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Random-anisotropy effects in the second-order phase transition of the 2D Blume-Capel model

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Abstract. *We report on the second-order phase transition of two-dimensional (2D) magnetic materials under the influence of random anisotropy in the context of the Blume-Capel model employing an effective field theory and the differential operator method. By analyzing the temperature dependence of magnetization, we thoroughly explore the second-order ferromagnetic-to-paramagnetic (FM-PM) phase transition at the critical temperature T_C. When the magnitude of the random anisotropy D and its probability p is sufficiently large, the magnetization equation becomes divergent and unsolvable at a critical temperature, indicating the emergence of a tricritical point and a first-order phase transition. Additionally, we produce a phase diagram for the second-order phase transition presenting the relation between the critical temperature and the anisotropy amplitude at various probabilities.*

Keywords: Blume-Capel model, random anisotropy, effective field theory, differential operator, second-order phase transition.

Classification numbers: 64.60.Cn –; 75.10.Hk; 75.30.Kz.

1. Introduction

Rich phase diagrams have been revealed in double perovskite metal oxides [1–3]. These materials are synthesized through chemical doping, which introduces multi-valent ions [4], leading to disordered spin systems. In such systems, the magnetic behavior becomes notably complex and distinct compared to materials with periodic, symmetric crystal structures. The presence of anisotropic interactions directly impacts the variation of spin interactions within the crystal lattice,

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greatly influencing the magnetic properties of the material. In particular, anisotropic interactions are often accompanied by various anomalous physical phenomena, such as multicritical phenomena, which have garnered considerable attention from researchers [5].

Among numerous efforts to explain the multicritical phenomena, the Blume-Capel (BC) model emerges as an ideal model with the ability to perfectly illustrate the critical behavior of ^{3}He–^{4}He mixtures in aerogel [6, 7]. This model was first introduced by Blume [8] and later independently by Capel [9–11] in 1966. It is a widely studied mathematical model in statistical mechanics, typically applied to spin-1 systems with additional anisotropic crystal field interactions. In this model, a variety of multicritical phenomena are exhibited, including a phase diagram where disordered paramagnetic and ordered paramagnetic phases are separated by a transition line, which shifts from a second-order phase to a first-order phase at the tricritical point (TCP). Various physical systems involving multicritical behavior, such as multicomponent fluids, ternary alloys, and several magnetic problems, have been explained within the context of this model [5].

To describe the disorder in double perovskite metal oxides, a random crystal field is introduced into the BC model. Several theoretical techniques have been used to study the BC model with a random crystal field, including the mean-field approximation (MFA) [12], Bethe lattice approximation (BLA) [13], cluster variational method (CVM) [7], pair approximation [14], finite cluster approach (FCA) [15], Monte Carlo simulation [16], renormalization group (RG) [17], and effective field theory (EFT) [18]. These studies have explored various random crystal field distributions, such as the Gaussian and bimodal distributions, however, the results consistently show the presence of multiple multicritical points. The bimodal distribution, due to its simplicity, provides a clearer understanding of the effects of dopants.

In addition, despite extensive research employing effective field theory [18, 19], the phase diagram of the BC model with a random crystal field remains a subject of debate, particularly regarding to the temperature dependence of magnetization - a crucial feature to validate the tricritical point. To address this, our current work aims to provide a transparent depiction of the temperature dependence of magnetization for various values of the random parameters from the perspective of the BC model with a bimodal distribution for random field. We also produce a phase diagram illustrating second-order magnetic phase transition with tricritical points and give comprehensive explanation underlying physical mechanisms of each regime.

2. Model and formalism

The Hamiltonian of the spin-1 Blume–Capel model with a random crystal field is given by

$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z + \sum_i D_i (S_i^z)^2, \tag{1}$$

where S_i^z is the z-component of spin variable associated with site i, which takes the values $S_i^z = 0, \pm 1$. The first term indicates ferromagnetic interactions among all pairs of nearest-neighbor spins, with the exchange interaction $J = 1$. The random anisotropic field D_i at site i follows the bimodal distribution law:

$$P(D_i) = p\delta(D_i - D) + (1-p)\delta(D_i). \tag{2}$$

In chemically doped double perovskites, the interactions among ions of the same valence generate one specific crystal field value, while interactions among ions of different valences create

another. Consequently, the distribution of the crystal field depends on the concentration of ions with different valences, which can be effectively described by a bimodal distribution. It was further demonstrated that the bimodal distribution can approximate the Gaussian distribution when studying the BC model with a random crystal field [20]. For its simplicity, the bimodal distribution has been widely adopted in the investigation of the Blume-Capel model with random crystal fields [16, 19].

Hamiltonian (1) is then rewritten in the form,

$$H = -\sum_i \left\{ E_i S_i^z - D_i (S_i^z)^2 \right\}, \tag{3}$$

where $E_i = J \sum_j' S_j^z$ expresses the interaction energy between the spin at site i and all of its nearest-neighbors. Then, the thermodynamic average of an arbitrary physical quantity $\langle\langle A \rangle\rangle_r$ is computed as a function of Hamiltonian (3):

$$\langle\langle A \rangle\rangle_r = \left\langle \left\langle \frac{\mathrm{Tr}(e^{-\beta H} \cdot A)}{\mathrm{Tr}(e^{-\beta H})} \right\rangle \right\rangle_r = \left\langle \left\langle \frac{\sum_{S_i^z=-1}^{1} e^{-\beta H} \cdot A}{\sum_{S_i^z=-1}^{1} e^{-\beta H}} \right\rangle \right\rangle_r \tag{4}$$

with the inverse temperature $\beta = 1/k_B T$, the canonical thermal average symbolized by the inner brackets $\langle ... \rangle$, and the random configurational average identified by the outer brackets $\langle ... \rangle_r$. Using the Callen identity [21], the average magnetic moment $m = \langle\langle S_k^z \rangle\rangle_r$, and the average squared moment $q = \langle\langle (S_k^z)^2 \rangle\rangle_r$ are obtained as follows:

$$m = \langle\langle S_k^z \rangle\rangle_r = \left\langle \left\langle \frac{2\sinh(\beta E_k)}{2\cosh(\beta E_k) + e^{\beta D_k}} \right\rangle \right\rangle_r, \tag{5}$$

$$q = \langle\langle (S_k^z)^2 \rangle\rangle_r = \left\langle \left\langle \frac{2\cosh(\beta E_k)}{2\cosh(\beta E_k) + e^{\beta D_k}} \right\rangle \right\rangle_r. \tag{6}$$

Using the differential operator method [22], we convert the right-hand sides of the two expressions above into algebraic equations involving different orders of the order parameters m, q, and the average value of the anisotropy coefficient D as a standard parameter.

$$m = \left\langle \left\langle e^{\beta E_k \nabla_x} f(x, D_k) \right\rangle \right\rangle_r \Big|_{x=0}, \tag{7}$$

$$q = \left\langle \left\langle e^{\beta E_k \nabla_x} g(x, D_k) \right\rangle \right\rangle_r \Big|_{x=0}, \tag{8}$$

where $\nabla_x = \frac{\partial}{\partial x}$ denotes the differential operator. The functions $f(x, D_k)$ and $g(x, D_k)$ are given by:

$$f(x, D_k) = \frac{2\sinh(x)}{2\cosh(x) + e^{\beta D_k}} \tag{9}$$

$$g(x, D_k) = \frac{2\cosh(x)}{2\cosh(x) + e^{\beta D_k}}. \tag{10}$$

Calculating the average over random configurations:

$$F(x, D) = \int P(D_k) f(x, D_k)\, dD_k = 2\sinh(x) \left[\frac{p}{2\cosh(x) + e^{\beta D}} + \frac{1-p}{2\cosh(x) + 1} \right], \tag{11}$$

$$G(x, D) = \int P(D_k) g(x, D_k)\, dD_k = 2\cosh(x) \left[\frac{p}{2\cosh(x) + e^{\beta D}} + \frac{1-p}{2\cosh(x) + 1} \right]. \tag{12}$$

Substituting $F(x,D)$ and $G(x,D)$ into the order parameters m, q (7) (8):

$$m = \left\langle \left\langle e^{\beta E_k \nabla_x} \right\rangle \right\rangle_r F(x,D)|_{x=0}\,, \tag{13}$$

$$q = \left\langle \left\langle e^{\beta E_k \nabla_x} \right\rangle \right\rangle_r G(x,D)|_{x=0}\,, \tag{14}$$

where the term $\left\langle \left\langle e^{\beta E_k \nabla_x} \right\rangle \right\rangle_r$ is defined using the van der Waerden identity [23] for spin-1 systems:

$$\left\langle \left\langle e^{\beta E_k \nabla_x} \right\rangle \right\rangle_r = \left\langle \left\langle \prod_j^z \left[1 + \sinh(\beta J \nabla_x) S_j^z + (\cosh(\beta J \nabla_x) - 1)(S_j^z)^2 \right] \right\rangle \right\rangle_r . \tag{15}$$

We now apply the approximation process from effective field theory (EFT) [24]:

$$\left\langle \left\langle s_1^z s_2^z s_3^z (s_4^z)^2 \right\rangle \right\rangle_r = \left\langle \langle s_1^z \rangle \right\rangle_r \left\langle \langle s_2^z \rangle \right\rangle_r \left\langle \left\langle s_3^z \right\rangle \right\rangle_r \left\langle \left\langle (s_4^z)^2 \right\rangle \right\rangle_r . \tag{16}$$

Thus, the order parameters m, q are described as follows:

$$m = \{1 + m\sinh(\lambda \nabla_x) + [\cosh(\lambda \nabla_x) - 1]q\}^z F(x,D)|_{x=0}, \tag{17}$$

$$q = \{1 + m\sinh(\lambda \nabla_x) + [\cosh(\lambda \nabla_x) - 1]q\}^z G(x,D)|_{x=0}, \tag{18}$$

where $\lambda = \beta J$, and the exponent z is the nearest-neighbor spin number.

For the 2D square lattice considered in this paper, $z = 4$, and the order parameters m, q are represented by a pair of self-consistent equations:

$$m = A_1(q)m + A_3(q)m^3, \tag{19}$$

$$q = B_0(q) + B_2(q)m^2 + B_4(q)m^4. \tag{20}$$

The solution to equation (19) is $m(q) = \sqrt{\frac{1-A_1(q)}{A_3(q)}}$, which is then substituted into equation (20) to derive a self-consistent function dependent only on q. The solution for q is subsequently substituted back into equation (19) to determine the average magnetic moment m.

3. Results and discussion

Firstly, we examine the temperature dependence of the magnetization for pure BC systems with $p = 1$, considering two non-positive cases of the random anisotropy magnitude $D = 0$ and $D \to -\infty$.

In Fig. 1, for $p = 1$ and $D = 0$, the spin-1 BC model is equivalent to a 3-state Ising model with spin values of 0, and ± 1. The system exhibits two distinct phases: ferromagnetic (FM) and paramagnetic (PM), which transition at the critical temperature $T_C = 2.19$. Below T_C, the strongly-coupled spins in parallel arrangement induce a non-zero magnetic moment characterizing for the FM state. Above T_C, thermal energy breaks this alignment, causing the spins to become randomly oriented, leading to a near-zero magnetic moment of the PM state. In the absence of anisotropy, the FM-PM phase transition is completely smooth, a typical indication of the second-order phase transition.

For $p = 1$ and $D \to -\infty$, the strong anisotropy, presented by the second term in Hamiltonian (1), forces all spins to align along the z-axis, with only two possible spin states ± 1, while the transverse state (spin value 0) is suppressed. Consequently, the spin-1 BC model reduces to the standard Ising model for spin-1/2. This leads to a second-order FM to PM phase transition at the critical temperature $T_C = 3.10$, between the exact value $2J/\ln(1+\sqrt{2}) \approx 2.269J$ [25] and the

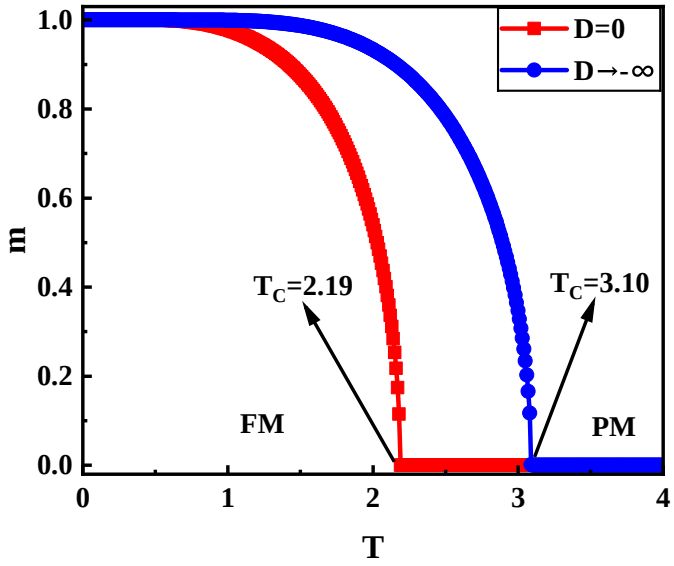

Fig. 1. The temperature dependence of the magnetization for a 2D square lattice with $p = 1$ in 2 cases: $D = 0$ and $D \to -\infty$.

Weiss-field result $4J$. Our calculated critical temperatures for the two non-positive values of the random anisotropy in the pure spin-1 BC model are consistent with Ref. [26].

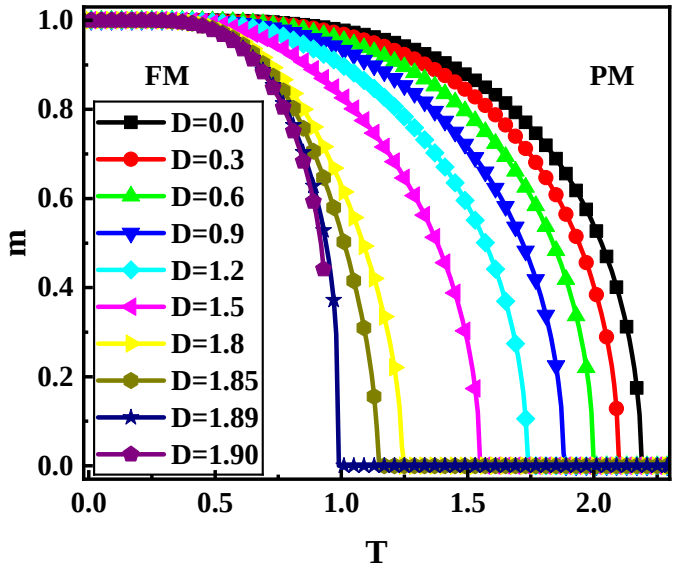

Fig. 2. The temperature dependence of the magnetization for a 2D square lattice with $p = 1$ and different values of the anisotropy magnitude D.

The impact of different positive anisotropy magnitudes on the second-order phase transition in the pure spin-1 BC model ($p = 1$) is explored in Fig. 2. For $0 < D \leq 1.89$, the system consistently undergoes a second-order FM-to-PM phase transition, with the critical temperature T_C decreasing as the anisotropy magnitude increases. This indicates that as the dopant introduces stronger anisotropy, the spins tend to align more along the transverse direction (spin value 0) rather than the z-direction. Consequently, the exchange interaction energy between spins weakens, requiring less thermal energy to disrupt the system's phase order, resulting in a lower critical temperature T_C.

In addition, for $D \geq 2$, magnetization is suppressed at all temperatures. These findings align with Ref. [9] using molecular field theory, suggesting that for $D < \frac{4}{3}\ln(4)$, the system consistently exhibits a second-order phase transition. Furthermore, as D approaches 2 ($1.89 < D < 2$), the self-consistent magnetization equation diverges, yielding no reasonable solution in this range.

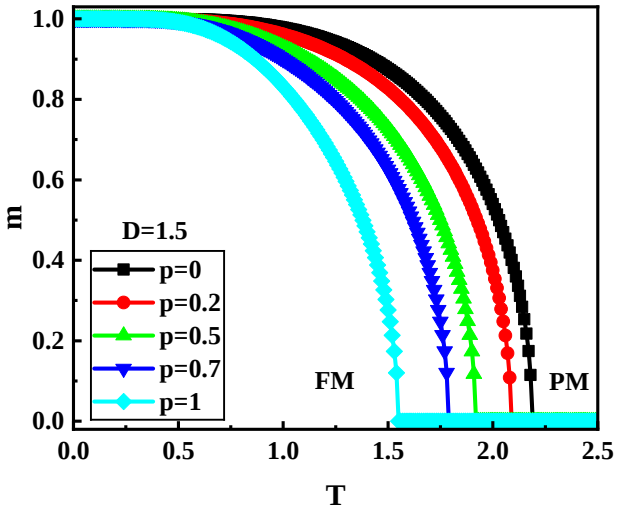

Fig. 3. The temperature dependence of the magnetization for a 2D square lattice with anisotropy amplitude $D = 1.5$ and different probabilities p.

In Fig. 3, we also examine the effect of disorder by analyzing how magnetization depends on temperature for a fixed anisotropy magnitude of $D = 1.5$, while varying the probability p. For this anisotropy value, a second-order phase transition occurs at every probability p. It implies that increasing the probability reduces the critical temperature T_C because of the spin tendency to align in the transverse direction (spin state 0) rather than along the z-axis.

The temperature dependence of magnetization is analyzed for different values of the probability p and the anisotropy amplitude D to determine the critical temperatures. These critical temperatures are then used to construct a T_C-D phase diagram, shown in Fig. 3. In this phase diagram, the solid lines represent the second-order phase transition. For each curve with $p \leq 0.6$, the phase diagram is clearly divided into two regions: the upper right corresponds to the paramagnetic (PM) phase, while the lower left represents the ferromagnetic (FM) phase. For $p = 0$, the phase transition line appears as a horizontal line at $T_C = 2.19$, as no anisotropy is present, effectively reducing the spin-1 BC model to a 3-state Ising model for spin-1.

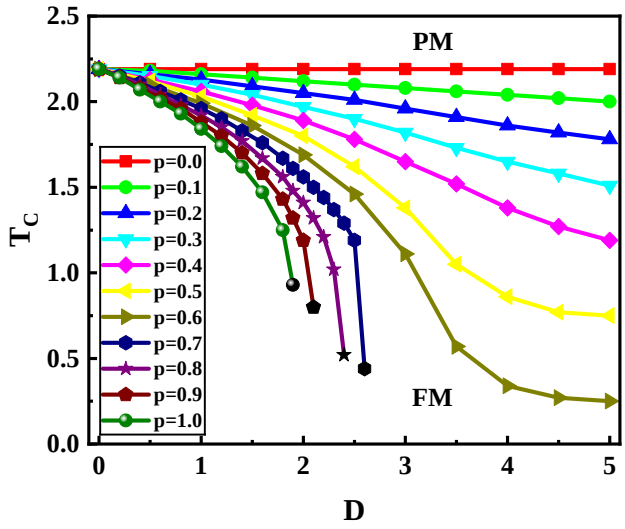

Fig. 4. T_C-D phase diagram of the spin-1 BC model with random anisotropy in a square lattice for different probabilities p. The black points represent the tri-critical points (TCP).

For $0 < p \leq 0.6$, the self-consistent equation for magnetization has a unique solution at every temperature, regardless of the anisotropy magnitude D. This behavior is accompanied by a second-order FM to PM phase transition, where the critical temperature T_C decreases as D increases for a given p. As the anisotropy parameter D becomes sufficiently large for each p, the critical temperature T_C saturates and remains constant. This occurs because, at high enough values of D, the lowest energy state consists entirely of transverse spins (spin state 0), which remains unchanged even with further increases in D. For example, when $p = 0.6$ and $D \geq 5$, the critical temperature stabilizes at $T_C = 0.25$.

For $p \geq 0.7$, as the anisotropy parameter D increases, the phase transition curves break at the black points. Indeed, in the vicinity of $D \lesssim zJ/2p$, the self-consistent equation for magnetization becomes divergent and unsolvable at a particular temperature. The horizontal coordinate of these black points represents the anisotropy value D where this divergence begins, while the vertical coordinate corresponds to the specific temperature at which it occurs. According to Landau's theory of phase transitions, at the critical temperature of a first-order phase transition, multiple magnetization values satisfy the self-consistent equation, meaning this divergence signals the occurrence of a first-order phase transition. Thus, the temperature where this divergence takes place is the critical temperature T_C. Additionally, since the black points indicate where the phase transition changes from second-order to first-order, they are the tricritical points (TCP).

For $p \geq 0.7$ and $D \geq zJ/2p$, magnetization is suppressed at every temperature.

4. Conclusions

Using the EFT formalism and the differential operator method, we have studied the magnetism of two-dimensional disordered magnetic systems, such as double perovskites, within the

framework of the spin-1 BC model with a random crystal field. For various values of the probability p and the anisotropy parameter D, which are directly related to the concentration of dopants and the doping element, we analyzed the temperature dependence of magnetization. This dependence reveals the nature of the phase transition and the critical temperature T_C, which is used to construct a phase diagram in the T_C–D plane.

This phase diagram is distinctly separated into two parts by a second-order FM to PM phase transition line for each probability value in the range $p \leq 0.6$. For $p = 0$, this line is horizontal due to the absence of anisotropy. For $0 < p \leq 0.6$, as the anisotropy parameter D grows, the critical temperature T_C declines. However, once D reaches a certain threshold, T_C stops decreasing and remains constant.

For $p \geq 0.7$, as D increases, the phase transition curves become discontinuous and terminate at the black points shown in Fig. 4. At these points, the divergence of the self-consistent magnetization equation indicates the presence of a first-order phase transition, identifying these points as tricritical points (TCPs). Furthermore, the behavior of the first-order phase transition curves in the phase diagram inspires further research.

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Authors contributions

Quan D. Nguyen: Resources, Methodology, Investigation, Validation, Visualization. **Son N. Bui**: Methodology, Investigation, Validation, Data Curation. **Phong H. Nguyen**: Writing - Review - Editing, Investigation, Validation, Funding acquisition. **Giang H. Bach**: Validation, Visualization, Editing, Formal analysis, Supervision.

Conflict of interest

The authors have no conflict of interest to declare.

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