnetic correlations are sensitive to the system size. As shown in Fig. 3(a), for a fixed $L_{\text{TCA}} = 4$, the temperature dependence of $S(\pi, \pi, \pi)$ exhibits only a weak dependence on lattice sizes $L^3 \geq 8^3$. This demonstrates that our choice of $L^3 = 10^3$ is sufficient and that finite-size effects do not qualitatively or quantitatively affect the extracted T_N or the nature of the magnetic order. In Fig. 3(b), we compare results obtained using different TCA cluster sizes ($L_{\text{TCA}} = 4$ versus $L_{\text{TCA}} = 6$) while keeping the system size fixed

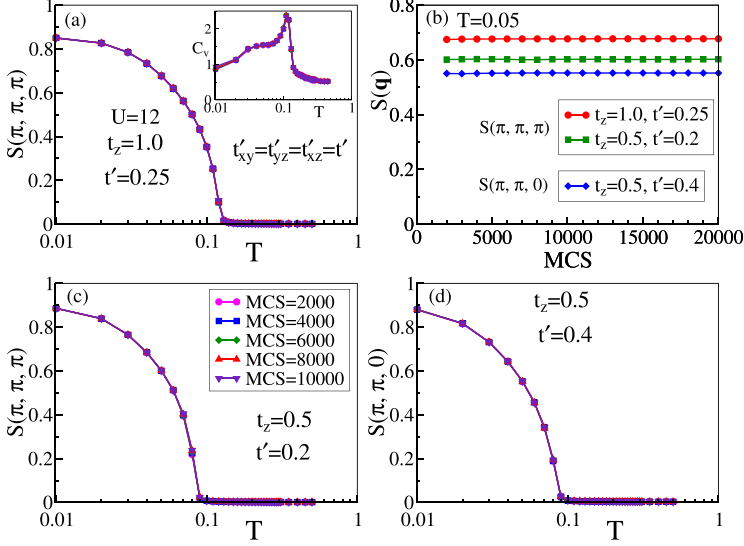


FIG. 2. MCS convergence checks at $U = 12$ (system size $L^3 = 10^3$ and TCA cluster size $L_{\text{TCA}}^3 = 4^3$). (a) Temperature dependence of $S(\pi, \pi, \pi)$ for the isotropic case ($t_z = 1$ and $t'_{xy} = t'_{yz} = t'_{xz} = 0.25$) is shown for different numbers of MCS. The value of $S(\pi, \pi, \pi)$ remains consistent at all temperatures as MCS increases. For each calculation, the first half of the total MCS is used for equilibration, while the second half is utilized for calculating observables. Inset: Temperature dependence of C_v computed using different MCS values also exhibits excellent agreement with each other. (b) Evolution of $S(\pi, \pi, \pi)$ as a function of MCS at a fixed low temperature $T = 0.05$ ($< T_N$). The first 1000 MCS are used for equilibration. Absence of any systematic drift in the subsequent measurements confirms that 2000 MCS is sufficient for our calculations. (c), (d) Temperature dependence of the relevant magnetic structure factors [$S(\pi, \pi, \pi)$ for panel (c) and $S(\pi, \pi, 0)$ for panel (d)] under compressive strain ($t_z = 0.5$) for different MCS, demonstrating a good agreement with each other. Legends are identical for panels (a), (c), and (d).

at $L^3 = 10^3$. The identical behavior of the magnetic structure factor confirms that the chosen cluster size $L_{\text{TCA}}^3 = 4^3$ accurately captures long-range magnetic correlations. These checks ensure that the magnetic phase boundaries reported in the subsequent sections are intrinsic properties of the system and not artifacts of numerical approximations.

III. EFFECT OF ANISOTROPIC HOPPING: MODELING THE COMPRESSIVE STRAIN

To uncover the microscopic evolution of magnetotransport properties under this anisotropic hopping, we examine finite-temperature observables for $U = 12$ while fixing the out-of-plane NN hopping to $t_z = 0.5$, and varying the isotropic NNN hopping t' . Note that, in a later section, we systematically vary U to investigate the robustness of the strain-driven magnetic phase transitions. The magnetic structure factors shown in Fig. 4(a) clearly distinguish the competing magnetic states. For small t' ($=0.0$ and 0.2), $S(\pi, \pi, \pi)$ exhibits a well-defined transition into a G-type AF state, with the corresponding Néel temperature T_N decreasing slightly as t' increases. This decrease reflects enhanced magnetic frustration introduced by NNN hopping, which weakens the three-dimensional AF correlations. For larger t' ($=0.4$), the magnetic correlations shift to $S(\pi, \pi, 0)$, signaling a transition from G-type AF to C-type AF($\pi, \pi, 0$) order.

The specific heat C_v curves, shown in Fig. 4(b), display sharp low-temperature peaks, which track the magnetic transitions identified in Fig. 4(a). These peaks, related to spin fluctuations, thermodynamically verify the ordering temperatures. A broad high-temperature peak, originating from charge fluctuations, persists across all t' , indicating the robust formation of local

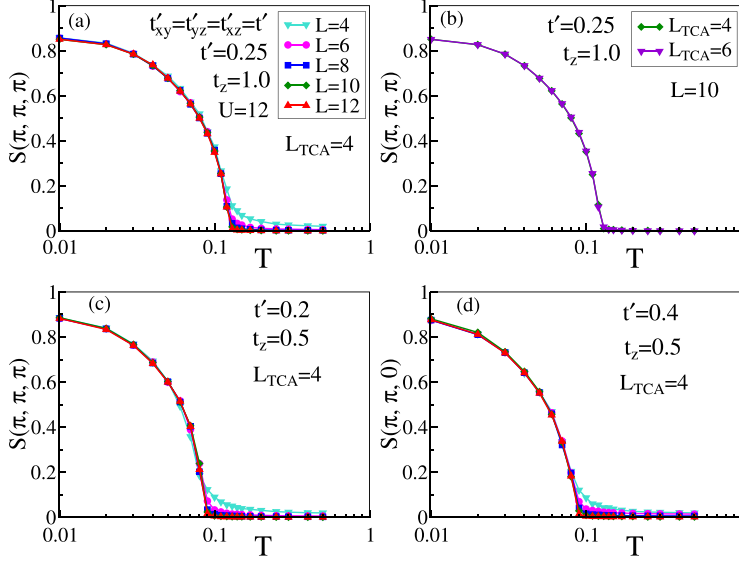


FIG. 3. Analysis of finite-size effects. (a) Temperature dependence of the G-type AF structure factor $S(\pi, \pi, \pi)$ for different system sizes L (using a fixed TCA cluster size $L_{TCA} = 4$). The results are nearly indistinguishable for $L \geq 8$, indicating that finite-size effects are negligible for our adopted 10^3 system. (b) Comparison of $S(\pi, \pi, \pi)$ obtained using different L_{TCA} for a fixed system size $L = 10$. The overlap of the data confirms that the chosen TCA cluster size ($L_{TCA}^3 = 4^3$) reliably captures long-range magnetic correlations. (c), (d) Temperature evolution of the relevant magnetic structure factors under compressive strain ($t_z = 0.5$) for various L at a fixed $L_{TCA} = 4$. The results show negligible size dependence, further confirming the stability of the observed magnetic correlations. Legends are same for panels (a), (c), and (d).

magnetic moments [109]. The temperature dependence of the local magnetic moment, M , shown in the inset of Fig. 4(c), further confirms that moments are well formed at low temperatures for all three t' values. The main panel of Fig. 4(c) shows that the resistivity along the z direction, ρ_z , remains insulating at low temperatures for all t' values, although T_{MIT} decreases slightly with increasing t' . This observed insulating behavior is consistently supported by the low-temperature DOS in Fig. 4(d), which reveals a gap around the Fermi level ($\omega = 0$). Although the gap is reduced for the C-type AF($\pi, \pi, 0$) phase ($t' = 0.4$), it remains large. As a result, both G-type AF and C-type AF($\pi, \pi, 0$) phases retain their insulating character, and the G-type AF to C-type AF transition leads only to quantitative changes in the resistivity. Consequently, both phases exhibit a qualitatively similar insulating response at low temperatures, making a clear identification of the magnetic transition via transport measurements alone highly challenging. Furthermore, we note that T_{MIT} matches well with the temperature at which the high-temperature peak in C_v appears. Importantly, T_{MIT} always exceeds T_N , which ensures the existence of a substantial PM insulator (PM-I) regime between the PM metal (PM-M) and AF insulating states.

To validate the robustness of the strain-driven magnetic transition identified in Fig. 4, we also performed a systematic analysis using increasing MCS and varying the size of system. These calculations are performed to ensure that the ordered phases stabilized under compressive strain ($t_z = 0.5$) are intrinsic properties and not artifacts of Monte Carlo sampling or finite-size effects. We focus on two representative cases: $t' = 0.2$ (G-type AF order) and $t' = 0.4$ (C-type AF order). To verify the stability of these results, we examine the temperature dependence of the magnetic structure factors as a function of the total number of MCS. In both cases, the results remain insensitive to the total MCS count, where the first half of the sweeps is utilized for equilibration

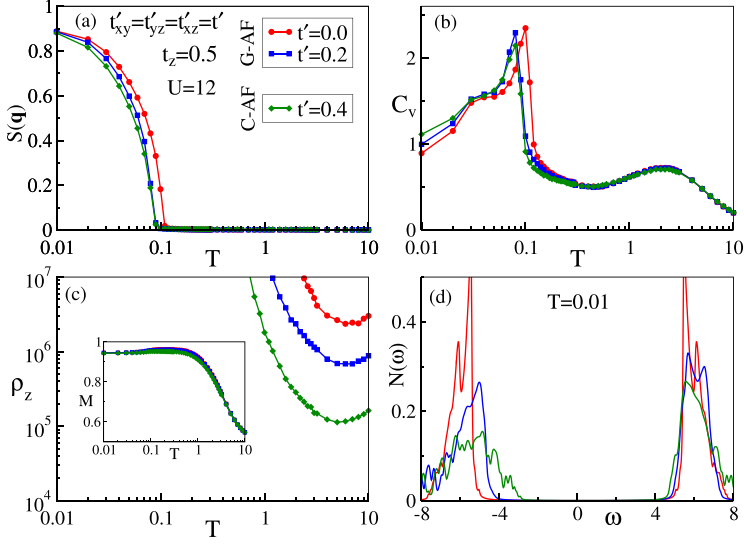


FIG. 4. Magnetic and transport properties for $t_z = 0.5$, with varying isotropic NNN hopping $t' = 0.0, 0.2$, and 0.4 ($t' = t'_{xy} = t'_{yz} = t'_{xz}$). (a) Magnetic structure factor $S(\mathbf{q})$ indicating G-type AF(π, π, π) ordering for $t' = 0$ and 0.2 and C-type AF($\pi, \pi, 0$) order at $t' = 0.4$. (b) Specific heat C_v displaying low- T peaks that align with the magnetic transitions in panel (a) and high- T peaks related to moment formation near T_{MIT} . (c) Resistivity ρ_z showing insulating behavior for all t' . Notably, $T_{\text{MIT}} \gg T_N$, leading to a PM-I regime between the PM-M and magnetically ordered phases. Inset: Temperature dependence of the local magnetic moment M , which saturates at low T , reflecting moment formation well above T_N . (d) DOS at $T = 0.01$ confirming insulating states with a finite gap at $\omega = 0$. Legends are consistent across all panels.

and the second half is used for measurements [see Figs. 2(c) and 2(d)]. Furthermore, we evaluate finite-size effects by varying the system size while keeping the total simulation length fixed at 2000 MCS. As shown in Figs. 3(c) and 3(d), the temperature dependence of the relevant magnetic structure factors exhibits only a weak dependence on the lattice size for $L^3 \geq 8^3$, confirming that finite-size effects are negligible for our adopted 10^3 system. The reproducibility of the magnetic structure factors across varying MCS and system sizes confirms that the magnetic phases inferred from Fig. 4 are numerically stable and well converged.

We now map out the $t'-T_N$ phase diagram for isotropic NNN hopping ($t'_{xy} = t'_{yz} = t'_{xz} = t'$) in Fig. 5(a). As the temperature is lowered, the system evolves from the high-temperature PM-I regime, transitioning into a G-type AF insulator for small t' but stabilizing a C-type AF($\pi, \pi, 0$) insulating state for moderate-to-large t' . Increasing t' monotonically suppresses the G-type AF ordering temperature (T_N) due to the enhanced magnetic frustration introduced by the NNN hopping. This G-type AF order persists up to $t' = 0.27$, beyond which the system stabilizes the C-type AF($\pi, \pi, 0$) phase, and T_N subsequently increases with further increments in t' . The evolution of the corresponding magnetic structure factors, $S(\pi, \pi, \pi)$ for G-type AF order and $S(\pi, \pi, 0)$ for C-type AF order, at $T = 0.01$ is shown in the inset of Fig. 5(a). For small t' , $S(\pi, \pi, \pi)$ remains large and nearly unchanged, indicating robust G-type AF order. With increasing t' , $S(\pi, \pi, \pi)$ remains stable up to $t' = 0.27$, while $S(\pi, \pi, 0)$ becomes dominant for $t' \geq 0.28$, indicating the emergence of the C-type AF($\pi, \pi, 0$) phase. Thus, increasing NNN hopping drives a sharp change in the dominant magnetic correlations from G-type AF to C-type AF($\pi, \pi, 0$) order. Based on these low-temperature magnetic structure factors, we place the phase boundary at $t' = 0.275$, between the G-type and C-type AF($\pi, \pi, 0$) phases. We use similar criterion to identify the phase boundaries throughout the phase diagrams.

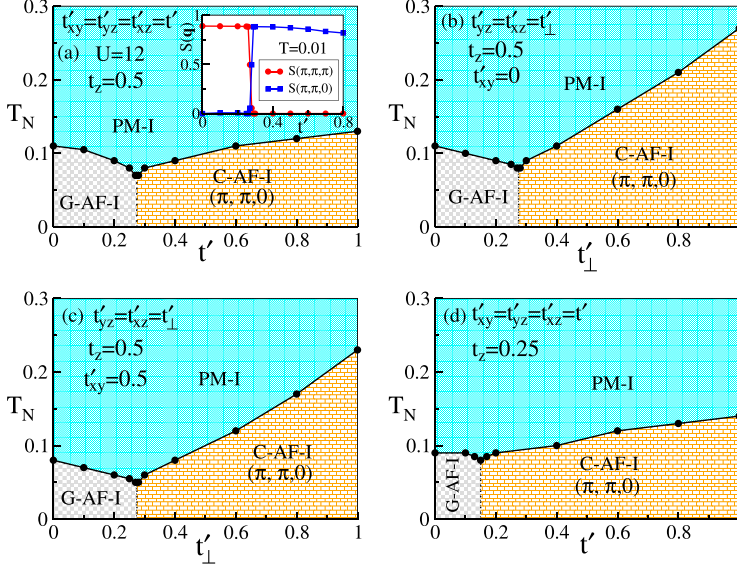


FIG. 5. (a) The t' - T_N phase diagram for isotropic NNN hopping ($t'_{xy} = t'_{yz} = t'_{xz} = t'$) at $t_z = 0.5$. Small t' favors a G-type AF insulating phase, while moderate-to-large t' stabilizes a C-type AF($\pi, \pi, 0$) insulating phase. As t' increases, T_N decreases within the G-type AF regime but increases for the C-type AF phase. Inset: Low-temperature magnetic structure factors, $S(\pi, \pi, \pi)$ and $S(\pi, \pi, 0)$, at $T = 0.01$. With increasing t' , the dominant magnetic order changes from G-type AF at $t' = 0.27$ to C-type AF($\pi, \pi, 0$) at $t' = 0.28$. For details, see the main text. The $t'_\perp$ - T_N phase diagrams ($t'_{yz} = t'_{xz} = t'_\perp$), with $t_z = 0.5$ for two in-plane NNN hoppings: (b) $t'_{xy} = 0$ and (c) $t'_{xy} = 0.5$. In both cases, increasing $t'_\perp$ drives a transition from G-type AF at small $t'_\perp$ to C-type AF($\pi, \pi, 0$) at larger values. The transition point is essentially identical to that in panel (a), suggesting the in-plane NNN hopping does not shift the transition boundary, though T_N is suppressed for $t'_{xy} = 0.5$. (d) The t' - T_N phase diagram for isotropic NNN hopping at a smaller out-of-plane hopping $t_z = 0.25$. Reducing t_z shifts the G-type AF to C-type AF($\pi, \pi, 0$) transition to lower t' values. In all cases, $T_{MIT} \gg T_N$, giving rise to a PM-I regime above T_N . The G-type and C-type AF phases are labeled as G-AF-I and C-AF-I, respectively; notably, all magnetic phases reported in this work are insulating.

Crucially, the anisotropy in the NN hopping ($t_x = t_y \neq t_z$) explicitly lifts the degeneracy of the C-type AF orders [i.e., between the $(\pi, \pi, 0)$, $(0, \pi, \pi)$, and $(\pi, 0, \pi)$ variants] that arises from cubic symmetry. Since $t_z < t_x$, the out-of-plane AF order is weaker than the in-plane AF order; consequently, only the C-type AF($\pi, \pi, 0$) configuration is stabilized in the phase diagram for large t' , while the symmetry-related $(0, \pi, \pi)$ and $(\pi, 0, \pi)$ variants are suppressed. Throughout this evolution, T_{MIT} remains higher than T_N , which maintains a broad PM-I intermediate regime, consistent with the magnetic and transport behavior reported in Fig. 4.

At this point, it is important to mention that while the isotropic t' analysis identifies the dominant role of NNN hopping in controlling the magnetic phase competition, realistic epitaxial strain environments are expected to modify the in-plane and out-of-plane NNN hopping amplitudes differently. This raises a critical question: Which NNN hopping component [the out-of-plane component ($t'_\perp = t'_{yz} = t'_{xz}$) or the in-plane component (t'_{xy})] plays the major role in driving the magnetic phase transition? To address this, we analyze the $t'_\perp$ - T_N phase diagrams for anisotropic NNN hopping configurations shown in Figs. 5(b) and 5(c). In these plots, the out-of-plane component $t'_\perp$ is varied at a fixed $t_z = 0.5$ (compressive strain) for two representative in-plane values: $t'_{xy} = 0$ [Fig. 5(b)] and $t'_{xy} = 0.5$ [Fig. 5(c)]. In both cases, increasing $t'_\perp$ drives a transition from a G-type AF state to a C-type AF($\pi, \pi, 0$) phase. Remarkably, the transition point for the G-type AF to C-type AF($\pi, \pi, 0$) is essentially identical to that found in the isotropic NNN hopping case [Fig. 5(a)]. This strongly

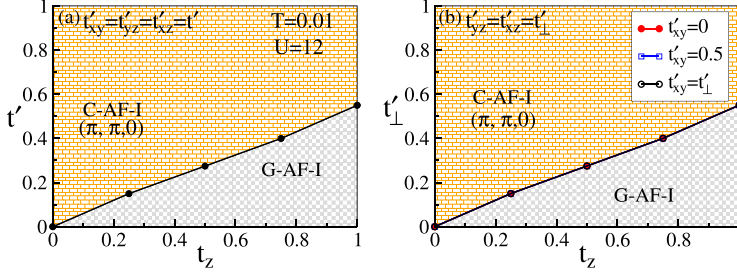


FIG. 6. (a) Low-temperature ($T = 0.01$) t_z - t' phase diagram for isotropic NNN hoppings. Increasing t' drives a transition from the G-type AF insulating state to a C-type AF($\pi, \pi, 0$) insulating state. The critical t' value increases linearly as t_z increases. (b) The t_z - $t'_\perp$ phase diagrams ($t'_y = t'_z = t'_\perp$) shown for $t'_{xy} = 0$ and $t'_{xy} = 0.5$; the isotropic NNN hopping case ($t'_{xy} = t'_\perp$) is replotted for comparison. In all cases, increasing $t'_\perp$ destabilizes the G-type AF phase in favor of C-type AF($\pi, \pi, 0$) order, while the phase boundary remains nearly independent of t'_{xy} .

suggests that the boundary is governed primarily by the out-of-plane NNN hopping $t'_\perp$ rather than the in-plane component t'_{xy} , a result that is physically viable in real systems given that the required $t'_\perp$ is around $t_z/2$ to drive this transition.

However, t'_{xy} does influence the ordering temperature: When the in-plane competition is absent ($t'_{xy} = 0$), the T_N corresponding to the C-type AF($\pi, \pi, 0$) phase grows rapidly with increasing $t'_\perp$. Conversely, when a finite in-plane NNN hopping is included ($t'_{xy} = 0.5$), the overall Néel temperature decreases across all $t'_\perp$. This confirms that the in-plane NNN hopping t'_{xy} mainly modulates the ordering temperature under compressive strain ($t_z = 0.5$).

Next, we investigate the isotropic NNN hopping case by setting the out-of-plane NN hopping to $t_z = 0.25$ to focus on the effects of stronger compressive strain. This allows us to quantify how strain shifts the balance between competing AF orders. The resulting $t'-T_N$ phase diagram is displayed in Fig. 5(d). Under these conditions, the transition from G-type AF to C-type AF($\pi, \pi, 0$) occurs at a smaller critical t' (≈ 0.15), confirming that compressive strain enhances the tendency toward C-type AF($\pi, \pi, 0$) order at much smaller t' . Similar to the behavior observed at $t_z = 0.5$, in this more extreme compressive regime ($t_z = 0.25$), the primary role of the in-plane NNN hopping, t'_{xy} , is to modulate the magnetic ordering temperature. However, crucially, t'_{xy} does not significantly control the magnetic phase transition point at low temperatures, which is predominantly controlled by the out-of-plane NNN hopping, $t'_\perp$.

The finite-temperature analysis above demonstrates that the competition between G-type AF and C-type AF($\pi, \pi, 0$) orders is strongly controlled by the strengths of both out-of-plane NN and NNN hopping amplitudes. To present the complete picture of how the low-temperature phases behave with t_z and t' , we show the t_z - t' phase diagram at a low temperature ($T = 0.01$) in Fig. 6(a). Note that, in this section, our analysis focuses only on the $t_z < t_x$ regime, which corresponds to compressive strain. As the isotropic NNN hopping t' increases, the system evolves from a G-type AF insulator to a C-type AF($\pi, \pi, 0$) insulator in the whole range. The critical t' separating these phases grows monotonically with increasing t_z , as a larger out-of-plane NN hopping t_z stabilizes AF alignment along the z axis and delays the ferromagnetic stacking required for the C-type AF($\pi, \pi, 0$) state.

Next, focusing on the relative roles of in-plane and out-of-plane NNN hopping, we show the t_z - $t'_\perp$ phase diagram at $T = 0.01$ with varying t'_{xy} in Fig. 6(b). In all cases shown ($t'_{xy} = 0$, $t'_{xy} = 0.5$, and $t'_{xy} = t'_\perp$), increasing the out-of-plane NNN hopping $t'_\perp$ destabilizes the G-type AF phase and stabilizes the C-type AF($\pi, \pi, 0$) order. Notably, the phase boundary between the G-type AF and C-type AF($\pi, \pi, 0$) order remains nearly unchanged across all three t'_{xy} values. This highlights that for $t_z < t_x$ (under compressive strain), the out-of-plane NNN hopping $t'_\perp$ is the main driver of the G-type AF to C-type AF($\pi, \pi, 0$) transition, while variations in in-plane NNN hopping t'_{xy} primarily

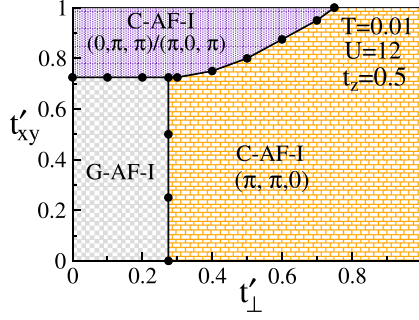


FIG. 7. The $t'_\perp$ - t'_{xy} phase diagram at $T = 0.01$ for $t_z = 0.5$ (representing compressive strain). At small t'_{xy} , increasing $t'_\perp$ drives a transition from the G-type AF insulating state to the C-type AF($\pi, \pi, 0$) insulating phase. Conversely, for large in-plane NNN hopping ($t'_{xy} \gtrsim 0.72$), a twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase is stabilized at small $t'_\perp$. Within this large- t'_{xy} regime, increasing $t'_\perp$ induces a switching between the C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] and C-type AF($\pi, \pi, 0$) phases.

influence the ordering temperature (as seen in Fig. 5). As we discuss later, this behavior changes qualitatively in the tensile strain regime, where the variation of t'_{xy} plays a crucial role in determining the magnetic states.

Finally, to present the full magnetic phase behavior across the parameter space, we show the $t'_\perp$ - t'_{xy} phase diagram in Fig. 7 for $t_z = 0.5$. Here, we varied t'_{xy} up to a value of 1 for completeness, though we acknowledge that such a large magnitude relative to t_x is highly improbable in realistic material systems. Beyond a critical, high value of t'_{xy} (~ 0.72), the twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase appears, particularly for small values of the out-of-plane NNN hopping, $t'_\perp$. Furthermore, in this high t'_{xy} regime (e.g., around $t'_{xy} \sim 0.8$), increasing $t'_\perp$ triggers a subtle intra-C-type phase transition, causing a switching of the ground state between the C-type variants: AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] and AF($\pi, \pi, 0$) phase.

Having established the strain-induced magnetic phase diagram, we now examine how the anisotropic hopping parameters influence the corresponding transport response. In particular, we focus on the in-plane (ρ_x) and out-of-plane (ρ_z) resistivities, which provide direct insight into the role of hopping anisotropy in charge transport. We first consider $t_z = 0.5$ (compressive strain) and uniform NNN hopping $t' = 0.2$ [Fig. 8(a)], which corresponds to the G-type AF phase [see Fig. 5(a)]. In this case, the metal-insulator transition temperature remains significantly higher than the magnetic ordering temperature ($T_{MIT} \gg T_N$) [for T_N , see Fig. 5(a)]. A transport anisotropy with $\rho_z > \rho_x$ is observed over the entire accessible temperature range. Since the NNN hopping is isotropic, the anisotropy originates solely from the reduced out-of-plane NN hopping ($t_z < t_x$), which suppresses charge transport along the z direction and results in a larger out-of-plane resistivity ρ_z . The finite separation between ρ_z and ρ_x persists across both the PM-M and PM-I regimes, indicating that the observed transport anisotropy is not directly associated with the G-type AF order.

To further emphasize the role of the NN hopping anisotropy, we increase t_z from 0.5 toward the isotropic limit ($t_z = 1$), as shown in the inset of Fig. 8(a). As t_z increases to 0.9, the difference between ρ_z and ρ_x is negligible, while for $t_z = 1.0$ (not shown), the two resistivity components overlap perfectly. This demonstrates that the transport anisotropy is directly controlled by the degree of hopping anisotropy and vanishes as hopping becomes isotropic. To investigate the effect of anisotropic NNN hopping, we next suppress the in-plane NNN hopping ($t'_{xy} = 0$) while keeping $t'_\perp = 0.2$ and $t_z = 0.5$, as shown in Fig. 8(b). Compared to Fig. 8(a), the separation between ρ_z and ρ_x is significantly reduced. This behavior originates from the competition between two distinct anisotropic hopping channels. While $t_z < t_x$ favors $\rho_z > \rho_x$, the anisotropic NNN hopping ($t'_\perp > t'_{xy}$) enhances charge transport along the z direction and therefore tends to favor $\rho_z < \rho_x$. The partial cancellation between these two effects leads to a weaker transport anisotropy.

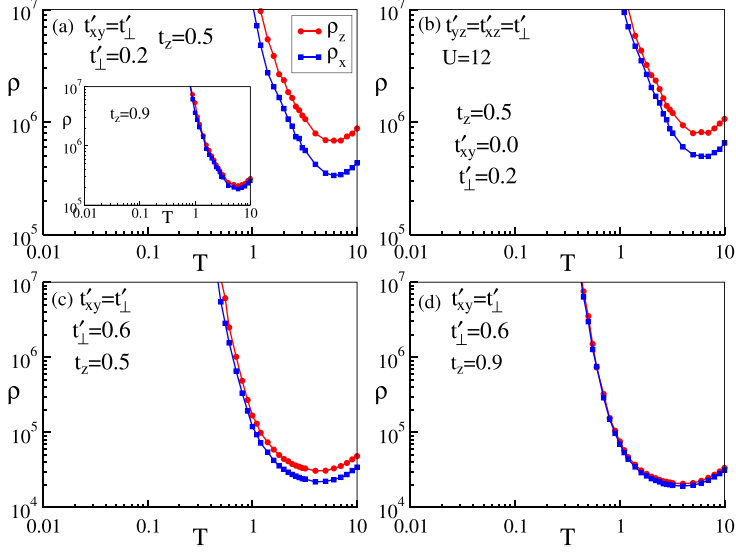


FIG. 8. Temperature evolution of the in-plane (ρ_x) and out-of-plane (ρ_z) resistivities for $U = 12$. In all cases, $T_{\text{MIT}} \gg T_N$ [for T_N , see Fig. 5(a)] and the transport response is probed entirely in the PM regime. (a) For compressive strain ($t_z = 0.5$) and isotropic NNN hopping ($t'_{xy} = t'_\perp = 0.2$), an anisotropy with $\rho_z > \rho_x$ is observed. This behavior is a direct consequence of the asymmetry in the kinetic terms, specifically that $t_z < t_x$. The inset shows that this anisotropy is suppressed as t_z increases to 0.9. (b) Anisotropic NNN hopping ($t'_{xy} = 0$, $t'_\perp = 0.2$) reduces the separation between ρ_z and ρ_x through competition between the anisotropic NN and NNN hopping channels. (c) For larger isotropic NNN hopping ($t'_{xy} = t'_\perp = 0.6$), the transport anisotropy is further reduced compared to panel (a). (d) For weaker compressive strain ($t_z = 0.9$) and $t'_{xy} = t'_\perp = 0.6$, the two resistivity components nearly overlap, indicating an almost isotropic transport response. Legends are identical in all panels.

Next, we increase the isotropic NNN hopping to $t'_{xy} = t'_\perp = 0.6$ [Fig. 8(c)], which stabilizes the C-type AF($\pi, \pi, 0$) state [for magnetic order, see Fig. 5(a)]. Although ρ_z remains larger than ρ_x , the transport anisotropy is considerably weaker than that in Fig. 8(a). Since $T_{\text{MIT}} \gg T_N$ and the transport response is only accessible well above the magnetic ordering temperature, this reduction cannot be unambiguously attributed to the change in magnetic order. Instead, it primarily reflects the enhanced electronic itinerancy introduced by the larger isotropic NNN hopping, which provides additional conduction pathways and reduces the relative influence of the anisotropic NN hopping on transport. For $t_z = 0.9$ and $t'_{xy} = t'_\perp = 0.6$, the separation between ρ_z and ρ_x is further suppressed and the two resistivity components nearly overlap over the entire temperature range, shown in Fig. 8(d). The combined effect of the larger isotropic NNN hopping and the reduced NN hopping anisotropy drives the transport response toward isotropy.

The above analysis indicates that the transport anisotropy is governed by the competition between anisotropic NN and NNN hopping channels. While the reduced out-of-plane NN hopping ($t_z < t_x$) favors $\rho_z > \rho_x$, a larger out-of-plane NNN hopping ($t'_\perp > t'_{xy}$) favors $\rho_z < \rho_x$, and the observed transport anisotropy is determined by their relative strengths. Notably, as the temperature approaches T_N , the resistivity values systematically exceed the numerical upper limit of our transport calculations. Consequently, distinguishing between these two distinct magnetic orders solely from their low-temperature transport responses remains intrinsically difficult due to the robustly insulating nature of both phases.

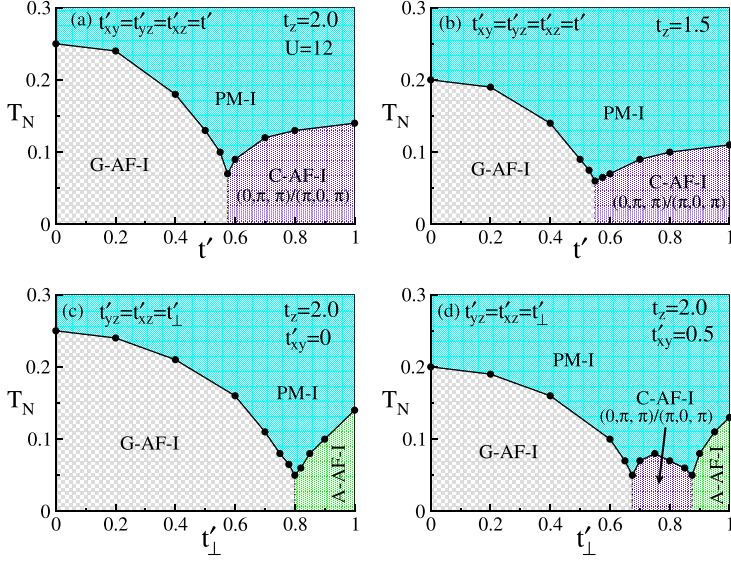


FIG. 9. Finite-temperature phase diagrams for isotropic and anisotropic NNN hoppings under tensile strain ($t_z > t_x$) at $U = 12$. (a), (b) The $t'-T_N$ phase diagrams for isotropic NNN hoppings ($t'_{xy} = t'_{yz} = t'_{xz} = t'$) at (a) $t_z = 2.0$ and (b) $t_z = 1.5$. For both t_z values, the system orders into a G-type AF insulating state at small t' , whereas larger t' stabilizes a twofold-degenerate C-type AF $[(0, \pi, \pi)/(\pi, 0, \pi)]$ insulating phase. Across the G-type AF region, T_N decreases monotonically with increasing t' , while in the C-type AF region, T_N increases with t' . Reducing t_z from 2.0 to 1.5 suppresses T_N overall, though the qualitative features of the phase diagram remain unchanged. (c), (d) The $t'_\perp-T_N$ phase diagrams for anisotropic NNN hopping ($t'_{yz} = t'_{xz} = t'_\perp$) at $t_z = 2.0$ with (c) $t'_{xy} = 0$ and (d) $t'_{xy} = 0.5$. In the absence of in-plane NNN hopping, the twofold-degenerate C-type AF $[(0, \pi, \pi)/(\pi, 0, \pi)]$ phase is fully suppressed; instead, an A-type AF $(0, 0, \pi)$ insulating phase emerges at large $t'_\perp$, and the G-type AF region expands relative to panel (a). With finite in-plane hopping ($t'_{xy} = 0.5$), the phase diagram becomes richer: The G-type AF insulating phase persists up to intermediate $t'_\perp$, followed by a narrow window of the twofold-degenerate C-type AF $[(0, \pi, \pi)/(\pi, 0, \pi)]$ phase, and finally an A-type AF $(0, 0, \pi)$ state at large $t'_\perp$. Interestingly, for $t'_{xy} = 0.5$, T_N exhibits a nonmonotonic trend within the twofold-degenerate C-type AF $[(0, \pi, \pi)/(\pi, 0, \pi)]$ region, while it continues to decrease monotonically for G-type AF and increases for A-type AF $(0, 0, \pi)$ orders. In all panels, T_{MIT} remains significantly higher than T_N , resulting in a finite-temperature PM-I regime. A-type AF $(0, 0, \pi)$ insulating phase is labeled as A-AF-I in all figures.

IV. EFFECT OF ANISOTROPIC HOPPING: MODELING THE TENSILE STRAIN

Our calculations in the previous section established that compressive epitaxial strain ($t_z < t_x$) strongly enhances the competition between two types of magnetic order, namely, G-type and C-type AF order, with NNN hopping selectively stabilizing the C-type AF $(\pi, \pi, 0)$ state; however, the magnetic competition is expected to be qualitatively modified under tensile strain ($t_z > t_x$), where the out-of-plane NN hopping becomes the dominant coupling. To determine how this balance evolves, we now examine the finite-temperature phase diagram for a representative large value, $t_z = 2.0$, at $U = 12$ and analyze its interplay with both isotropic and anisotropic NNN hopping. For isotropic NNN hopping, $t'_{xy} = t'_{yz} = t'_{xz} = t'$ [see Fig. 9(a)], the system shifts from a high-temperature PM-I phase into a low-temperature G-type AF insulator at small t' , but the low-temperature state switches to a twofold-degenerate C-type AF phase, corresponding to ordering vectors $(0, \pi, \pi)$ and $(\pi, 0, \pi)$, at large t' .

The analysis of the tensile strain regime ($t_z > t_x$) reveals three primary consequences arising from the dominant out-of-plane NN hopping. The first key finding is the overall enhancement of

T_N of the G-type AF phase, directly attributable to the large t_z that drives the AF order to higher temperatures. The second key finding is the complete absence of the C-type AF($\pi, \pi, 0$) phase [which was present in the small- t_z regime (see Fig. 5)] when t_z is large. This difference also stems from the large out-of-plane NN hopping: Since $t_z > t_x$, the NN AF coupling along the z direction becomes dominant over in-plane NN AF interactions. Consequently, the system naturally favors magnetic orders that preserve out-of-plane antiferromagnetism, leading to the stabilization of the twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase at large t' . The third key finding is that the G-type AF order persists up to significantly larger NNN hopping (t') values compared to the small- t_z case [see Fig. 5(a)]. The G-type AF phase maintains its stability over an extended intermediate range of t' due to two combined effects: the increasing influence of the NN hopping parameters with larger t_z , and the degeneracy of the competing C-type AF phase between the ($0, \pi, \pi$) and ($\pi, 0, \pi$) ordering vectors. Consistent with the small- t_z regime, T_N decreases monotonically with t' in the G-type AF phase, while it increases monotonically in the twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase. The qualitative scenario remains the same for $t_z = 1.5$, as shown in Fig. 9(b).

While the analysis of the isotropic NNN hopping case effectively demonstrates that large out-of-plane NN hopping ($t_z > t_x$) fundamentally reshapes the magnetic competition, it does not by itself identify which NNN hopping channel is responsible for this restructuring. In particular, large t_z removes the C-type AF($\pi, \pi, 0$) phase and stabilizes the twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] order at large t' , but it remains unclear whether this behavior is driven by the out-of-plane NNN hopping $t'_\perp$ or by the in-plane NNN hopping t'_{xy} . To disentangle these effects, we selectively remove the in-plane NNN hopping ($t'_{xy} = 0$) and analyze the regime where only the out-of-plane NNN hopping, $t'_\perp$, competes with the dominant out-of-plane NN hopping. Upon switching off the in-plane NNN hopping [see Fig. 9(c)], the twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase is completely suppressed, and an A-type AF($0, 0, \pi$) insulating state is stabilized instead at large $t'_\perp$. This shift is physically intuitive: The large t_z favors AF alignment between NNs along the z direction, and a large $t'_\perp$ also promotes AF alignment between NNNs along z . The resulting A-type AF($0, 0, \pi$) order accommodates both tendencies simultaneously, as spins are ferromagnetically aligned within each xy plane but alternate antiferromagnetically between adjacent planes. In this specific configuration, both out-of-plane NN and NNN bonds are antiferromagnetically satisfied, making the A-type AF($0, 0, \pi$) phase the energetically optimal solution in this regime. Notably, the G-type AF phase is also stabilized over a wider $t'_\perp$ range compared to the preceding isotropic case in Fig. 9(a).

For $t'_{xy} = 0.5$ [see Fig. 9(d)], the resulting phase diagram is significantly richer. The system exhibits a sequential transition: The G-type AF phase persists up to intermediate values of $t'_\perp$, followed by a narrow window of the twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] order, and finally transitioning to the A-type AF($0, 0, \pi$) phase at large $t'_\perp$. Within this complex landscape, T_N exhibits a nonmonotonic trend in the C-type AF region, while it continues to decrease for G-type AF and increase for A-type AF, indicating subtle competition between the different NNN couplings. The emergence of the degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] region is key, as it highlights the interplay of competing exchange channels: The presence of finite t'_{xy} introduces in-plane frustration that destabilizes the G-type AF state and promotes this intermediate C-type AF phase. Thus, the resulting phase sequence arises from two simultaneous competitions: first, the interplay between the out-of-plane NN (t_z) and NNN ($t'_\perp$) hopping, and second, the balance between the in-plane NN ($t_x = t_y$) and NNN (t'_{xy}) hopping. Crucially, these calculations demonstrate that the in-plane NNN hopping (t'_{xy}) plays a decisive role in stabilizing and modulating the magnetic orders across the phase space.

Next, we present the $t'_\perp$ - t'_{xy} phase diagram in Fig. 10, which clearly demonstrates that the complex emergence and competition of magnetic phases primarily occurs when the in-plane NNN hopping is significant ($t'_{xy} \gtrsim 0.35$). Notably, beyond a high value of t'_{xy} (~ 0.75), the twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase dominates, irrespective of the value of the out-of-plane NNN hopping, $t'_\perp$. It is important to note that such high t'_{xy} values may not be physically viable in

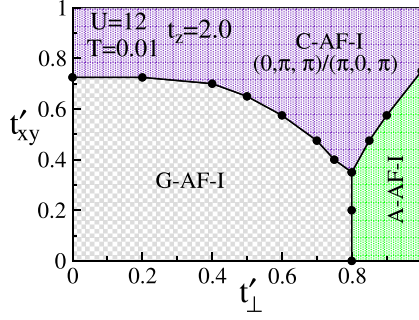


FIG. 10. The $t'_\perp$ - t'_{xy} phase diagram at $T = 0.01$ for $t_z = 2.0$ (representing tensile strain). For small t'_{xy} , the low-temperature magnetic state consists of G-type AF insulating state at small-to-moderate $t'_\perp$, followed by an A-type AF(0, 0, π) insulating state at sufficiently large $t'_\perp$ ($\gtrsim 0.8$). As t'_{xy} increases, in-plane frustration stabilizes a twofold-degenerate C-type AF[(0, π , π)/(π , 0, π)] phase over a broad parameter region.

real systems. Taken together, our calculations demonstrate that under tensile strain ($t_z = 2$), the dominance of out-of-plane NN hopping qualitatively reshapes the magnetic competition, leading to the emergence of distinct G-type, C-type, and A-type AF regimes, with the aid of t'_{xy} and $t'_\perp$, that were absent in the compressive limit (e.g., the $t_z = 0.5$ case). In comparison with the compressive strain regime ($t_z < 1$), where t'_{xy} has negligible influence on the low-temperature magnetic phase boundary (see Fig. 6), the in-plane NNN hopping plays a crucial role in determining the magnetic phase competition under tensile strain ($t_z > 1$), as will become more evident from the t_z - $t'_\perp$ phase diagrams discussed next.

Finally, for completeness, we analyze the low-temperature phase behavior over $0 \leq t_z \leq 2$ to present a unified understanding of how magnetic states evolve across the entire range of hopping, from compressive ($t_z < t_x$) to tensile ($t_z > t_x$) strain in Fig. 11. While $0 \leq t_z \leq 1$ was previously discussed, the full range is presented here for a detailed comparison across all magnetic phase transitions. The resulting low-temperature t_z - $t'_\perp$ phase diagram, where NNN hoppings are isotropic ($t'_{xy} = t'_\perp = t'$), is presented in Fig. 11(a). For any t_z , increasing $t'_\perp$, a transition from the G-type AF insulator to the C-type AF insulator is driven, as discussed earlier. Specifically, for $t_z < 1$, this C-type phase is the AF(π , π , 0), and the critical $t'_\perp$ value increases linearly with t_z . Conversely, for $t_z > 1$, the phase shifts to a doubly degenerate C-type AF[(0, π , π)/(π , 0, π)] state, and the critical $t'_\perp$ value remains nearly constant. For $t_z = 1$, the G-type AF order transitions to a threefold-degenerate C-type AF[(0, π , π)/(π , 0, π)/(π , π , 0)] phase for $t'_\perp \gtrsim 0.55$, due to the restoration of cubic symmetry in the NN and NNN hopping.

The nearly horizontal phase boundary between G-type AF and the doubly degenerate C-type AF[(0, π , π)/(π , 0, π)] phases for $t_z > 1$ arises from the underlying superexchange physics. In the strong-coupling regime, the magnetic interactions are governed by the superexchange couplings $J_z \sim t_z^2/U$ and $J' \sim t'^2/U$. Increasing t_z enhances the out-of-plane exchange interaction J_z , thereby strengthening the AF coupling along the z direction. Since both the G-type AF and the doubly degenerate C-type AF[(0, π , π)/(π , 0, π)] phases preserve antiferromagnetic alignment along the z direction, further enhancement of J_z (beyond $t_z > 1$) carries a negligible influence on the competition between these two states. As a result, the phase competition is governed primarily by t' , keeping the boundary nearly independent of t_z and leading to the flat, horizontal phase boundary observed at $t' \sim 0.55$.

We next vary the in-plane (t'_{xy}) and out-of-plane ($t'_\perp$) NNN hopping independently. For $t'_{xy} = 0$ [see Fig. 11(b)], as t_z increases, the critical $t'_\perp$ value required for the G-type to C-type transition increases linearly up to $t_z \sim 1.4$ (this was up to $t_z = 1$ for isotropic NNN hopping). Beyond $t_z \sim 1.4$, increasing $t'_\perp$ drives a transition from G-type AF to A-type AF(0, 0, π) order, where the critical $t'_\perp$ value remains nearly constant.

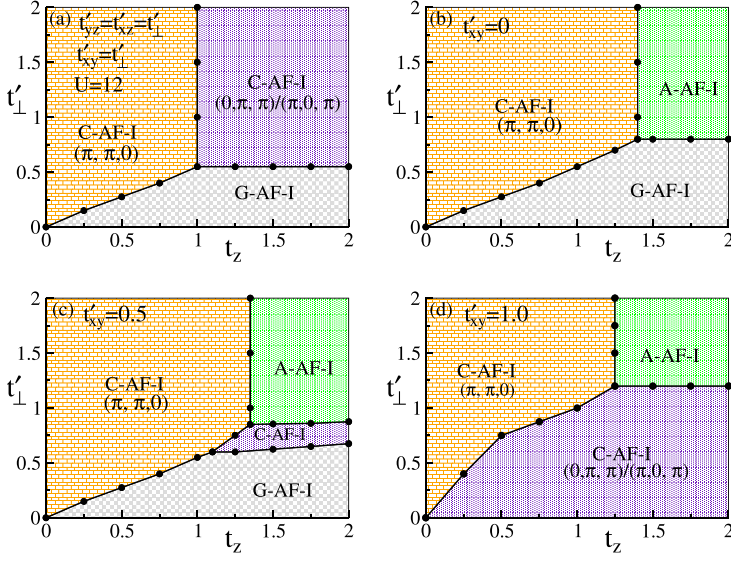


FIG. 11. The t_z - $t'_\perp$ phase diagrams at $T = 0.01$ for various t'_{xy} , illustrating the evolution of magnetic states from the compressive ($t_z < t_x$) to tensile ($t_z > t_x$) strain regimes. (a) Isotropic NNN hopping ($t'_{xy} = t'_\perp$): Increasing $t'_\perp$ (i.e., t' in this case) drives a transition from the G-type AF phase to a C-type AF phase for all t_z . For $t_z < 1$, the C-type AF($\pi, \pi, 0$) state is stabilized with a critical $t'_\perp$ that increases linearly with t_z . For $t_z > 1$, the system favors a doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase with a nearly constant critical $t'_\perp$. At $t_z = 1$, cubic symmetry is restored, and the G-type AF insulating phase transitions to a threefold-degenerate C-type AF[($\pi, \pi, 0$)/($0, \pi, \pi$)/($\pi, 0, \pi$)] insulating state for $t'_\perp \gtrsim 0.55$. (b) Anisotropic NNN hopping with $t'_{xy} = 0$: The critical out-of-plane hopping $t'_\perp$ required for the G-type AF to C-type AF($\pi, \pi, 0$) transition increases with t_z up to $t_z \sim 1.4$, beyond which an A-type AF($0, 0, \pi$) phase is stabilized at larger $t'_\perp$. (c) Moderate in-plane NNN hopping ($t'_{xy} = 0.5$): The low- t_z behavior is similar to that in panel (b); however, in the tensile strain regime, the G-type AF phase gives way first to the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase and subsequently to the A-type AF($0, 0, \pi$) phase at larger $t'_\perp$. (d) Large in-plane NNN hopping ($t'_{xy} = 1$): The doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase dominates the phase diagram, suppressing the G-type AF region and significantly reducing the stability of the A-type AF($0, 0, \pi$) phase.

Adding moderate in-plane frustration with $t'_{xy} = 0.5$ [see Fig. 11(c)] preserves the low- t_z behavior but substantially modifies the tensile-strain regime. For moderate tensile strain ($t_z \approx 1.2$), increasing $t'_\perp$ drives a two-step magnetic transition from the G-type AF phase to the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase, followed by the C-type AF($\pi, \pi, 0$) phase at larger $t'_\perp$. For stronger tensile strain ($t_z \gtrsim 1.4$), a different two-step sequence is observed: The G-type AF phase first transforms into the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase, which subsequently evolves into the A-type AF($0, 0, \pi$) phase with further increasing $t'_\perp$.

To complete our analysis of NNN hopping anisotropy, we present the results for large in-plane NNN hopping ($t'_{xy} = 1$) in Fig. 11(d). Here, the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase dominates a large portion of the phase diagram compared to the $t'_{xy} = 0.5$ case, effectively suppressing the entire G-type AF ordering region and part of the A-type AF($0, 0, \pi$) phase.

Finally, we present the evolution of the T_N as a function of the out-of-plane NN hopping t_z for different out-of-plane NNN hoppings $t'_\perp$, while fixing $t'_{xy} = 0.5$. This analysis complements the low-temperature phase diagram discussed in Fig. 11(c), which comprises all possible phases. For small and intermediate $t'_\perp$ values [Figs. 12(a) and 12(b)], T_N of the C-type AF($\pi, \pi, 0$) phase decreases with increasing t_z until it transitions to a G-type AF phase around $t_z \sim 2t'_\perp$. Upon further enhancing $t'_\perp$ to 0.75, the G-type AF phase is no longer stable at high t_z values; instead, the

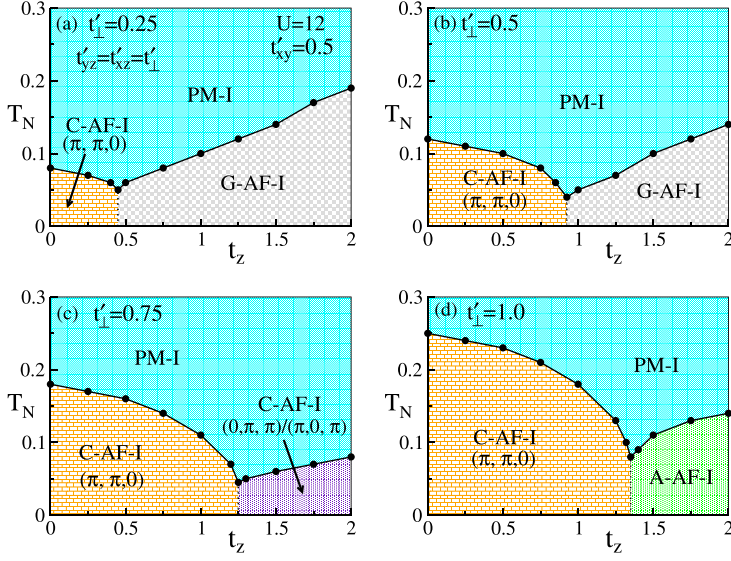


FIG. 12. The t_z - T_N phase diagrams for fixed in-plane NNN hopping $t'_{xy} = 0.5$ at various out-of-plane hoppings: (a) $t'_\perp = 0.25$, (b) $t'_\perp = 0.5$, (c) $t'_\perp = 0.75$, and (d) $t'_\perp = 1.0$. For small-to-moderate $t'_\perp$ (0.25 and 0.5), a C-type AF($\pi, \pi, 0$) phase is stabilized at low t_z ; its T_N decreases as t_z increases until a transition to the G-type AF phase occurs near $t_z \sim 2t'_\perp$. At $t'_\perp = 0.75$, the G-type AF phase is suppressed at large t_z , giving way to a twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase for $t_z \gtrsim 1.25$. In the large-hopping regime ($t'_\perp = 1.0$), an A-type AF($0, 0, \pi$) phase emerges beyond $t_z \approx 1.35$. In panels (c) and (d), T_N also decreases with t_z within the initial phase and then increases after the magnetic transition into the subsequent phase.

twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase becomes stabilized (beyond $t_z \approx 1.25$), as shown in Fig. 12(c). For a strong NNN hopping, $t'_\perp = 1$ [see Fig. 12(d)], the magnetic behavior is qualitatively distinct: The PM-I state evolves into the C-type AF($\pi, \pi, 0$) phase below $t_z \sim 1.35$, but an A-type AF($0, 0, \pi$) phase emerges above this threshold. Notably, in all cases, T_N decreases monotonically with t_z until the magnetic transition, after which it increases. Crucially, T_{MIT} consistently surpasses T_N , which ensures the existence of a stable PM-I regime at finite temperatures above the magnetically ordered phases.

V. EFFECT OF ON-SITE HUBBARD INTERACTION STRENGTH (U) ON STRAIN-DRIVEN MAGNETIC PHASES

In the preceding sections, we have primarily focused on $U = 12$ and demonstrated how compressive and tensile strain modify the magnetic properties of the system. Since the effective on-site repulsive Hubbard interaction strength U can vary significantly across different correlated materials, it is important to examine whether the strain-driven magnetic transitions obtained here remain robust against changes in U . Therefore, we now systematically investigate the evolution of the magnetic phases over a wider on-site Hubbard interaction regime. In particular, we perform a detailed finite-temperature analysis for intermediate interaction strengths $U = 9$ ($0.75W$) and $U = 6$ ($0.5W$) (where $W = 12$ denotes the noninteracting bandwidth of the system with $t_x = t_y = t_z = 1$ and $t' = 0$). We further examine the evolution of the low-temperature magnetic phase diagram across the entire interaction range to assess the robustness of the strain-driven magnetic competition.

To determine how the strain-induced magnetic phase competition evolves away from $U = 12$, we now investigate the low-temperature t_z - $t'_\perp$ phase diagrams for $U = 9$. Unlike the $U = 12$ phase diagrams, where $t'_\perp$ was explored up to 2, we restrict the present analysis to $0 \leq t'_\perp \leq 1$, which

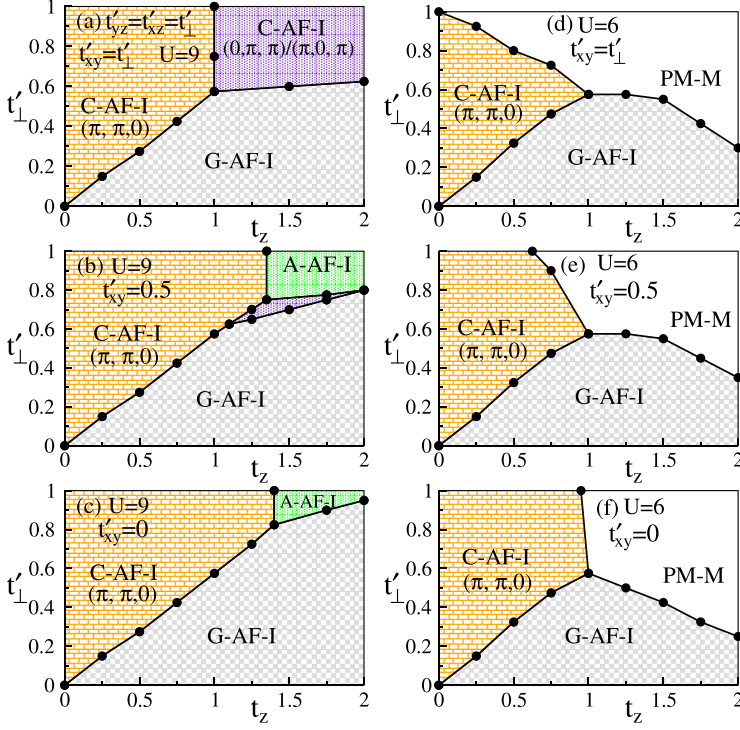


FIG. 13. Low-temperature t_z - $t'_\perp$ phase diagrams for different values of the on-site Hubbard interaction strength U and in-plane NNN hopping t'_{xy} . Panels (a)–(c) correspond to $U = 9$, while panels (d)–(f) correspond to $U = 6$. The top row [panels (a) and (d)] shows the case of uniform NNN hopping ($t'_{xy} = t'_\perp$), the middle row [panels (b) and (e)] corresponds to $t'_{xy} = 0.5$, and the bottom row [panels (c) and (f)] corresponds to $t'_{xy} = 0$. Under compressive strain ($t_z < t_x$), increasing $t'_\perp$ stabilizes the C-type AF($\pi, \pi, 0$) insulating phase in all interaction regimes. However, the tensile strain regime ($t_z > t_x$) exhibits a strong interaction dependence. For $U = 9$, tensile strain stabilizes doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] and/or A-type AF($0, 0, \pi$) insulating phases. However, for the weaker interaction strength $U = 6$, the degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] and A-type AF($0, 0, \pi$) phases are suppressed, and the G-type AF insulating phase converts to a PM-M phase with increasing $t'_\perp$.

captures the relevant magnetic phase competition. In Fig. 13(a), we consider uniform NNN hopping ($t'_{xy} = t'_\perp$) and find that the overall qualitative behavior remains similar to the $U = 12$ case shown in Fig. 11(a). As the uniform NNN hopping increases, the G-type AF phase transforms into the C-type AF($\pi, \pi, 0$) phase under compressive strain ($t_z < t_x$). On the other hand, for tensile strain ($t_z > t_x$), the G-type AF phase evolves into the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase. Importantly, all the magnetic phases remain insulating similar to $U = 12$. Compared to the $U = 12$ case, the main difference appears in the tensile strain regime ($t_z > t_x$), where the critical $t'_\perp$ required to stabilize the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase increases gradually with t_z , although slowly, instead of remaining nearly constant.

Next, we vary the in-plane (t'_{xy}) and out-of-plane ($t'_\perp$) NNN hoppings independently. For $t'_{xy} = 0.5$, increasing $t'_\perp$ under small tensile strain ($t_z \sim 1.2$) drives a two-step magnetic transition: The system first evolves from the G-type AF phase to the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase and subsequently transitions into the C-type AF($\pi, \pi, 0$) phase, as shown in Fig. 13(b). However, under larger tensile strain, an A-type AF($0, 0, \pi$) phase emerges directly at large $t'_\perp$, unlike the $U = 12$ case [see Fig. 11(c)]. Also, the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase is significantly reduced and the phase boundary separating it from the G-type AF phase becomes

t_z dependent. Finally, for $t'_{xy} = 0$, the doubly degenerate C-type AF phase completely disappears, leading to a direct G-type AF to A-type AF(0, 0, π) transition. This emphasizes the significant role of t'_{xy} under tensile strain ($t_z > 1$), unlike the compressive strain regime ($t_z < 1$), where it has little effect on the phase boundary. Moreover, unlike the nearly t_z -independent phase boundary observed for $U = 12$ [see Fig. 11(b)], the G-type AF to A-type AF(0, 0, π) phase boundary at $U = 9$ also becomes t_z dependent, indicating that a larger $t'_\perp$ is required to stabilize the A-type AF phase with increasing tensile strain.

To further examine the evolution of the strain-driven magnetic phases for the weaker interaction regime, we reduce the interaction strength to $U = 6$ and study the corresponding low-temperature t_z - $t'_\perp$ phase diagrams shown in Figs. 13(d)–13(f). Under compressive strain, the phase behavior remains qualitatively similar to the $U = 9$ [see Figs. 13(a)–13(c)] and $U = 12$ [see Figs. 11(a)–11(c)] cases, where increasing $t'_\perp$ stabilizes the C-type AF($\pi, \pi, 0$) phase over G-type AF phase. However, unlike the larger U cases, the C-type AF($\pi, \pi, 0$) phase is eventually suppressed at larger $t'_\perp$, giving rise to a PM-M phase. This C-type AF($\pi, \pi, 0$) to PM transition, particularly for $U = 6$, depends on the in-plane NNN hopping t'_{xy} : For uniform NNN hopping ($t'_{xy} = t'_\perp$), the C-type AF phase is rapidly destabilized, whereas reducing t'_{xy} suppresses the in-plane frustration and allows the C-type AF phase to remain stable over a broader range of $t'_\perp$. In comparison, the tensile strain regime undergoes a qualitative change at $U = 6$. Unlike the $U = 9$ and $U = 12$ cases, where increasing $t'_\perp$ stabilizes the doubly degenerate C-type AF or A-type AF phases, the G-type AF phase at $U = 6$ is suppressed in favor of a PM-M phase. This behavior originates from the reduced effective correlation strength, which makes the magnetic order more sensitive to the frustration induced by $t'_\perp$, particularly under tensile strain where the enhanced out-of-plane NN hopping t_z further increases the electronic itinerancy. Also note that the critical value of $t'_\perp$ required to suppress the G-type AF phase decreases systematically with increasing tensile strain.

We now turn to the temperature evolution of the strain-driven magnetic and transport properties for $U = 9$, focusing on representative compressive and tensile strain regimes with $t_z = 0.5$ and $t_z = 2.0$, respectively, as shown in Fig. 14. For the compressive strain case with uniform NNN hopping [$t'_{xy} = t'_\perp$; Fig. 14(a)], the low-temperature G-type AF insulating phase transforms into the C-type AF($\pi, \pi, 0$) insulating phase with increasing $t'_\perp$. Similar to the $U = 12$ case [see Fig. 5(a)], the magnetic transition temperature T_N remains substantially lower than T_{MIT} , leading to a broad PM-I regime at intermediate temperatures. Notably, at larger $t'_\perp$, the enhanced NNN hopping increases electronic itinerancy, causing T_{MIT} to approach T_N and thereby suppressing the intermediate PM-I regime. We next examine this effect by independently varying the in-plane NNN hopping. For $t'_{xy} = 0.5$ and 0 [Figs. 14(b) and 14(c)], the electronic itinerancy is reduced and the PM-I phase becomes more robust. The ordering temperature T_N of the C-type AF($\pi, \pi, 0$) phase increases with decreasing t'_{xy} due to the reduction of in-plane magnetic frustration, similar to the behavior observed for $U = 12$. We emphasize that, although t'_{xy} does not play a significant role in determining the low-temperature magnetic phase boundary under compressive strain ($t_z < 1$), it plays an important role in the intermediate-temperature magnetic and transport properties.

On the contrary, the tensile strain regime [$t_z = 2.0$; Figs. 14(d)–14(f)] exhibits qualitatively different behavior. For uniform NNN hopping [$t'_{xy} = t'_\perp$; Fig. 14(d)], increasing $t'_\perp$ drives a transition from the G-type AF insulating phase to the doubly degenerate C-type AF[(0, π, π)/($\pi, 0, \pi$)] insulating phase. Compared to the corresponding $U = 12$ case [Fig. 9(a)], the reduced interaction strength at $U = 9$ weakens the insulating behavior, causing T_{MIT} to approach T_N and significantly reducing the extent of the intermediate PM-I regime. For $t'_{xy} = 0.5$ [Fig. 14(e)], the doubly degenerate C-type AF[(0, π, π)/($\pi, 0, \pi$)] phase is completely suppressed and an A-type AF(0, 0, π) insulating phase emerges at large $t'_\perp$. This behavior differs from the corresponding $U = 12$ case [Fig. 9(d)], where both the doubly degenerate C-type AF and A-type AF phases remain stable. For $t'_{xy} = 0$ [Fig. 14(f)], the diagram is dominated by the G-type AF insulating phase, while only a narrow A-type AF(0, 0, π) insulating region survives at large $t'_\perp$. Compared to the corresponding $U = 12$ case [Fig. 9(c)], the stability region of the A-type AF(0, 0, π) phase is significantly reduced.

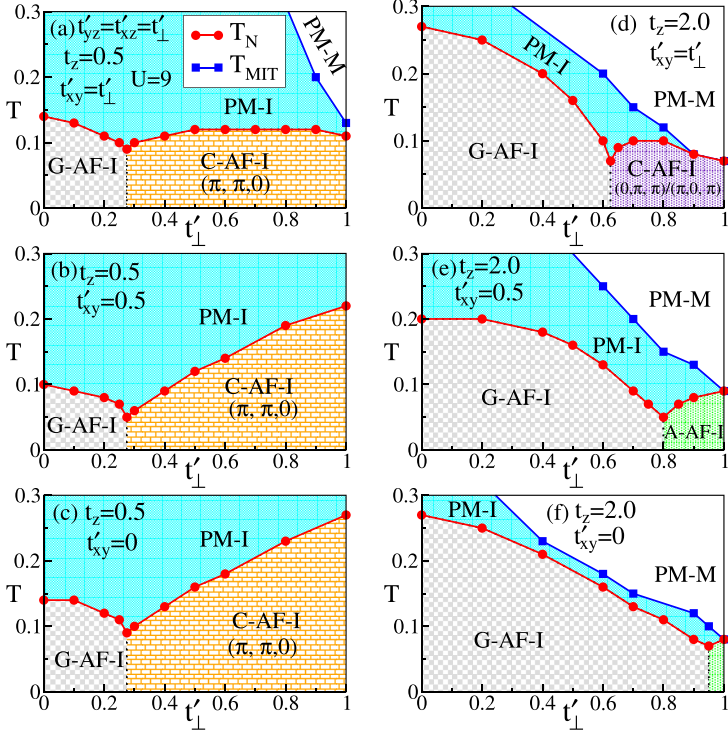


FIG. 14. The t' - T_N phase diagrams for $U = 9$ at representative compressive [$t_z = 0.5$; panels (a)–(c)] and tensile [$t_z = 2.0$; panels (d)–(f)] strain regimes. Panels (a) and (d) correspond to uniform NNN hopping ($t'_{xy} = t'_\perp$), panels (b) and (e) correspond to $t'_{xy} = 0.5$, and panels (c) and (f) correspond to $t'_{xy} = 0$. Under compressive strain, at low temperature, increasing $t'_\perp$ drives a transition from the G-type AF insulating phase to the C-type AF($\pi, \pi, 0$) insulating phase, while the intermediate-temperature region remains in PM-I phase. Conversely, at low temperature for uniform NNN hopping, tensile strain stabilizes the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] insulating phase, whereas reducing t'_{xy} suppresses the degenerate C-type AF phase and eventually stabilizes only a narrow A-type AF($0, 0, \pi$) insulating region at large $t'_\perp$. In this case, T_N and T_{MIT} become nearly comparable over a wide parameter range, leading to a strong suppression of the intermediate-temperature PM-I regime. The labeling and color scheme are identical in all panels.

Moreover, T_N and T_{MIT} become comparable over a wide parameter range, leading to a substantial narrowing of the intermediate-temperature PM-I regime.

We next investigate the temperature evolution of magnetotransport properties for interaction strength $U = 6$, as shown in Fig. 15. For the compressive strain regime [$t_z = 0.5$; Figs. 15(a)–15(c)], the system continues to exhibit a transition from the G-type AF insulating phase to the C-type AF($\pi, \pi, 0$) insulating phase with increasing $t'_\perp$ at low temperature. However, compared to the $U = 9$ case [see Figs. 14(a)–14(c)], the PM-I regime becomes considerably narrower. Furthermore, as $t'_\perp$ increases, the enhanced NNN frustration and electronic itinerancy weaken the C-type AF($\pi, \pi, 0$) order, resulting in a gradual reduction of T_N . Consequently, T_{MIT} approaches T_N , leading to the suppression of the intermediate PM-I regime. Particularly, for uniform NNN hopping [$t'_{xy} = t'_\perp$; Fig. 15(a)], both T_N and T_{MIT} are completely suppressed at large $t'_\perp$, resulting in the emergence of a low-temperature PM-M phase.

Conversely, the tensile strain regime [$t_z = 2.0$; Figs. 15(d)–15(f)] undergoes a qualitative change. Unlike the $U = 9$ [see Figs. 14(d)–14(f)] and $U = 12$ [see Fig. 9] cases, where the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] and/or A-type AF($0, 0, \pi$) phases remain stable under tensile

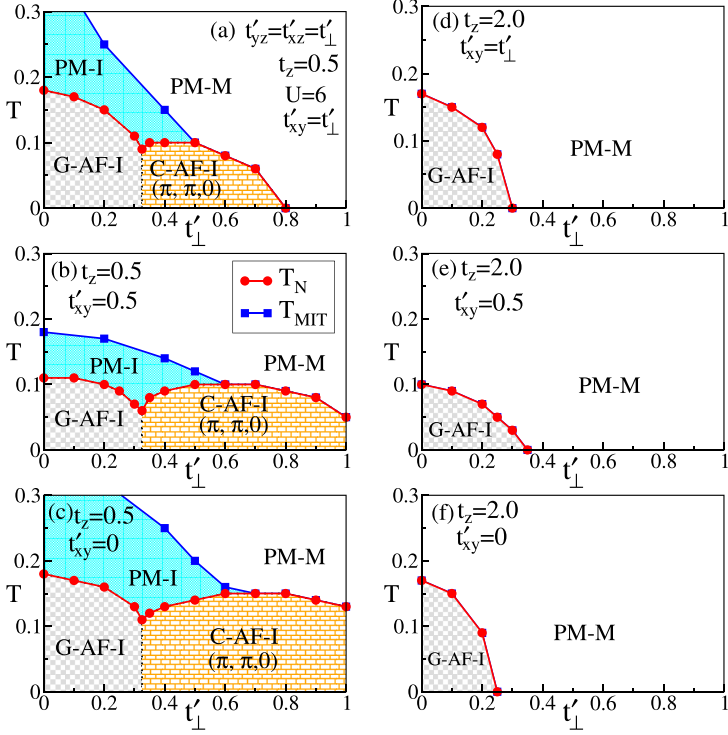


FIG. 15. The t' - T_N phase diagrams for $U = 6$ at representative compressive [$t_z = 0.5$; panels (a)–(c)] and tensile [$t_z = 2.0$; panels (d)–(f)] strain regimes. Panels (a) and (d) correspond to uniform NNN hopping ($t'_{xy} = t'_\perp$), panels (b) and (e) correspond to $t'_{xy} = 0.5$, and panels (c) and (f) correspond to $t'_{xy} = 0$. Under compressive strain, at low temperature, increasing $t'_\perp$ continues to stabilize the C-type AF($\pi, \pi, 0$) insulating phase. However, compared to the $U = 9$ case [see Fig. 14], the PM-M phase expands significantly and the PM-I regime becomes substantially narrower. However, the tensile strain regime exhibits a complete suppression of the C-type AF or A-type AF phases. The G-type AF insulating phase survives only in a small low- $t'_\perp$ region, while the PM-M phase dominates most of the phase diagram. The same legend convention is used throughout all panels.

strain, these AF phases are completely suppressed at $U = 6$. The G-type AF insulating phase survives only within a small low- $t'_\perp$ region, while the PM-M phase dominates most of the phase diagram. This demonstrates that the reduced interaction strength, combined with the enhanced bandwidth under tensile strain, strongly increases electronic itinerancy, thereby destabilizing the strain-induced AF ordered phases observed at larger U .

Finally, to present a comprehensive picture of the interplay between on-site Hubbard interaction strength and strain-induced magnetic frustration, we construct the low-temperature U - $t'_\perp$ phase diagrams for representative compressive ($t_z = 0.5$) and tensile ($t_z = 2.0$) strain regimes, as shown in Fig. 16. For the compressive strain case [$t_z = 0.5$; Figs. 16(a)–16(c)], the low-temperature phase diagrams exhibit a competition among PM-M, G-type AF insulating, and C-type AF($\pi, \pi, 0$) insulating phases as the interaction strength U and NNN hopping $t'_\perp$ are varied. At small U , increasing $t'_\perp$ suppresses the G-type AF insulating phase in favor of a PM-M phase. In particular, for $t'_{xy} = 0.5$ [Fig. 16(b)], the enhanced in-plane NNN frustration completely suppresses the G-type AF phase in the weak-coupling regime. At the same time, for moderate-to-large interaction strength, increasing $t'_\perp$ drives a transition from the G-type AF insulating phase to the C-type AF($\pi, \pi, 0$) insulating phase.

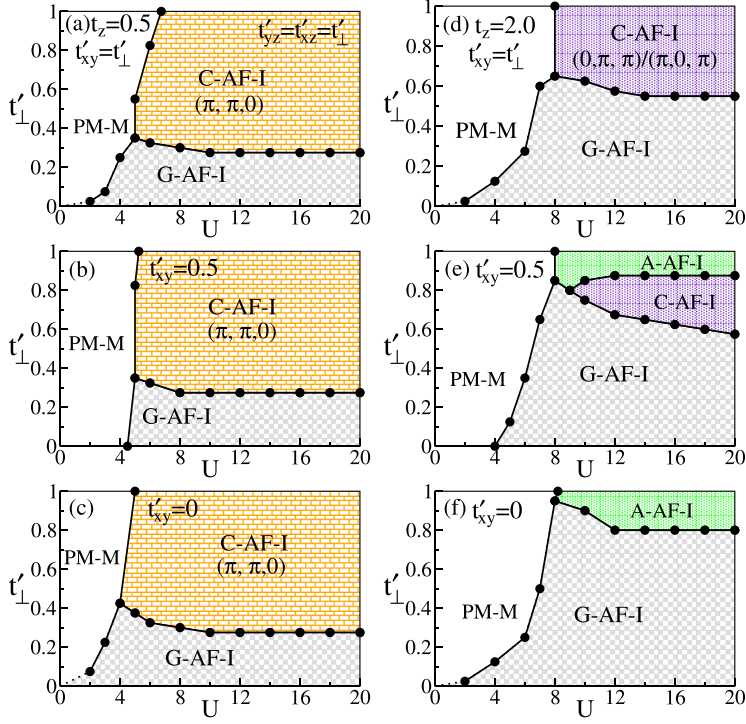


FIG. 16. Low-temperature U - $t'_\perp$ phase diagrams for representative compressive [$t_z = 0.5$; panels (a)–(c)] and tensile [$t_z = 2.0$; panels (d)–(f)] strain regimes. The top row [panels (a) and (d)] corresponds to uniform NNN hopping ($t'_{xy} = t'_\perp$), the middle row [panels (b) and (e)] to $t'_{xy} = 0.5$, and the bottom row [panels (c) and (f)] to $t'_{xy} = 0$. Under compressive strain, increasing $t'_\perp$ stabilizes the C-type AF($\pi, \pi, 0$) insulating phase over the G-type AF insulating phase at moderate-to-large interaction strength, while weak coupling favors a PM-M phase due to enhanced itinerancy. In comparison, the tensile strain regime, for uniform NNN hopping, increasing $t'_\perp$ drives a transition from the G-type AF insulating phase to the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] insulating phase. For $t'_{xy} = 0.5$, the system exhibits a sequence of transitions from G-type AF to doubly degenerate C-type AF and eventually to A-type AF($0, 0, \pi$). However, for $t'_{xy} = 0$, increasing $t'_\perp$ drives a direct transition from the G-type AF insulating phase to the A-type AF($0, 0, \pi$) insulating phase.

On the other hand, the tensile strain regime [$t_z = 2.0$; Figs. 16(d)–16(f)] exhibits qualitatively different behavior. In the weak-to-moderate U regime ($U \lesssim 8$), increasing $t'_\perp$ suppresses the G-type AF insulating phase in favor of a PM-M phase for all cases, reflecting the strong enhancement of itinerancy under tensile strain. For uniform NNN hopping [$t'_{xy} = t'_\perp$; Fig. 16(d)], increasing $t'_\perp$ at large U drives a transition from the G-type AF insulating phase to the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] insulating phase. For nonuniform NNN hopping with $t'_{xy} = 0.5$ [Fig. 16(e)], the system exhibits a sequence of magnetic transitions from the G-type AF insulating phase to the doubly degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] insulating phase and eventually to the A-type AF($0, 0, \pi$) insulating phase with increasing $t'_\perp$. Finally, for $t'_{xy} = 0$ [Fig. 16(f)], the doubly degenerate C-type AF phase disappears completely and increasing $t'_\perp$ drives a direct transition from the G-type AF insulating phase to the A-type AF($0, 0, \pi$) insulating phase. This indicates the crucial role of the in-plane NNN hopping t'_{xy} in determining the magnetic phase competition under tensile strain ($t_z > 1$), unlike the compressive strain regime ($t_z < 1$), where its influence on the low-temperature magnetic phase boundary remains limited.

VI. CONCLUSIONS

We investigated how anisotropic hopping modifies the competition among magnetic phases in a three-dimensional one-band Hubbard model using s-MC simulations. We find a systematic competition among G-type, C-type, and A-type AF states controlled by the interplay of the anisotropic hoppings. In the compressive strain regime, the G-type AF to C-type AF($\pi, \pi, 0$) phase boundary demonstrates that the out-of-plane NN and NNN hoppings (t_z and $t'_\perp$) play a dominant role in driving this transition. Furthermore, tensile strain reorganizes the AF phase landscape, ultimately stabilizing an A-type AF($0, 0, \pi$) phase as well as a twofold-degenerate C-type AF[($0, \pi, \pi$)/($\pi, 0, \pi$)] phase. We also show that the strain-driven magnetic phase competition evolves systematically with the on-site Hubbard interaction strength U . While the overall mechanism governing the strain-induced magnetic transitions remains robust, reducing U modifies the phase boundaries and qualitatively reorganizes the competing AF phases. Our study thus establishes a mechanism wherein epitaxial strain, by tuning directional hopping anisotropies, acts as a powerful tool for engineering competing AF states.

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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.

APPENDIX A: DERIVATION OF THE EFFECTIVE SPIN-FERMION HAMILTONIAN

To implement the s-MC framework, we begin by reformulating the quartic on-site interaction term in the Hubbard Hamiltonian [in Eq. (1)] using the Hubbard-Stratonovich transformation. This decoupling introduces auxiliary fields that facilitate a tractable quadratic form. First, we express the on-site interaction term as

$$n_{i,\uparrow}n_{i,\downarrow} = \frac{1}{4}n_i^2 - S_{iz}^2 = \frac{1}{4}n_i^2 - (\mathbf{S}_i \cdot \hat{\Omega}_i)^2, \quad (\text{A1})$$

where $\mathbf{S}_i = \frac{1}{2} \sum_{\alpha\beta} c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{i,\beta}$ is the spin operator at site i (with $\hbar = 1$) and $\boldsymbol{\sigma}$ denotes the Pauli matrices. The arbitrary unit vector $\hat{\Omega}_i$ appears due to SU(2) symmetry, allowing rotational invariance: $S_{ix}^2 = S_{iy}^2 = S_{iz}^2 = (\mathbf{S}_i \cdot \hat{\Omega}_i)^2$ for any $\hat{\Omega}_i$.

The partition function for the Hamiltonian stated in Eq. (1) is defined as $Z = \text{Tr}[e^{-\beta H}]$, with the trace taken over all particle numbers and site occupations. The inverse temperature is $\beta = 1/T$, and we set $k_B = 1$. To evaluate Z numerically, we discretize the imaginary-time interval $[0, \beta]$ into M steps of width $\Delta\tau$ such that $\beta = M\Delta\tau$ and apply a first-order Suzuki-Trotter decomposition:

$$e^{-\beta(H_0+H_I)} \approx (e^{-\Delta\tau H_0} e^{-\Delta\tau H_I})^M + \mathcal{O}(\Delta\tau^2). \quad (\text{A2})$$

Using Eq. (A1), the interaction term at a single time slice l can be decoupled into a path integral over scalar and vector auxiliary fields:

$$\int d\phi_i(l) d\Delta_i(l) d^2\Omega_i(l) \exp \left[-\Delta\tau \sum_i \left\{ \frac{\phi_i^2(l)}{U} + i\phi_i(l)n_i + \frac{\Delta_i^2(l)}{U} - 2\Delta_i(l)\hat{\Omega}_i(l) \cdot \mathbf{S}_i \right\} \right], \quad (\text{A3})$$

where $\phi_i(l)$ and $\Delta_i(l)$ are the auxiliary fields for charge and spin density, respectively. We define a vector auxiliary field $\mathbf{m}_i(l) = \Delta_i(l)\hat{\Omega}_i(l)$ to simplify notation. The full partition function becomes

$$Z \propto \text{Tr} \prod_{l=M}^1 \int d\phi_i(l) d^3\mathbf{m}_i(l) \exp \left[-\Delta\tau \left\{ H_0 + \sum_i \left(\frac{\phi_i^2(l)}{U} + i\phi_i(l)n_i + \frac{\mathbf{m}_i^2(l)}{U} - 2\mathbf{m}_i(l) \cdot \mathbf{S}_i \right) \right\} \right]. \quad (\text{A4})$$

At this stage, the formulation is exact, preserving full SU(2) spin symmetry, with auxiliary fields depending on both space and imaginary time.

To make the problem computationally feasible within the s-MC approach, we adopt two approximations: (1) We drop the imaginary-time dependence of the auxiliary fields, treating ϕ_i and $\mathbf{m}_i$ as classical fields; and (2) we fix the charge field to its saddle-point value, $i\phi_i = \frac{U}{2}\langle n_i \rangle$. With a rescaling $\mathbf{m}_i \rightarrow \frac{U}{2}\mathbf{m}_i$, we obtain the following effective Hamiltonian:

$$H_{\text{eff}} = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + \frac{U}{2} \sum_i (\langle n_i \rangle n_i - \mathbf{m}_i \cdot \boldsymbol{\sigma}_i) + \frac{U}{4} \sum_i (\mathbf{m}_i^2 - \langle n_i \rangle^2) - \mu \sum_i n_i, \quad (\text{A5})$$

as presented earlier in Eq. (2). The resulting spin-fermion model describes itinerant electrons interacting with classical auxiliary fields $\{\mathbf{m}_i\}$, which are sampled using Monte Carlo techniques.

APPENDIX B: DEFINITIONS OF PHYSICAL OBSERVABLES

To characterize the magnetic and transport properties of the system, we compute several observables, including the magnetic structure factor, local magnetic moment, specific heat, density of states, and resistivity. These quantities serve as key indicators of phase transitions and ordering tendencies within the spin-fermion model governed by Eq. (2).

Magnetic correlations. The magnetic ordering is quantified using the spin structure factor $S(\mathbf{q})$, which captures long-range spin correlations. It is defined as

$$S(\mathbf{q}) = \frac{1}{(L^3)^2} \sum_{k,l} \langle \mathbf{S}_k \cdot \mathbf{S}_l \rangle e^{-i\mathbf{q} \cdot (\mathbf{r}_k - \mathbf{r}_l)}, \quad (\text{B1})$$

which is measured in units of $\hbar^2$. $\mathbf{S}_k$ denotes the spin operator at site k and the angular brackets indicate combined quantum and thermal averages. The sum runs over all pairs of lattice sites on a system of volume L^3 , where L is the length of the sides of the simple cubic lattice. Within the parameter space investigated, we find only the commensurate wave vectors corresponding to the G-, C-, and A-type AF states; no additional incommensurate magnetic ordering vectors are found. Specifically, $\mathbf{q} = (\pi, \pi, \pi)$ corresponds to G-type AF order; $\mathbf{q} = (\pi, \pi, 0)$, $(0, \pi, \pi)$, and $(\pi, 0, \pi)$ correspond to the three symmetry-related C-type AF orders; and $\mathbf{q} = (0, 0, \pi)$, $(\pi, 0, 0)$, and $(0, \pi, 0)$ correspond to the three symmetry-related A-type AF orders. These characteristic ordering wave vectors are illustrated in Fig. 1.

Local moment. The local magnetic moment M is defined as the average of the square of quantum magnetization:

$$M = \langle (n_\uparrow - n_\downarrow)^2 \rangle = \langle n \rangle - 2\langle n_\uparrow n_\downarrow \rangle, \quad (\text{B2})$$

and is measured in units of $\hbar^2$. $\langle n \rangle = \langle n_\uparrow + n_\downarrow \rangle$ is the average electron density of the system. At half filling ($\langle n \rangle = 1$), the moment is bounded between $M = 0.5$ (uncorrelated or high-temperature limit) and $M = 1$ (large coupling $U \rightarrow \infty$, where double occupancy vanishes). Thus, the evolution of M with temperature and interaction strength provides insight into local moment formation.

Specific heat. The specific heat C_v is computed as the derivative of the total energy with respect to temperature:

$$C_v = \frac{dE}{dT}. \quad (\text{B3})$$

Here, E includes contributions from both fermionic degrees of freedom (quantum energy) and the classical auxiliary fields (classical energy). Numerically, we evaluate C_v using central difference scheme.

Density of states. To probe the electronic spectrum, we calculate the DOS, defined as

$$N(\omega) = \sum_{i=1}^{2L^3} \delta(\omega - \omega_i), \quad (\text{B4})$$

where ω_i are the eigenvalues of the effective Hamiltonian in Eq. (2). In practice, the δ function is replaced by a Lorentzian with a broadening of $\sim W/(2L^3)$, where W denotes the bandwidth of the noninteracting model. The factor $2L^3$ corresponds to the total number of single-particle states. The Fermi energy is taken to be at $\omega = 0$ in all spectral analyses.

Resistivity. Transport properties are evaluated via the dc limit of the optical conductivity, which is computed using the Kubo-Greenwood formula [94,110]:

$$\sigma_z(\omega) = \frac{\pi e^2}{L^3 \hbar a_0} \sum_{\alpha, \beta} (n_\alpha - n_\beta) \frac{|f_{\alpha\beta}^z|^2}{\omega_\beta - \omega_\alpha} \delta(\omega - (\omega_\beta - \omega_\alpha)), \quad (\text{B5})$$

where a_0 is the lattice parameter and we have expressed σ_z in units of $\frac{e^2}{\hbar a_0}$. $n_\alpha = \mathcal{F}(\mu - \omega_\alpha)$ is the Fermi-Dirac distribution and $f_{\alpha\beta}^z = \langle \psi_\alpha | J_z | \psi_\beta \rangle$ denotes the current matrix element along the z direction. The current operator along the z direction is defined as

$$J_z = i a_0 \sum_{i, \sigma} t_z (c_{i, \sigma}^\dagger c_{i+a_0 \hat{z}, \sigma} - \text{H.c.}) + t'_{xz} (c_{i, \sigma}^\dagger c_{i+a_0 \hat{z}+a_0 \hat{x}, \sigma} - \text{H.c.}) + t'_{yz} (c_{i, \sigma}^\dagger c_{i+a_0 \hat{z}+a_0 \hat{y}, \sigma} - \text{H.c.}).$$

The eigenvalues ω_α and corresponding eigenstates ψ_α are obtained from diagonalizing H_{eff} . The dc conductivity (along the z axis) σ_{dc}^z is estimated by integrating $\sigma_z(\omega)$ over a small low-frequency interval:

$$\sigma_{\text{dc}}^z = \frac{1}{\Delta\omega} \int_0^{\Delta\omega} \sigma_z(\omega) d\omega. \quad (\text{B6})$$

The parameter $\Delta\omega$ is chosen to be approximately 4–5 times larger than the system's average finite-size gap, which is estimated as the total bandwidth divided by the number of eigenvalues. The resistivity along the z direction is defined as $\rho_z = 1/\sigma_{\text{dc}}^z$.

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