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[Satoru Hayami](#)*

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Article

Transitions from Coplanar Double- Q to Noncoplanar Triple- Q States Induced by High-Harmonic Wave-Vector Interaction

Satoru Hayami 

Graduate School of Science, Hokkaido University, Sapporo 060-0810, Japan; hayami@phys.sci.hokudai.ac.jp

Abstract

We theoretically investigate topological transitions between coplanar and noncoplanar magnetic states in centrosymmetric itinerant magnets on a square lattice. A canonical effective spin model incorporating bilinear and biquadratic exchange interactions at finite wave vectors is analyzed to elucidate the emergence of multiple- Q magnetic orders. By taking into account high-harmonic wave-vector interactions, we demonstrate that a coplanar double- Q spin texture continuously evolves into a noncoplanar triple- Q state carrying a finite scalar spin chirality. The stability of these multiple- Q states is examined using simulated annealing as a function of the relative strengths of the high-harmonic coupling, the biquadratic interaction, and the external magnetic field. The resulting phase diagrams reveal a competition between double- Q and triple- Q states, where the noncoplanar triple- Q phase is stabilized through the cooperative effect of the high-harmonic and biquadratic interactions. Real-space spin textures, spin structure factors, and scalar spin chirality distributions are analyzed to characterize the distinct magnetic phases and the topological transitions connecting them. These findings provide a microscopic framework for understanding the emergence of noncoplanar magnetic textures driven by the interplay between two- and four-spin interactions in centrosymmetric itinerant magnets.

Keywords: multiple- Q state; scalar spin chirality; multi-spin interaction; itinerant magnets; magnetic frustration; square lattice

1. Introduction

Magnetic systems exhibiting noncollinear or noncoplanar spin arrangements have attracted tremendous attention due to their rich variety of emergent phenomena, including unconventional transport responses, complex spin dynamics, and topologically protected magnetic textures [1–8]. Such spin configurations often arise from the superposition of multiple spin density waves, giving rise to so-called multiple- Q states, in which competing exchange interactions and crystalline symmetry determine the relative phases and amplitudes of the constituent ordering wave vectors. Depending on the lattice geometry, a wide variety of multiple- Q spin textures have been realized in triangular [9–16], square [17], cubic [18], kagome [19,20], honeycomb [21,22], and Shastry-Sutherland lattices [23].

A particularly prominent manifestation of multiple- Q order is the formation of skyrmion and vortex crystals with a finite scalar spin chirality, which acts as an emergent magnetic field for conduction electrons [24–28]. This emergent field gives rise to the topological Hall effect and other anomalous transport phenomena [29–37]. Such noncoplanar magnetic lattices have been identified in a wide class of materials, including the chiral magnetic compound MnSi [38–45] and other B20-type compounds [46–54], where the Dzyaloshinskii-Moriya (DM) interaction [55,56] plays a central role in stabilizing multiple- Q skyrmion crystals [57–59]. Beyond these chiral systems, similar noncollinear and noncoplanar states have also been discovered in centrosymmetric itinerant magnets such as Gd₂PdSi₃ [60–65], Gd₃Ru₄Al₁₂ [66–69], and GdRu₂Si₂ [70–74], where nontrivial multiple- Q spin textures emerge from competing exchange interactions [75–78], sublattice-dependent DM interactions [79,80], and bond-dependent magnetic anisotropies [81–85].

In itinerant magnets, the emergence of such complex spin textures can be traced back to the momentum-space structure of conduction electrons. The geometry of the Fermi surface determines the momentum-dependent spin exchange interaction, and nesting dictated by symmetry-related wave vectors enhances spin susceptibility at those wave vectors [86,87]. When several nesting vectors become degenerate due to crystal symmetry, the system tends to develop multiple- Q magnetic instabilities, giving rise to noncollinear and noncoplanar textures even without relativistic spin-orbit coupling [14,15]. This mechanism provides a purely electronic route to complex magnetic order, distinct from DM-driven mechanisms in noncentrosymmetric systems, and directly links Fermi-surface topology to emergent spin structures and transport phenomena.

To capture these Fermi-surface-driven instabilities, effective spin models with bilinear and biquadratic exchange interactions have been developed [88]. The biquadratic interaction, originating from higher-order spin correlations mediated by conduction electrons, plays a crucial role in stabilizing noncoplanar spin configurations such as the four-sublattice triple- Q state on the triangular lattice [14]. More recently, the inclusion of high-harmonic wave-vector interactions—arising from a similar Fermi-surface instability mechanism—has been shown to further stabilize multiple- Q states, including double- Q square skyrmion crystals [89–91]. These interactions can drive the transformation from collinear or coplanar spin configurations to noncoplanar ones with a finite scalar spin chirality, even in centrosymmetric itinerant magnets.

Motivated by these developments, in this work, we theoretically investigate the topological transition between coplanar and noncoplanar magnetic states in itinerant magnets by focusing on the role of high-harmonic wave-vector two-spin interaction as well as the four-spin one. We construct and analyze a canonical effective spin model on a square lattice that includes bilinear and biquadratic exchange interactions at finite ordering wave vectors, supplemented by additional higher-harmonic interactions. Through simulated-annealing calculations, we establish the phase diagrams under zero and finite magnetic fields, elucidating how the interplay among these competing interactions dictates the stability and transformation of multiple- Q magnetic states. The results demonstrate that the noncoplanar triple- Q phase is stabilized cooperatively by the combined action of the high-harmonic and biquadratic couplings, whereas coplanar double- Q states dominate when such coupling is weak. By analyzing real-space spin configurations, spin structure factors, and scalar spin chirality distributions, we elucidate the microscopic mechanism through which momentum-space interactions give rise to noncoplanar spin textures in centrosymmetric itinerant systems.

The rest of this paper is organized as follows. Section 2 presents the effective spin model originating from the Kondo lattice Hamiltonian and outlines the simulated annealing approach used to obtain the ground-state spin configurations. Section 3 discusses the results in three parts: Section 3.1 examines the system without the biquadratic interaction, Section 3.2 explores the effect of the biquadratic term and the resulting phase diagram, and Section 3.3 analyzes the influence of an external magnetic field on the multiple- Q states. Finally, Section 4 summarizes the main conclusions and implications of this study.

2. Model and Method

We consider the Kondo lattice model on a two-dimensional square lattice under the D_{4h} symmetry, which serves as a prototypical framework for studying itinerant magnetism in centrosymmetric metals. The model describes conduction electrons coupled to localized classical spins S_i with $|S_i| = 1$, and is expressed as

$$\mathcal{H}_{\text{KLM}} = - \sum_{i,j,\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + J_K \sum_{i,\sigma,\sigma'} c_{i\sigma}^\dagger \sigma_{\sigma\sigma'} \cdot S_i c_{i\sigma'}, \quad (1)$$

where $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) denotes the creation (annihilation) operator of an itinerant electron with spin σ at site i , t_{ij} is the hopping amplitude between i th and j th sites, and J_K represents the exchange coupling between itinerant electron spins and localized moments. Because the triangular lattice preserves

inversion symmetry, no antisymmetric spin-orbit coupling leading to the DM interaction appears in this Hamiltonian.

In the weak-coupling regime where J_K is much smaller than the electronic bandwidth, the conduction electron degrees of freedom can be integrated out, resulting in a spin-only effective Hamiltonian with long-range multi-spin interactions [14,15]. Up to fourth order in J_K , the effective Hamiltonian is written as

$$\mathcal{H} = - \sum_q J_q \mathbf{S}_q \cdot \mathbf{S}_{-q} + \frac{1}{N} \sum_{q_1, q_2, q_3, q_4} K_{q_1, q_2, q_3, q_4} \delta_{q_1+q_2+q_3+q_4, G} \times [(\mathbf{S}_{q_1} \cdot \mathbf{S}_{q_2})(\mathbf{S}_{q_3} \cdot \mathbf{S}_{q_4}) + (\mathbf{S}_{q_1} \cdot \mathbf{S}_{q_4})(\mathbf{S}_{q_2} \cdot \mathbf{S}_{q_3}) - (\mathbf{S}_{q_1} \cdot \mathbf{S}_{q_3})(\mathbf{S}_{q_2} \cdot \mathbf{S}_{q_4})], \quad (2)$$

where $\mathbf{S}_q$ is the Fourier component of the localized spin $\mathbf{S}_i$, N is the total number of lattice sites, and G is a reciprocal-lattice vector. The first term represents the bilinear exchange interaction proportional to J_K^2 , which corresponds to the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [92–94], while the second term arises from the fourth-order perturbation in J_K and corresponds to the effective four-spin interaction proportional to J_K^4 . Because inversion symmetry forbids antisymmetric spin-orbit coupling, the DM and the bond-dependent anisotropic interactions do not appear in this model [95].

To capture the essential physics of multiple- Q magnetic instabilities, we focus on the situation where the dominant interactions appear at the symmetry-related wave vectors $\mathbf{Q}_1 = (\pi, 0)$ and $\mathbf{Q}_2 = (0, \pi)$ to satisfy the fourfold rotational symmetry of the square-lattice system. Such a situation can be achieved by considering appropriate hopping parameters and the chemical potential μ . For example, by taking $t_1 = 1$ (t_1 is the nearest-neighbor hopping) and $\mu = -2$, the susceptibility of itinerant electrons that corresponds to the interaction J_q is maximized at $\mathbf{Q}_1$ and $\mathbf{Q}_2$, owing to the presence of the partial nesting of the Fermi surfaces [15]. Retaining only the contributions from two wave-vector points, the effective Hamiltonian simplifies to

$$\mathcal{H}_{\text{eff}} = -J \sum_{\nu} \mathbf{S}_{\mathbf{Q}_{\nu}} \cdot \mathbf{S}_{-\mathbf{Q}_{\nu}} + \frac{K}{N} \sum_{\nu} (\mathbf{S}_{\mathbf{Q}_{\nu}} \cdot \mathbf{S}_{-\mathbf{Q}_{\nu}})^2. \quad (3)$$

where $\nu = 1, 2$ labels the two ordering wave vectors. The first term describes the RKKY interaction with the coupling constant J , while the second term represents the biquadratic interaction with the coupling constant K . For the latter, we consider the most dominant contribution among the four-spin interactions that works on the same ordering wave vectors [14,15]. The energy unit is set by $J = 1$. In the absence of the four-spin interactions ($K = 0$), the ground-state spin configuration is degenerate between single- Q and double- Q structures, as detailed below. This type of effective spin Hamiltonian has been used to explore unconventional multiple- Q states discovered in itinerant electron systems [96–98] and reproduce the experimental phase diagram, including multiple- Q states, as found in $\text{Y}_3\text{Co}_8\text{Sn}_4$ [99], EuPtSi [100], and EuNiGe_3 [101].

In addition to the Hamiltonian in Equation (3), we consider additional contributions at high-harmonic wave vectors $\mathbf{Q}_3 = \mathbf{Q}_1 + \mathbf{Q}_2$ as follows:

$$\mathcal{H}_{\mathbf{Q}_3} = -J_{\mathbf{Q}_3} \mathbf{S}_{\mathbf{Q}_3} \cdot \mathbf{S}_{-\mathbf{Q}_3}. \quad (4)$$

It is noted that $\mathbf{Q}_3$ is not symmetry related to $\mathbf{Q}_1$ and $\mathbf{Q}_2$, which indicates that the coupling constant $J_{\mathbf{Q}_3}$ is different from J ; we set $J_{\mathbf{Q}_3} = \gamma J$ for $\gamma \leq 1$. We ignore the biquadratic interaction at $\mathbf{Q}_3$ for simplicity. The ordering wave vectors we consider in the present study are presented in Figure 1. We show that such a high-harmonic wave-vector interaction can lead to the instability toward noncoplanar triple- Q ordering in the following section.

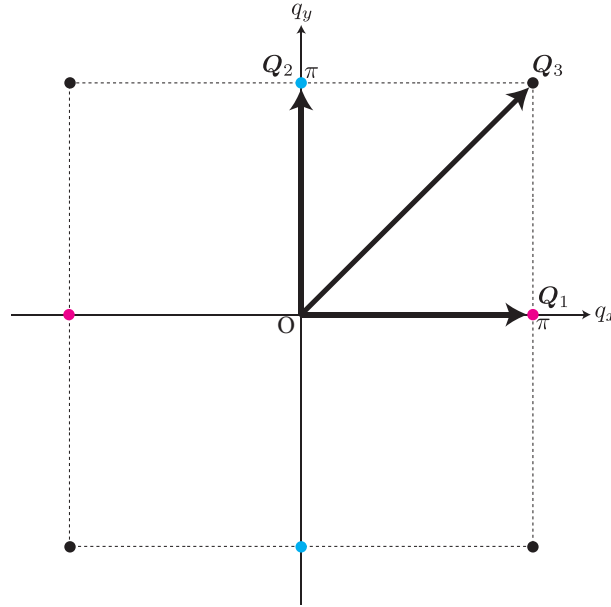


Figure 1. Schematic picture of the relevant ordering wave vectors in the first Brillouin zone. $Q_1 = (\pi, 0)$ and $Q_2 = (0, \pi)$ are the primary ordering wave vectors, and $Q_3 = (\pi, \pi)$ is the high-harmonic wave vectors of Q_1 and Q_2 .

Furthermore, we consider the Zeeman coupling to investigate the effect of an external magnetic field. The Zeeman Hamiltonian is given by

$$\mathcal{H}_Z = -H \sum_i S_i^z. \quad (5)$$

We take the field direction as the out-of-plane (z) direction.

The equilibrium spin configurations of the total Hamiltonian $\mathcal{H}_{\text{eff}} + \mathcal{H}_{Q_3} + \mathcal{H}_Z$ are obtained using simulated annealing combined with Monte Carlo sampling based on the standard single-spin-flip Metropolis algorithm. The simulations begin from a random configuration at high temperature ($T_0 = 1$), and the temperature is gradually reduced according to $T_{n+1} = \alpha T_n$ with $\alpha = 0.999999$ until the final temperature $T_f = 0.01$ is reached. At each temperature step, 10^5 to 10^6 Monte Carlo sweeps are performed for equilibration and measurements, and additional runs are independently initiated from low-temperature spin configurations near phase boundaries to confirm stability and reproducibility.

To characterize the resulting spin textures, we compute the magnetic moment at the Q_ν component, which is defined as

$$m_{Q_\nu} = \frac{1}{N} \sqrt{\sum_{\eta=x,y,z} \sum_{i,j} S_i^\eta S_j^\eta e^{iQ_\nu \cdot (r_i - r_j)}}, \quad (6)$$

where r_i denotes the position of site i . The uniform magnetization along the field direction is evaluated as

$$M^z = \frac{1}{N} \sum_i S_i^z. \quad (7)$$

The topological nature of the spin configurations is examined through the scalar spin chirality, defined as

$$\chi^{\text{sc}} = \frac{1}{N} \sum_{i,\delta=\pm 1} \mathbf{S}_i \cdot (\mathbf{S}_{i+\delta\hat{x}} \times \mathbf{S}_{i+\delta\hat{y}}), \quad (8)$$

where $\hat{x}$ ($\hat{y}$) is the unit vector in the x (y) direction [58]. A finite χ^{sc} indicates a noncoplanar magnetic texture associated with an emergent magnetic field, which gives rise to the topological Hall effect in itinerant electron systems.

3. Results

3.1. Without Biquadratic Interaction

We first discuss the case without the biquadratic interaction and external magnetic field, namely $K = H = 0$. Since the effective interaction includes contributions at Q_1 , Q_2 , and Q_3 , the ground state is expected to take one of the single-, double-, or triple- Q configurations depending on the parameter γ .

The single- Q spin configuration is given by

$$S_i = (\cos(Q_1 \cdot r_i), 0, 0), \quad (9)$$

representing a collinear structure characterized by a single ordering wave vector Q_1 (or equivalently Q_2). As illustrated in Figure 2(a), the spins are aligned along one direction, forming a simple collinear sinusoidal modulation without any finite scalar spin chirality.

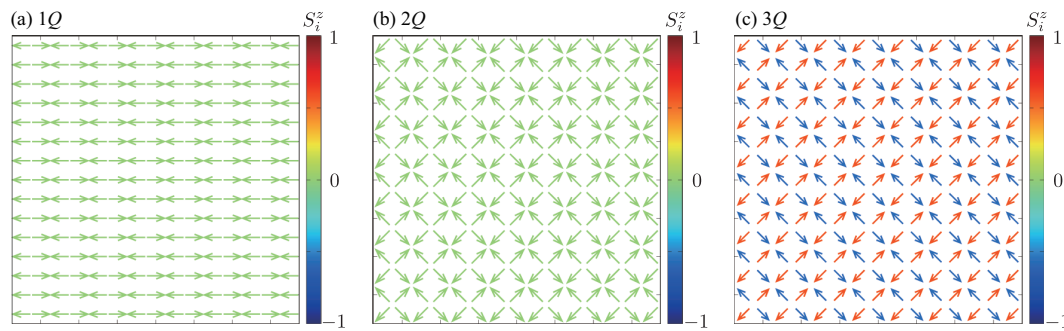


Figure 2. Spin configurations of (a) the single- Q (1Q) collinear state, (b) the double- Q (2Q) coplanar state, and (c) the triple- Q (3Q) noncoplanar state. The arrows denote the direction of spin moment, and their color indicates the z -spin component.

The double- Q configuration is expressed as

$$S_i = \frac{1}{\sqrt{2}}(\cos(Q_1 \cdot r_i), \cos(Q_2 \cdot r_i), 0). \quad (10)$$

This state corresponds to a coplanar texture resulting from the coherent superposition of two orthogonal spin density waves with ordering wave vectors Q_1 and Q_2 . The resulting interference generates a periodic vortex–antivortex array within the plane, as shown in Figure 2(b). All spins lie in a common plane, and hence both the local and net scalar spin chirality vanish. This type of noncollinear spin texture has also been found in iron-based materials [102–113].

In the absence of K and for $\gamma < 1$, the energies of the single- Q and double- Q states are degenerate. This degeneracy arises because the bilinear exchange interaction contributes equally to both configurations, as neither exhibits a component at the higher-harmonic wave vector Q_3 . As will be shown later, this degeneracy is lifted when the biquadratic interaction K is introduced.

For $\gamma = 1$, the triple- Q state becomes energetically degenerate with the single- Q and double- Q states without the biquadratic interaction. The corresponding spin configuration is given by

$$S_i = \frac{1}{\sqrt{3}}(\cos(Q_1 \cdot r_i), \cos(Q_2 \cdot r_i), \cos(Q_3 \cdot r_i)), \quad (11)$$

which represents a noncoplanar spin arrangement, as shown in Figure 2(c). This state exhibits a finite and uniform scalar spin chirality, signaling the emergence of a topologically nontrivial magnetic texture. Meanwhile, for $\gamma < 1$, the triple- Q configuration becomes energetically unfavorable compared

with the single- Q and double- Q states due to the loss of the exchange energy by the high-harmonic contribution at Q_3 .

3.2. Effect of Biquadratic Interaction

We next examine how the biquadratic interaction influences the stability of magnetic states in the absence of an external magnetic field. Figure 3 shows the ground-state phase diagram on the plane of the high-harmonic wave-vector interaction ratio $\gamma = J_{Q_3}/J$ and the biquadratic interaction strength K , obtained via simulated-annealing calculations at low temperatures. When $K = 0$, the ground state is degenerate between the collinear single- Q and coplanar double- Q configurations for $\gamma < 1$, while a noncoplanar triple- Q state becomes energetically degenerate at $\gamma = 1$, consistent with the discussion in the previous section. Introducing an infinitesimally small K lifts this degeneracy and generates a distinct phase boundary between the double- Q and triple- Q regions. The double- Q phase dominates for small γ and K , whereas the triple- Q phase is stabilized when both parameters are sufficiently large. Meanwhile, the single- Q state is not realized for $K \neq 0$. These results demonstrate that the cooperative effect between the high-harmonic wave-vector interaction and the biquadratic interaction drives the emergence of noncoplanar spin textures with a finite scalar spin chirality.

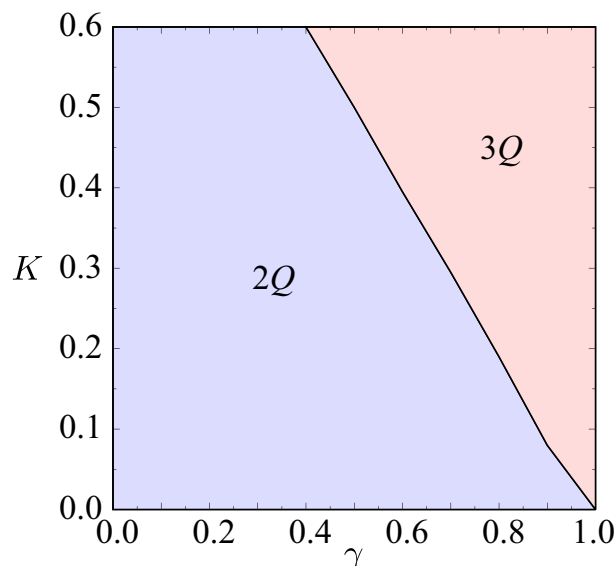


Figure 3. Magnetic phase diagram at low temperatures and zero magnetic field, which is obtained by simulated annealing. The horizontal axis represents the ratio of the high-harmonic wave-vector interaction to the ordering-wave-vector interaction, γ , and the vertical axis represents the biquadratic interaction, K . $2Q$ and $3Q$ stand for the double- Q and triple- Q states, respectively.

The quantitative evolution of the order parameters with K is presented in Figure 4. Figure 4(a)–(d) show the K dependence of the squared magnetic moments $(m_{Q_i})^2$ at Q_1 – Q_3 and the spatially averaged scalar spin chirality χ^{sc} for representative values of $\gamma = 0.4, 0.6, 0.8$, and 1 . For $\gamma = 0.4$ in Figure 4(a), both $(m_{Q_1})^2$ and $(m_{Q_2})^2$ remain nearly constant, while $(m_{Q_3})^2$ and χ^{sc} remain negligible throughout the entire range of K , indicating the robustness of the coplanar double- Q state. At $\gamma = 0.6$ in Figure 4(b), a transition occurs around $K \simeq 0.4$, where $(m_{Q_3})^2$ and χ^{sc} gradually increase while $(m_{Q_1})^2$ and $(m_{Q_2})^2$ slightly decrease, signaling the onset of a noncoplanar triple- Q configuration. As γ increases to 0.8 in Figure 4(c), this transition shifts to smaller K , reflecting the facilitation of the triple- Q ordering by the enhanced high-harmonic wave-vector interaction. For $\gamma = 1$ in Figure 4(d), both $(m_{Q_3})^2$ and χ^{sc} remain finite even for small K , confirming that the triple- Q state is naturally stabilized so as to prevent the energy loss of the positive biquadratic interaction. The continuous increase of χ^{sc} near the boundary indicates that the transition from the double- Q to triple- Q phase proceeds smoothly through gradual spin canting rather than a discontinuous jump.

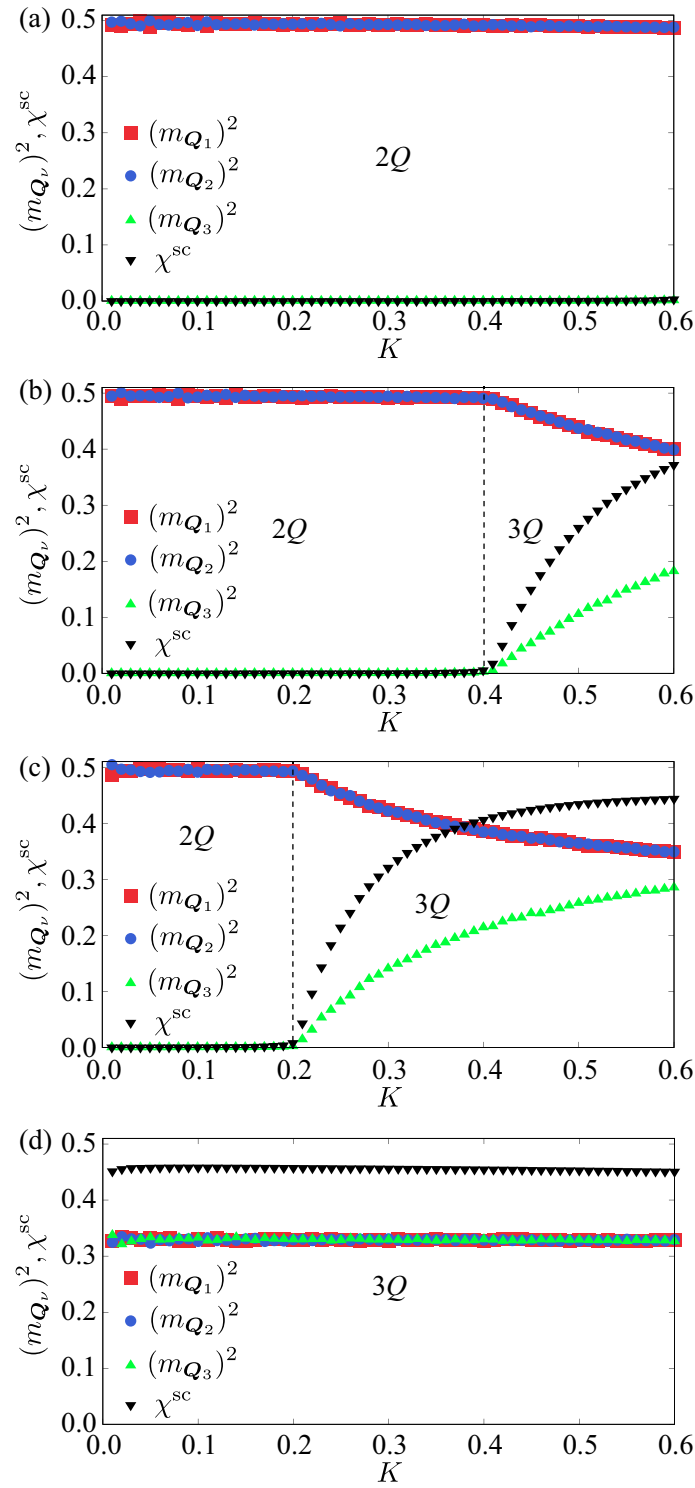


Figure 4. K dependence of the squared magnetic moments at Q_1 – Q_3 , $(m_{Q_\nu})^2$, and the scalar spin chirality χ^{sc} at (a) $\gamma = 0.4$, (b) $\gamma = 0.6$, (c) $\gamma = 0.8$, and (d) $\gamma = 1$. The vertical dashed lines denote the phase boundaries separating double- Q and triple- Q phases.

The real-space spin textures corresponding to these parameter sets are shown in Figure 5. Because the model preserves $SU(2)$ spin-rotational symmetry, the spin orientation can be freely rotated without changing the energy in the simulations. At $\gamma = 0.4$ [Figure 5(a)], the system exhibits the characteristic coplanar double- Q vortex–antivortex pattern confined within a single plane. When γ is increased to 0.6 [Figure 5(b)], a small component perpendicular to the double- Q structure develops periodically, producing a weakly noncoplanar arrangement with finite local solid angles. For $\gamma = 0.8$ and 1 [Figures 5(c) and 5(d)], this perpendicular component becomes more pronounced, leading to a fully

developed triple-Q spin texture accompanied by a uniform scalar spin chirality. These results clearly show that the biquadratic interaction, in conjunction with the high-harmonic wave-vector interaction, induces a continuous topological transition from the coplanar double-Q phase to the noncoplanar triple-Q phase.

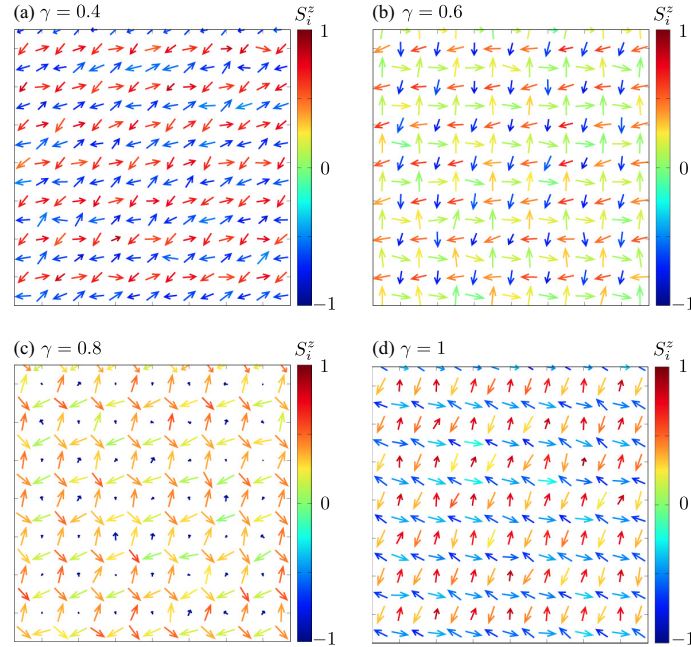


Figure 5. Real-space spin configurations of (a) the double-Q state at $\gamma = 0.4$, (b) the triple-Q state at $\gamma = 0.6$, (c) the triple-Q state at $\gamma = 0.8$, and (d) the triple-Q state at $\gamma = 1$ for $K = 0.5$. The arrows denote the direction of spin moment, and their color indicates the z-spin component.

3.3. Effect of Magnetic Field

We now examine the evolution of the multiple-Q states under an external magnetic field applied along the z axis. Figures 6, 7, and 8 summarize the field-dependent magnetic responses and the corresponding real-space spin and scalar spin chirality textures for a fixed $K = 0.2$, where the ground state at zero field corresponds to the coplanar double-Q state for small γ and the noncoplanar triple-Q state for larger γ , the latter of which accompanies a finite scalar spin chirality. The application of the magnetic field induces a continuous transformation of this state, sequentially reducing the magnetic moments at Q_i as well as the scalar spin chirality as the Zeeman coupling tends to align the spins along the field direction.

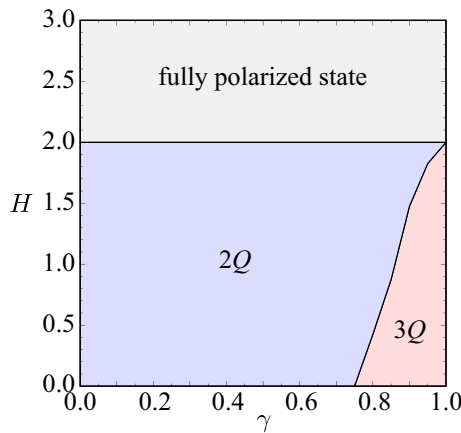


Figure 6. Magnetic phase diagram in the plane of γ and the magnetic field H at $K = 0.2$. 2Q and 3Q stand for the double-Q and triple-Q states, respectively.

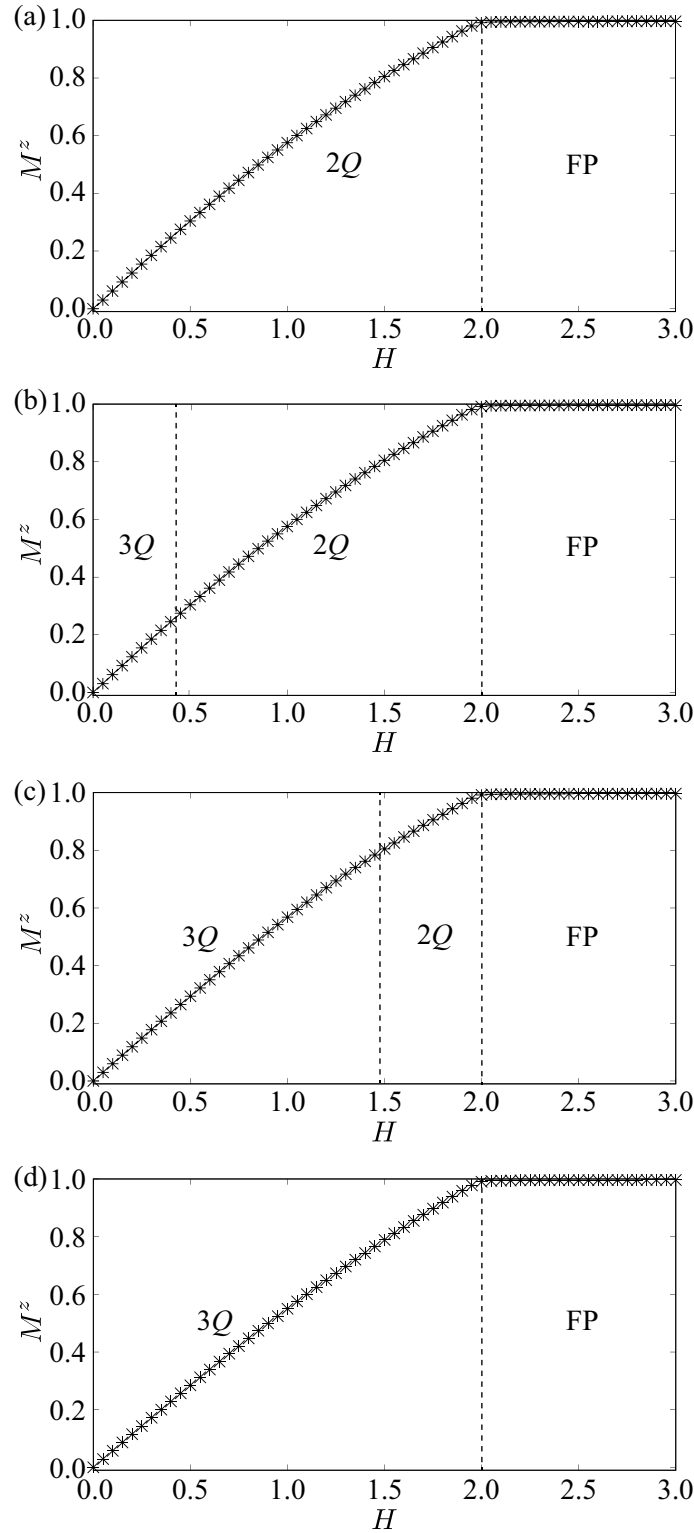


Figure 7. H dependence of the magnetization along the z direction at (a) $\gamma = 0.7$, (b) $\gamma = 0.8$, (c) $\gamma = 0.9$, and (d) $\gamma = 1$. The vertical dashed lines denote the phase boundaries separating different magnetic phases. FP stands for the fully polarized state.

The field dependence of the uniform magnetization M^z is plotted in Figure 7 for representative values of $\gamma = 0.7, 0.8, 0.9$, and 1 . At $\gamma = 0.7$, the magnetization increases smoothly with H until saturation around $H \simeq 2$, where the system transitions from the coplanar double- Q to a fully polarized state, as shown in Figure 7(a). For $\gamma = 0.8$, the ground state at $H = 0$ is the triple- Q phase, which persists up to $H \approx 0.4$ before transforming into the double- Q configuration and subsequently into the fully polarized phase near $H \approx 2$, as shown in Figure 7(b). This two-step evolution indicates

that the Zeeman field initially suppresses the high-harmonic wave-vector components responsible for noncoplanarity, converting the noncoplanar triple- Q state into the coplanar double- Q state, and only at higher fields aligns all spins parallel to the field direction. A similar trend is seen at $\gamma = 0.9$, where the triple- Q region widens, extending up to $H \approx 1.5$ before giving way to the double- Q and fully polarized phases, as shown in Figure 7(c). At $\gamma = 1$, the triple- Q phase remains robust over a broad field range, illustrating that the competition of the interactions between the ordering wave vectors and their high-harmonic one stabilizes noncoplanarity against Zeeman alignment, as shown in Figure 7(d). In all cases, the smooth increase of M^z with H signifies a continuous transformation of the spin texture rather than an abrupt metamagnetic transition.

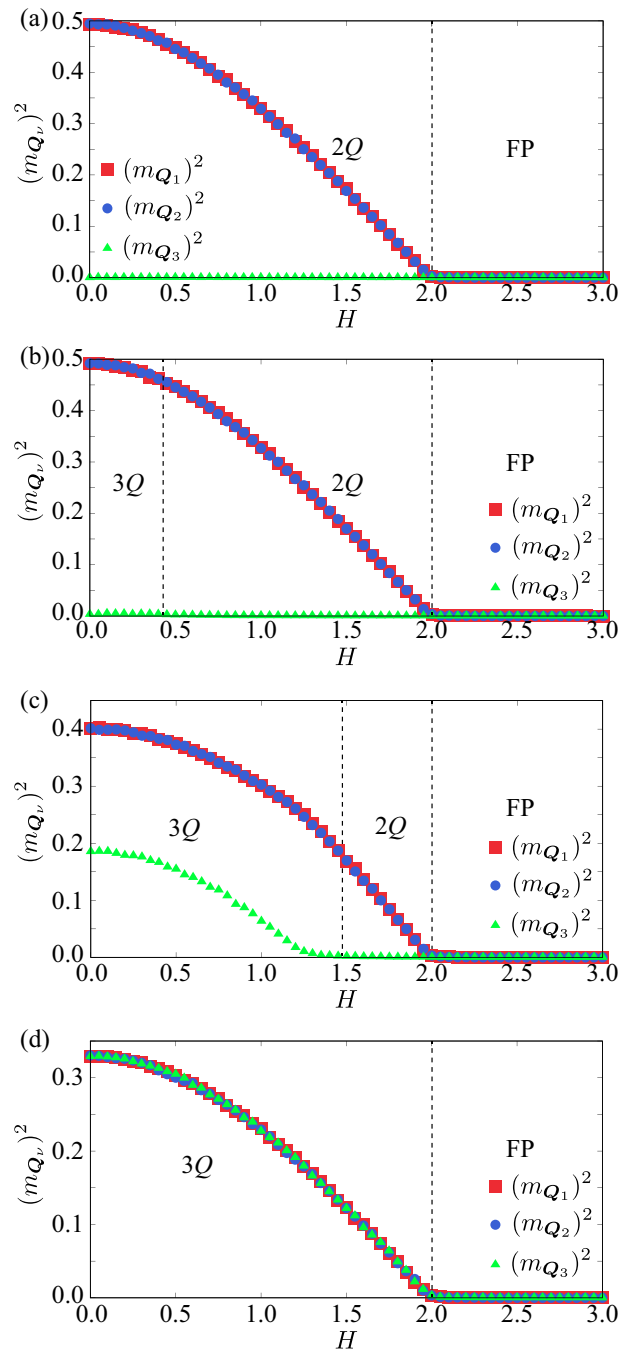


Figure 8. H dependence of the squared magnetic moments at Q_1 – Q_3 , $(m_{Q_i})^2$, at (a) $\gamma = 0.7$, (b) $\gamma = 0.8$, (c) $\gamma = 0.9$, and (d) $\gamma = 1$. The vertical dashed lines denote the phase boundaries separating different magnetic phases. FP stands for the fully polarized state.

The microscopic mechanism underlying these transitions is presented in Figure 8, which shows the H dependence of the squared magnetic moments $(m_{Q_i})^2$ at Q_1 – Q_3 . For $\gamma = 0.7$, the intensities at Q_1 and Q_2 remain nearly equal and gradually decrease with increasing field, while $(m_{Q_3})^2$ stays negligible throughout, consistent with a purely coplanar double- Q structure, as shown in Figure 8(a). At $\gamma = 0.8$, the triple- Q state at low fields is characterized by finite $(m_{Q_3})^2$, which drops to zero near $H \approx 0.4$, marking the transition to the double- Q phase, as shown in Figure 8(b). This suppression of the Q_3 component corresponds to the loss of the high-harmonic wave-vector modulation and hence of the scalar spin chirality. As γ increases to 0.9 and 1, the $(m_{Q_3})^2$ amplitude remains significant over a wider field range before vanishing near $H \approx 2$, demonstrating that strong high-harmonic wave-vector interactions enhance the resilience of the triple- Q noncoplanar state, as shown in Figures 8(c),(d). Beyond these critical magnetic fields, all $(m_{Q_i})^2$ components diminish simultaneously, leading to the fully polarized phase. The smooth evolution of $(m_{Q_3})^2$ across the boundaries also supports that the topological triple- Q phase is continuously deformed into a topologically trivial coplanar double- Q phase or fully polarized state. These results indicate that the external magnetic field suppresses the noncoplanar spin components and scalar spin chirality by favoring spin alignment along the field direction; the sequence of field-driven transitions from the triple- Q to the double- Q and the fully polarized states arises from the gradual reduction of the high-harmonic Q_3 component.

4. Conclusions

In this study, we have theoretically investigated the topological transition between coplanar and noncoplanar multiple- Q magnetic states in centrosymmetric itinerant magnets by employing a canonical effective spin model on a two-dimensional square lattice. The model incorporates bilinear and biquadratic exchange interactions at finite ordering wave vectors, supplemented by a high-harmonic wave-vector component that originates from the effects of Fermi-surface nesting and its higher-order contribution. By performing simulated-annealing calculations, we systematically mapped out the phase diagrams under zero and finite magnetic fields and clarified how the interplay among these competing interactions governs the emergence and evolution of multiple- Q phases.

At zero magnetic field, the cooperative action of the high-harmonic wave-vector interaction and the biquadratic coupling stabilizes a noncoplanar triple- Q state carrying a finite scalar spin chirality. When either coupling is weak, the system instead favors a coplanar double- Q configuration characterized by vortex–antivortex arrays without net scalar spin chirality. As the biquadratic term increases, the double- Q phase continuously evolves into the triple- Q phase through gradual spin canting, signifying a smooth topological transition rather than a first-order jump. The corresponding real-space and momentum-space spin structures reveal that the high-harmonic wave-vector contribution plays an important role in generating a scalar spin chirality, thereby lifting the degeneracy between coplanar and noncoplanar spin configurations. Under an external magnetic field, the Zeeman coupling further modifies these multiple- Q states. The field tends to suppress the noncoplanar components and scalar spin chirality, inducing a continuous sequence of transitions from the triple- Q state to the double- Q state and finally to the fully polarized state. The robustness of the triple- Q phase over a wide field range at a large high-harmonic wave-vector interaction underscores its stabilizing influence against field-driven alignment. These results demonstrate that the magnetic field acts as a tuning parameter that continuously deforms the topologically nontrivial spin textures toward topologically trivial coplanar and collinear ones.

Our findings establish a microscopic mechanism for the formation and field evolution of noncoplanar spin textures in centrosymmetric itinerant magnets, highlighting the crucial role of high-harmonic wave-vector and multi-spin interactions originating from Fermi-surface nesting in order to stabilize triple- Q topological magnetism even in the absence of spin–orbit coupling under inversion-asymmetric environments.

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Data Availability Statement: The original contributions presented in the study are included in the article, further inquiries can be directed to the corresponding author.

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