Research Progress on Higher-Order Transitions in Finite Systems – Statistical Structural Rearrangement, Geometric Characterization, and Critical Precursors

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Abstract

Traditional phase transition theory is mainly based on singularities in derivatives of the free energy in the thermodynamic limit. For finite systems, however, the vicinity of a primary phase transition is often accompanied by more detailed structural reorganization and asymmetric fluctuation behavior, which cannot be fully characterized by singularities in low-order derivatives of conventional thermodynamic quantities. In recent years, microcanonical inflection-point analysis has provided a systematic framework for identifying higher-order transitions in finite systems and has revealed independent and dependent third-order transitions in models such as Ising, Baxter–Wu, Potts, and Blume–Capel. Furthermore, geometric observables such as the number of isolated spins, cluster area, and perimeter have endowed higher-order transitions with a more intuitive structural picture; canonical criteria based on energy cumulants have advanced the study of higher-order transitions from reliance on density-of-states reconstruction toward more general equilibrium and nonequilibrium scenarios; and intrinsic microstate spectral statistics further characterize higher-order structural rearrangements at the level of the overall organization of configuration space. This paper reviews research progress on third- and higher-order transitions in finite systems, focusing on microcanonical identification, geometric characterization, complex-network and nonequilibrium extensions, and canonical criteria, with particular emphasis on the relationship between higher-order transitions and primary phase transitions, their physical significance as precursor signals, and key issues that remain to be clarified in current research.

Full Text

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Research Progress on Higher-Order Transitions in Finite Systems

–Statistical Structural Rearrangement, Geometric Characterization, and Critical Precursors

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Abstract: Traditional phase-transition theory is mainly founded on the singularities of derivatives of the free energy in the thermodynamic limit. For finite systems, however, the vicinity of a primary phase transition is often accompanied by more subtle structural reorganization and asymmetric fluctuation behavior, which are difficult to characterize completely through singularities of low-order derivatives of conventional thermodynamic quantities. In recent years, microcanonical inflection-point analysis has provided a systematic framework for identifying higher-order transitions in finite systems, and has revealed independent and dependent third-order transitions in models such as the Ising, Baxter-Wu, Potts, and Blume-Capel models. Furthermore, geometric observables such as the number of isolated spins, cluster area, and perimeter have endowed higher-order transitions with a more intuitive structural picture. Canonical criteria based on energy cumulants have advanced the study of higher-order transitions from reliance on density-of-states reconstruction toward more general equilibrium and nonequilibrium scenarios, while intrinsic microstate spectral statistics further characterize higher-order structural rearrangements from the perspective of the overall organization of configuration space. Focusing on third- and higher-order transitions in finite systems, this article reviews research progress in microcanonical identification, geometric characterization, complex networks and nonequilibrium extensions, and canonical criteria. It emphasizes the relationship between higher-order transitions and primary phase transitions, their physical significance as precursor signals, and key issues that remain to be clarified in current research.

Keywords: higher-order transitions; microcanonical inflection-point analysis; geometric characterization; canonical criteria; finite systems

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1 Introduction

Phase transitions are among the most central research topics in statistical physics and thermodynamics. Traditional phase-transition theory is primarily built upon the thermodynamic limit, namely the assumption that the system size tends to infinity, so that the free energy and its derivatives exhibit strict non-analytic behavior near the critical point [1]. Within this framework, a first-order phase transition is usually associated with a discontinuity in the first derivative of the free energy, whereas a second-order phase transition is characterized by singularities in higher-order derivatives [2]. The Ehrenfest classification [3], Landau theory [4], and the later renormalization-group theory [5] were precisely the principal structures of modern phase-transition theory gradually established on this basis. In recent years, many machine-learning methods have also played a major role in advances in the study of phase transitions [6–9]. For macroscopic systems, these theoretical frameworks have been extraordinarily successful: they can not only explain classical phenomena such as magnetic materials and liquid-gas transitions, but also provide a unified language for core concepts such as critical exponents, scaling relations, and universality classes.

However, as research objects have continuously expanded from ideal macroscopic systems to nanoscale materials [10, 11], polymers [12, 13], complex networks [14], and various nonequilibrium cooperative systems [15–18], traditional phase-transition theory has gradually revealed a fundamental limitation: singularity criteria in the thermodynamic limit cannot be directly applied to finite systems. In finite systems, many originally

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Quantities that, in the thermodynamic limit, should diverge, jump, or become discontinuous are all smoothed out, instead appearing as broad peaks, skewness, local extrema, or splitting of response intervals [2]. At this point, a system' s "transition" is often no longer equivalent to an obvious abrupt change in a single thermodynamic quantity; rather, it is more like the superposition of a series of cross-scale structural reorganization processes [19]. Precisely for this reason, the problem of identifying phase transitions in finite systems has gradually shifted from searching for singular points to identifying cooperative rearrangement signals with physical meaning.

Against this background, the importance of microcanonical analysis has rapidly increased. Unlike the canonical system, which mainly focuses on response functions such as the distribution function, free energy, heat capacity, and magnetic susceptibility, the microcanonical method starts directly from the density of states $g(E)$ (DOS) and encodes the system' s phase behavior in the microcanonical entropy $S(E) = k_B \ln g(E)$. Because $S(E)$ contains complete information about the system' s phase behavior, even when a finite system lacks genuine thermodynamic singularities, changes in the system' s phase-related structure may still be manifested through more delicate variations in the curvature and monotonicity of the entropy and its hierarchy of derivatives. In other words, although phase-change quantities in finite systems are no longer strictly singular, they are not necessarily blurred and structureless; as long as a stable cooperative reorganization process exists, that process may leave traceable signals in the entropy derivatives [20].

Based on this idea, in 2018 Qi and Bachmann proposed the microcanonical inflection-point analysis (MIPA) method [23], in combination with the principle of minimal sensitivity [21, 22]. The core idea of this method is that transition signals in finite systems need not appear as genuine thermodynamic singularities, but can still be identified through the "least-sensitive inflection points" in the microcanonical entropy and its derivative hierarchy. More importantly, this method can not only locate traditional first- and second-order phase transitions, but can also systematically distinguish and identify independent and dependent transitions of arbitrary order. Its application to the two-dimensional ferromagnetic Ising model and polymer adsorption models showed that the phase-related structures inside finite systems may be richer than those implied by the classical picture. From this point on, studies of higher-order transitions began to move from scattered individual cases toward systematization.

The introduction of MIPA in fact changed the way people discuss transition problems in finite systems. From the traditional perspective, finite systems are often regarded as blurred approximations to the thermodynamic limit, and their extra peaks, secondary extrema, or local bending are often easily interpreted as finite-size errors or as additional details on a smoothing background. Within the framework of MIPA, however, these additional structures are no longer automatically treated as noise, but are re-examined as cooperative reorganization signals that may have independent physical significance. In particular, the distinction between independent and dependent types provides a new language for understanding additional phenomena near a primary phase transition: the former are closer to independently existing higher-order reorganizations, while the latter coexist with lower-order phase transitions and are usually located on the higher-energy or higher-temperature side, thus naturally carrying the meaning of a certain "precursor signal" or "additional information" and therefore can be regarded as harbingers of a lower-order primary phase transition. Thus, research on higher-order transitions gradually formed a developmental trajectory of "method proposal—model validation—geometric interpretation—canonical extension."

Around this method, two-dimensional finite-size spin models became the most important starting platform for research on higher-order transitions. First, work on the two-dimensional Ising [24] and Baxter–Wu models [25] [26–28] used Wang–Landau sampling [29, 30] to obtain the density of states, and combined it with MIPA to systematically analyze finite-size pseudo-transitions. The relevant results showed that, in addition to the second-order phase transition, the Ising model also exhibits identifiable third-order independent and dependent transition signals, while the Baxter–Wu model, at finite size, likewise displays a structure in which first-order and third-order transitions coexist. More importantly, these results suggested that higher-order transitions possess a certain "universality" in different spin models. This step moved higher-order-transition research from methodological proposal to the stage of model validation.

Subsequently, research on the Potts [31] model pushed this issue further. What makes the Potts model special compared with the Ising model is that it allows continuous phase transitions and first-order phase transitions to be examined within the same theoretical framework, and is therefore highly suitable for studying how higher-order transition signals change with the nature of the primary phase transition. Related work in 2024 used a comparison between Wang–Landau and parallel tempering [32, 33] to obtain the DOS [34], and determined the positions of third-order transitions through MIPA. The microcanonical and canonical results showed good consistency in the locations of higher-order transitions, thereby further supporting that higher-order transitions are not accidental additional peaks, but structural levels that can be stably tracked. This further advanced a stronger question: what actual physical organization processes do these higher-order transitions correspond to?

It is precisely from this point onward that research on higher-order transitions has gradually shifted from criterion-based identification to interpretation in terms of physical images. An increasing number of studies indicate that merely relying on traditional canonical quantities such as heat capacity, magnetic susceptibility, and Binder cumulants is not sufficient to fully reveal these additional

the connotation of higher-order signals; by contrast, geometric and morphological observables such as isolated spins, cluster area, mean cluster perimeter, and boundary density often correspond more directly to the structural reorganization processes reflected by higher-order transitions. Taking the Ising model and the Potts model as examples, geometric studies have shown that independent third-order transitions are better characterized by isolated spins, whereas dependent third-order transitions are more closely associated with the rapid rearrangement of cluster area or perimeter [26, 27, 35]. This indicates that higher-order transitions are not merely a simple refinement of a single thermodynamic peak, but may instead correspond to two distinct mechanisms: local rupture on the ordered side and precursor boundary reorganization on the disordered side.

On this basis, the Blume–Capel model [36] further reveals the relationship between higher-order signals and changes in the type of the primary phase transition. Because this model contains a tricritical point, it allows the coupled evolution among continuous phase transitions, first-order phase transitions, and higher-order signals to be examined within the same system. Relevant studies show that when the crystal-field parameter crosses the tricritical point and the system enters a region with a stronger first-order phase transition, the dependent third-order transition no longer appears, while a fourth-order independent transition can be identified in the high-temperature region. This suggests that higher-order transitions are not fixed structures statically attached to the two sides of the primary phase transition, but instead may undergo order elevation, disappearance, or rearrangement as the strength of the primary transition and the topology of the phase diagram change.

At the same time, this field has also continued to break through the methodological limitation of having to rely on the microcanonical density of states. Although

MIPA provides a clear language for classification, it is still microcanonical in essence and often requires explicit construction of the DOS, which is a clear limitation for large systems, complex energy landscapes, and nonequilibrium steady states. To address this problem, recent work has proposed a canonical criterion based on energy cumulants [37],

$$\Xi(T) = \frac{\kappa_3(T)}{[\kappa_2(T)]^3} \tag{1.1}$$

thereby establishing a fluctuation-based canonical expression for third-order transitions. This framework allows higher-order signals to be extracted directly from canonical energy cumulants and to correspond asymptotically to the microcanonical classification in the single-saddle-point region; more importantly, it does not require explicit DOS reconstruction and remains operational in nonequilibrium steady states. This marks the movement of higher-order-transition research from microcanonical identification toward canonical–microcanonical bridging.

On the basis of the above methodological and model studies, the significance of higher-order-transition problems has also gradually extended beyond traditional equilibrium spin systems themselves. Related models and methods were first successfully used in fundamental theoretical topics such as partition-function zeros [38], Fisher zeros [39, 40], inherent microstates [41], and basic models, for example the XY model [42], neural-network models [43], spin models [44], and topology [45–48]; subsequently, they were widely applied to various complex systems, including nanosystems, small-size systems, small ideal gases, small molecules, polymer adsorption, community-structure analysis in complex networks, and protein-folding networks [49–57]. At the same time, the precursor significance of higher-order signals has also been increasingly emphasized: studies of majority-vote models and networks link them to opinion formation, cultural dynamics, language dynamics, and the early identification of large-scale social disturbances [58-60]; Potts and Blume–Capel models further extend this problem to precursor scenarios in complex systems such as artificial populations, active bacterial colonies, climate change, and ecological collapse [35, 36]. Furthermore, the proposal of canonical criteria also shows that the scope of higher-order-transition research is no longer limited to equilibrium lattice models, but is gradually entering the problem of generalized fluctuation diagnosis in strongly nonequilibrium steady states [37].

In summary, research on higher-order transitions has evolved from the question of whether additional third- or fourth-order signals exist in finite systems into a research thread centered on the reorganization of statistical structure: microcanonical inflection-point analysis provides a classification language for higher-order transitions; equilibrium spin models verify the stability of these signals under different primary phase-transition backgrounds; geometric observables further reveal the corresponding defect, cluster, and boundary reorganization processes; and canonical cumulants together with spectral-statistical methods attempt to transform microcanonical signals into more general observable characterizations. Following this line, this paper first introduces the theoretical basis of higher-order transitions in finite systems, then reviews the main evidence in models such as Ising, Baxter–Wu, Potts, Blume–Capel, and Clock, and subsequently discusses geometric characterization, canonical response, spectral statistics of inherent microstates, complex networks, and nonequilibrium extensions. Finally, it summarizes the key issues that remain to be solved in this field. Figure 1 presents the cross-statistical-level interpretive framework adopted in this paper.

Research roadmap for statistical-structural criteria for higher-order pseudo–phase transitions

Scientific question: Do observable, verifiable, and generalizable statistical-structural criteria exist for higher-order pseudo–phase transitions?

- **Route 1 –Theoretical positioning**
  - Higher-order derivatives of the microcanonical entropy
  - Construction of canonical response quantities
  - Proof of positioning consistency
  - Observable positioning in the canonical ensemble
- **Route 2 –Structural criteria**
  - Configuration-ensemble representation
  - Extraction of statistically correlated modes
  - Stability assessment
  - Structural criteria for critical precursors
- **Route 3 –Nonequilibrium extension**
  - Nonequilibrium steady-state configuration ensembles
  - Equilibrium–nonequilibrium comparison
  - Tests in nonequilibrium systems
  - Boundaries of applicability

Overall output: Statistical-structural mechanisms of higher-order pseudo-phase transitions, observable canonical criteria, and boundaries of applicability in nonequilibrium systems

Figure 1 Cross-statistical-level characterization framework for higher-order transitions in finite systems. The microcanonical entropy and its higher-order derivatives provide a thermodynamic prototype for statistical structural rearrangement; canonical response functions, energy cumulants, and geometric observables transform this prototype into observable criteria; spectral-statistical projections further characterize the carrier modes of structural rearrangement at the level of the overall organization of configuration ensembles.

2 The theoretical foundations of higher-order transitions

This section mainly reviews the evidentiary basis and observable representations of higher-order transitions in finite systems. It first explains why phase-transition criteria in finite systems must shift from thermodynamic singularities to structural rearrangements; then introduces how microcanonical inflection-point analysis (MIPA) identifies independent and dependent transitions through derivatives of the microcanonical entropy; and further discusses how canonical cumulants, geometric observables, and spectral-statistical methods form complementary relations across different statistical levels and microcanonical classifications.

2.1 Rewriting the language of phase transitions in finite systems

Classical phase-transition theory is built upon the thermodynamic limit. Within this framework, phase transitions are usually defined by the nonanalytic behavior of thermodynamic potentials and their derivatives: a first-order phase transition corresponds to a discontinuity in the first derivative of the free energy, a second-order phase transition corresponds to a singularity in the second derivative, and higher-order transitions can, in form, be extended upward in the same way. Such a description is natural and effective in macroscopic systems, but for finite systems it immediately encounters a fundamental difficulty: in finite systems there are no genuinely strict thermodynamic singularities. Many quantities that, in infinite systems, would appear as divergences, jumps, or cusps are smoothed out in finite systems, leaving only peaks, shoulders, bends, local extrema, or even broad response intervals. This has been pointed out directly for the Potts model [34]. Traditional phase-transition theory focuses on macroscopic infinite systems, whereas many real systems—including nanomaterials, biological systems, social systems, and complex systems [61–65]—all have finite size. Therefore, the thermodynamic singularities on which traditional phase-transition definitions rely do not exist in these systems, and new definitions of phase transitions in finite systems must be sought.

Precisely for this reason, the study of phase transitions in finite systems cannot simply be understood as a low-precision version of thermodynamic-limit theory. More accurately, the transition problem in finite systems asks: after strict singularities have disappeared, does the system still possess a reproducible, comparable, and physically meaningful level of cooperative reorganization? Recent work on canonical physical quantities has given a very clear summary of this [37]: in finite systems, neighborhoods of the primary transition often still contain "additional transitions" that are not accompanied by singularities. These higher-order features correspond to precursor behavior on the disordered side and reorganizations on the ordered side; they carry, from the perspective of conventional low-order observables,

information on otherwise invisible defect formation, mesoscopic organization, and fluctuation rearrangement.

This shift in definitional perspective is crucial. It means that the goal of studying high-order transitions is not to forcibly seek rounded singularities in finite systems, but to establish a new language capable of describing how finite systems accomplish organizational rearrangements in a hierarchical manner. Small-world networks also clearly indicate [59] that, in finite systems, beyond the primary critical features there may also exist additional reorganizations beyond the main low-order critical characteristics. The importance of such high-order behavior lies precisely in the fact that it reflects changes in domains, boundaries, and mesoscopic correlations that conventional thermodynamic quantities cannot adequately characterize.

2.2 Microcanonical Inflection-Point Analysis and Independent/Dependent Transitions

Microcanonical analysis has rapidly become a theoretical foundation for the study of high-order transitions because it does not rely on divergences of response functions in the canonical ensemble, but instead starts directly from the density of states $g(E)$ and the microcanonical entropy

$$S(E) = k_B \ln g(E) \tag{2.1}$$

and interprets phase transitions as changes in curvature and breakdowns of monotonicity in the entropy and its higher-order derivatives. Formally, the first-level object of microcanonical analysis is the inverse microcanonical temperature,

$$\beta(E) = \frac{dS(E)}{dE} \tag{2.2}$$

followed by the second derivative,

$$\gamma(E) = \frac{d^2S(E)}{dE^2} \tag{2.3}$$

and the third derivative,

$$\delta(E) = \frac{d^3S(E)}{dE^3}. \tag{2.4}$$

Within a single-phase interval, these functions usually maintain relatively regular monotonic and curvature properties; once the system undergoes cooperative reorganization, the corresponding derivative hierarchy exhibits the least-sensitive inflection point or local extremum. The least-sensitive inflection point in $\beta(E)$ marks the energy corresponding to the phase transition; $\gamma(E)$ exhibits a pronounced extremum at the primary transition; and $\delta(E)$ exhibits a positive minimum located at $T < T_c$ and a negative maximum located at $T > T_c$, corresponding respectively to third-order independent and third-order dependent transitions.

Theoretically, this formulation has two direct advantages. First, it bypasses the obstacle that finite systems have no true singularities, because what it concerns is not divergence itself but the reorganization of curvature structures within the derivative hierarchy. Second, it is naturally suited for extension to higher orders: whether first-order, second-order, third-order, or still higher-order transitions, all can be described uniformly within the same derivative–inflection-point–extremum language. Qi and Bachmann combined precisely this line of thought with the principle of minimal sensitivity, thereby forming the later microcanonical inflection-point analysis, as shown in Table 1.

Table 1 Sign criteria for transitions of different orders in microcanonical inflection-point analysis

Category	Even-order transition	Odd-order transition
Independent type	$d^{2k}S(E)/dE^{2k} < 0$	$d^{2k-1}S(E)/dE^{2k-1} > 0$
Independent type	negative local maximum	positive local minimum
Dependent type	$d^{2k}S(E)/dE^{2k} > 0$	$d^{2k-1}S(E)/dE^{2k-1} < 0$
Dependent type	positive local minimum	negative local maximum

Because the core input of MIPA is the density of states $g(E)$ or the microcanonical entropy $S(E)$, while high-order transition signals also depend on higher-order derivatives of $S(E)$, numerical reliability occupies a particularly important position in this field. Compared with conventional canonical analysis, microcanonical higher-order derivatives are more sensitive to statistical noise, energy discretization, smoothing methods, and sampling coverage. If the density of states

Near the transition interval, systematic bias may exist, or smoothing may introduce artificial oscillations; these can produce spurious extrema in $\gamma(E)$, $\delta(E)$, and even higher-order derivatives. Therefore, in reviewing studies of higher-order transitions, one cannot merely ask "whether a higher-order signal has been observed" ; one must also discuss how such signals are confirmed through reliable sampling and cross-validation.

At present, the most commonly used routes are Wang-Landau sampling, multiple-histogram reweighting, and parallel tempering. The advantage of the Wang-Landau method is that it performs a random walk directly in energy space and gradually estimates $g(E)$ according to the flat-histogram idea, thereby reconstructing canonical thermodynamic quantities at different temperatures after a relatively complete sampling of energy space [29, 30, 66–68]. This is especially important for MIPA, because MIPA is not concerned only with the peak and drop near a fixed temperature, but instead needs to extract the curvature structure of the entropy derivative from the entire energy interval. Parallel tempering improves ergodicity in complex energy landscapes through exchanges between replicas at different temperatures, and is particularly suitable for systems with multi-valley structures, phase coexistence, or relatively high energy barriers [32, 33]. In studies of the Potts model, the authors used both Wang-Landau and parallel tempering to obtain the DOS, and compared the higher-order transition positions obtained by the two methods; this point is crucial for excluding artifacts of a single algorithm [34].

In addition to sampling algorithms, smoothing derivatives is also a key step in higher-order transition analysis. The density of states or entropy function is usually obtained in the form of discrete energy points, whereas MIPA requires it to be continuousized, smoothed, and differentiated. Bézier curves, polynomial fitting, local smoothing, and histogram reweighting may all change the shapes of local extrema in higher-order derivatives. Therefore, different studies usually need to combine error estimation, size variation, peaks of canonical thermodynamic quantities, and geometric observables for cross-confirmation. Bachmann' s work on the statistical mechanics of macromolecular systems also emphasizes that microcanonical analysis of finite systems requires combining generalized-ensemble sampling, histogram reconstruction, and smoothing procedures in order to obtain interpretable phase behavior in finite-size structural transitions.

Accordingly, this paper treats numerical reliability as part of the study of higher-order transitions, rather than as a technical appendix. For a higher-order signal to be regarded as physically meaningful, it usually needs to satisfy at least three conditions: first, it has a traceable temperature or energy location under different system sizes or different sampling methods; second, it exhibits mutually corroborating relations among microcanonical derivatives, canonical fluctuations, and geometric observables; third, it can correspond to some interpretable structural reorganization process, rather than merely being an isolated numerical oscillation appearing in higher-order derivatives. This standard also explains why recent work has increasingly emphasized the complementary relationship among MIPA, canonical criteria, and geometric order parameters.

2.3 From Microcanonical to Observable Characterization: Canonical Responses, Geometric Quantities, and Spectral Statistics

Although MIPA provides a clear classification framework, it essentially relies on the density of states or derivatives of the microcanonical entropy, while constructing the density of states is not always feasible in large systems, complex energy landscapes, and nonequilibrium steady states. Therefore, an important recent advance has been to translate higher-order transitions from classification by entropy derivatives into directly computable canonical fluctuation criteria, and further to establish connections with geometric observables and spectral-statistical characterizations.

Figure 2 summarizes this research logic. Higher-order derivatives of the microcanonical entropy first provide the classification basis for higher-order transitions; canonical cumulants convert the third-order information in entropy derivatives into the asymmetry of the energy-fluctuation distribution; geometric quantities such as isolated spins, cluster area, and perimeter further explain the structural reorganization processes corresponding to these fluctuation signals; spectral statistics and nonequilibrium models are then used to test the applicability boundaries of this criterion in complex systems.

Figure 2 (flowchart text). Technical route for statistical-structural criteria of higher-order pseudo-phase transitions.

Scientific question: What statistical-structural criteria allow higher-order pseudo-phase transitions to be observed, verified, and generalized?

- **Theoretical basis**
  - Microcanonical system: microcanonical entropy
    [Phys. Rev. Lett. 120, 180601 (2018)]
  - Derivation via saddle-point expansion
  - Canonical system: canonical generalized response quantities
    [arXiv.2603.09124 (2026)]
  - Universal theoretical basis for third-order phase transitions
- **Microstate structure**
  - Statistical structure of microstate ensembles
    [Phys. Rev. E. 106, 014314 (2022)
    Phys. Rev. E. 111, 054128 (2025)]
  - Eigen-microstate analysis
  - Evolution of spectral weights and modal morphology
  - Observable structural criteria are observable
- **Cross-dynamical tests and mechanistic analysis**
  - Spin models on complex networks
    [J. Stat. Mech. 2024, 083402 (2024)]
  - Comparative tests of generalized responses and structural criteria
  - Validity analysis in complex systems
    [Phys. Rev. Lett. 135, 138401 (2025)]
  - Explanation of deviation mechanisms

Overall output: statistical-structural mechanisms of higher-order pseudo-phase transitions, canonical observable criteria, and boundaries of applicability in nonequilibrium settings.

Figure 2. Research logic from microcanonical criteria to observable characterization for higher-order transitions. Higher-order derivatives of the microcanonical entropy provide the basis for classification; canonical cumulants and geometric statistical quantities convert them into observable signals; spectral statistics, complex networks, and nonequilibrium models are then used to test the generalizability and applicability boundaries of these structural criteria.

Taking the canonical partition function

$$Z(\beta) = \sum_E g(E) e^{-\beta E} \tag{2.5}$$

as the starting point, introduce the cumulant generating function

$$K(\beta) = \ln Z(\beta), \tag{2.6}$$

and define the energy cumulants

$$\kappa_n(\beta) = (-1)^n \frac{\partial^n K(\beta)}{\partial \beta^n}. \tag{2.7}$$

Here,

$$\langle E \rangle = -\frac{\partial K}{\partial \beta}, \qquad \kappa_2 = \frac{\partial^2 K}{\partial \beta^2}, \qquad \kappa_3 = -\frac{\partial^3 K}{\partial \beta^3}. \tag{2.8}$$

On this basis, one may construct the third-order canonical diagnostic quantity

$$\Xi(T) = \frac{\kappa_3(T)}{[\kappa_2(T)]^3}. \tag{2.9}$$

Below we explain the bridging relation between this canonical criterion and the microcanonical classification. Let $E = Ne$, and define the microcanonical entropy per degree of freedom as

$$s(e) = \frac{1}{N} \ln g(E). \tag{2.10}$$

In the thermodynamic limit, the partition function can be approximately written as

$$Z(\beta) \simeq \int de \, \exp\left[N\phi_\beta(e)\right], \qquad \phi_\beta(e) = s(e) - \beta e. \tag{2.11}$$

In a single-saddle region, the integral is governed by the condition

$$\left.\frac{d\phi_\beta(e)}{de}\right|_{e=e^*} = 0. \tag{2.12}$$

is governed by the dominant energy density e^*, and therefore

$$s'(e^*) = \beta. \tag{2.13}$$

This indicates that the canonical temperature corresponds to a dominant energy position on the microcanonical entropy curve.

Differentiating the saddle-point condition $s'(e^*) = \beta$ with respect to β, one obtains

$$s''(e^*)\frac{de^*}{d\beta} = 1, \tag{2.14}$$

that is,

$$\frac{de^*}{d\beta} = \frac{1}{s''(e^*)}. \tag{2.15}$$

Since

$$\langle E \rangle \simeq Ne^*, \tag{2.16}$$

the second-order energy cumulant is

$$\kappa_2 = -\frac{d\langle E \rangle}{d\beta} \simeq -N\frac{de^*}{d\beta} = -\frac{N}{s''(e^*)}. \tag{2.17}$$

On a thermodynamically stable concave entropy branch, $s''(e^*) < 0$, and therefore $\kappa_2 > 0$, consistent with the physical requirement for energy fluctuations.

Further differentiating κ_2, one obtains the third-order energy cumulant

$$\kappa_3 = -\frac{d\kappa_2}{d\beta} \simeq -N\frac{s^{(3)}(e^*)}{[s''(e^*)]^3}. \tag{2.18}$$

Thus one obtains

$$N^2\frac{\kappa_3}{\kappa_2^3} \simeq s^{(3)}(e^*). \tag{2.19}$$

Therefore, when the single-saddle-point approximation holds, there exists an asymptotic bridge between the canonical cumulant criterion and the third derivative of the microcanonical entropy:

$$N^2\Xi(T) \to s^{(3)}(e^*), \qquad \Xi(T) = \frac{\kappa_3(T)}{[\kappa_2(T)]^3}. \tag{2.20}$$

This relation shows that $\Xi(T)$ is not an empirical higher-order moment; rather, under the single-saddle-point condition, it has an asymptotic correspondence with the third derivative of the microcanonical entropy. Since $\kappa_2 > 0$, the sign of $\Xi(T)$ is determined by κ_3, and it inherits the classification information contained in $s^{(3)}(e^*)$. Therefore, a negative local maximum of $\Xi(T)$ corresponds to a dependent-type third-order transition, whereas a positive local minimum corresponds to an independent-type third-order transition. In other words, the microcanonical classification given by MIPA can be read from the asymmetry of energy fluctuations in the canonical system, thereby avoiding an explicit reconstruction of the density of states.

From a physical perspective, κ_2 describes the width of the energy distribution, i.e., the ordinary energy fluctuation, whereas κ_3 describes the asymmetry of the energy distribution. A third-order transition does not necessarily correspond to a low-order response anomaly such as a heat-capacity peak; instead, it manifests as a local rearrangement of the skew direction and skew strength of the energy distribution. Thus $\Xi(T)$ can be understood as a normalized indicator of the asymmetry of energy fluctuations. It is not the usual skewness $\kappa_3/\kappa_2^{3/2}$, but adopts the normalization κ_3/κ_2^3, so as to ensure that in the single-saddle-point limit it can correspond directly to the third derivative $s^{(3)}(e^*)$ of the microcanonical entropy. This is precisely the key point distinguishing the canonical criterion from empirical higher-order moment analysis.

Moreover, from the canonical-system identity

$$\kappa_2(T) = T^2 C_V(T) \tag{2.21}$$

and

$$\kappa_3(T) = -\frac{d\kappa_2}{d\beta} \tag{2.22}$$

we obtain

$$\kappa_3(T) = T^4 \frac{dC_V}{dT} + 2T^3 C_V(T). \tag{2.23}$$

Therefore, the third-order energy cumulant contains not only the energy fluctuation strength itself, but also the reorganization information associated with the temperature dependence of that fluctuation strength. This also explains why a third-order transition can manifest, in addition to a conventional heat-capacity peak, as a more refined asymmetric signal of fluctuation rise and fall.

The above relation has a clear illustration in the exact Onsager solution of the two-dimensional Ising model [69]. As shown in Figure 3, the positive local minimum of $\Xi(T)$ corresponds to an independent-type third-order signal on the low-temperature side, the negative local maximum corresponds to a dependent-type third-order signal on the high-temperature side, and the gray mark denotes the main critical point. Correspondingly, the isolated-spin number n_1 exhibits a stable feature near the independent-type signal, reflecting the emergence of local defects within an ordered background; the cluster-average area change rate dA/dT shows a pronounced response near the dependent-type signal, indicating that the cluster structure and boundary organization on the high-temperature side have already undergone rearrangement. Thus, the figure demonstrates a direct correspondence from the canonical cumulant criterion to geometric structural images.

No.	Point	Color	T	Meaning
1	Critical transition	Gray	2.269	Criticality
2	Independent third-order	Green	2.229	Ordered-side reorganization
3	Dependent third-order	Orange	2.567	Disordered precursor

Figure 3. Correspondence between the canonical third-order criterion and geometric observables in the two-dimensional Ising model. (a) Temperature dependence of the canonical cumulant ratio $\Xi = \kappa_3/\kappa_2^3$, where the positive local minimum corresponds to the independent-type third-order signal, the negative local maximum corresponds to the dependent-type third-order signal, and the gray mark denotes the main critical point; (b) response of the isolated-spin number n_1 to the independent-type signal on the low-temperature side; (c) response of the cluster-average area change rate dA/dT to the dependent-type signal on the high-temperature side. Different curves correspond to different system sizes. Adapted from Ref. [37].

It can thus be seen that $\Xi(T)$ gives the positions and types of the third-order signals, whereas the geometric observables further reveal the specific structural processes corresponding to these signals. The former provides a criterion, and the latter provides a physical picture; the two are not substitutes for one another. Independent-type and dependent-type transitions should also not be understood as purely mathematical names. In existing studies of two-dimensional spin models, third-order independent-type transitions are usually located on the low-temperature side of the main phase transition and can be interpreted as local loosening, defect nucleation, or micro-fracturing of clusters within an ordered background; third-order dependent-type transitions are usually located on the high-temperature side of the main phase transition and are closer to precursor-like fluctuation reorganization on the disordered side, cluster disintegration, or boundary rearrangement. Therefore, the sign rules of MIPA provide classification criteria, the canonical criterion provides an observable route, and the geometric quantities further endow these classifications with structural images.

In addition to canonical cumulants and geometric observables, spectral-statistical methods provide another possible characterization of higher-order transitions. The basic idea is to regard the sampled microscopic configurations as an ensemble of configurations, and to characterize the overall organization of their statistical structure through covariance structures, eigenmodes, or distributions of spectral weights. Unlike local geometric quantities, spectral statistics focuses on how statistical weights are redistributed among different modes in configuration space; it may therefore be applicable to complex systems in which an explicit order parameter is difficult to define and geometric observables are not easy to construct. At present, however, the correspondence between spectral statistics and higher-order transitions remains at an exploratory stage. How to distinguish genuine structural rearrangements from finite-sampling noise, and how to establish stable correspondences between spectral quantities and microcanonical and canonical criteria, still require further study.

2.4 Spectral Statistics and Eigen-Microstate Characterization

In addition to canonical cumulants and geometric observables, recent eigen-microstate methods further describe higher-order transitions as redistributions of spectral weights in configuration space [41]. This method first organizes microscopic configurations sampled at fixed temperature into a configuration matrix, and obtains a set of eigen-microstates and their spectral weights through singular-value decomposition. Unlike ordinary principal-component analysis, the eigen-microstate framework is not mainly used for dimensional reduction; rather, it interprets spectral weights as the way in which a statistical system is organized in configuration space. Ordinary phase transitions correspond to the condensation of dominant eigenmodes, whereas higher-order pseudo-transitions correspond to more delicate rearrangements of spectral weights in the subspace of fluctuations beyond the dominant modes.

Within this framework, let the normalized spectral weight be w_α, and define the spectral cumulants with respect to the uniform weight $\bar{w}$ as

$$K_n = \sum_\alpha (w_\alpha - \bar{w})^n. \tag{2.24}$$

Here, K_2 characterizes the overall degree of concentration of the spectral weights, while K_3 describes the asymmetric redistribution of weights among different fluctuation modes. Thus one can construct the third-order spectral response

$$R_3 = \frac{K_3}{(K_2)^3}. \tag{2.25}$$

The role of this ratio is analogous to that of the third-order ratio in canonical energy-cumulant criteria, but its object is no longer energy fluctuations; rather, it is the rearrangement of the weights of eigenmodes in configuration space. Therefore, extrema of R_3 can serve as spectral-statistical signals of third-order pseudo-transitions.

More importantly, spectral projection also provides an operational way to distinguish independent-type and dependent-type third-order pseudo-transitions. If, after removal of the dominant eigenmodes, the characteristic extremum of R_3 still exists, this indicates that the signal mainly arises from weight rearrangements inside the subspace of secondary fluctuations, and may be attributed to an independent-type higher-order reorganization. If the extremum is significantly weakened or disappears after removal of the dominant modes, this indicates that the signal is still attached to the leading ordered channel of the primary phase transition, and is closer to a dependent-type higher-order precursor. Thus, higher-order transitions can no longer be understood only as local extrema in derivatives of the free energy; they can also be interpreted as redistributions of statistical weight among different fluctuation modes in configuration space.

The significance of this spectral-statistical viewpoint lies in the fact that it further connects microcanonical, canonical, and geometric characterizations. Microcanonical methods provide the geometric prototype of higher-order transitions in terms of entropy; canonical cumulants provide observable fluctuation criteria; real-space geometric quantities reveal defect and boundary rearrangements; and eigen-microstate spectra start from the organization of the entire ensemble of configurations, depicting the transfer of statistical weight behind higher-order transitions. Therefore, spectral-statistical methods are particularly suitable for inclusion in a cross-level characterization framework for higher-order transitions in finite systems, serving as a supplement that moves from local geometric structures toward the global organization of configuration space.

In summary, from microcanonical entropy derivatives to canonical cumulants, geometric observables, and spectral-statistical characterizations, the study of higher-order transitions is forming an analytical framework that spans statistical levels. Microcanonical methods provide a language of classification, canonical criteria provide computable fluctuation diagnoses, geometric quantities provide structural images, and spectral statistics offers a further possibility for analyzing the overall configurational organization of complex systems. The following sections will first review the main evidence for these signals in the equilibrium Ising model, and then discuss their geometric mechanisms and extensions to complex systems.

Table 2 Comparison of Major Characterization Methods for High-Order Transitions in Finite Systems

Method	Core object	Main advantages	Main limitations
Microcanonical inflection-point analysis	Entropy density and microcanonical entropy derivatives	Clear classification; can distinguish independent and dependent types	Relies on high-precision DOS; high-order derivatives are sensitive to noise
Canonical cumulant criterion	Energy jumps and their high-order cumulants	Reconstructs the DOS implicitly; facilitates canonical simulations and extension to nonequilibrium data	The correspondence with microcanonical classification depends on a single saddle point or approximation conditions
Geometric statistics	Isolated spins, cluster area, perimeter, and boundary density	Structural images are intuitive; can explain defects and boundary rearrangement	Observables are model-dependent and cannot be simply transferred across models
Spectral statistical methods	Eigen-microstate spectral weights and their projections	Characterizes the redistribution of statistical weights from the overall organization of configuration space	Affected by the number of samples, projection depth, and spectral resolution
Nonequilibrium and network extensions	Network topology, dynamical response, and absorbing-state structure	Can be used for early-warning signals and structural-reorganization analysis in complex systems	Do not necessarily have a strict thermodynamic order meaning

3 High-Order Transitions in Equilibrium Spin Models

Figure 4 Schematic illustration of microcanonical inflection-point analysis (MIPA) for the Ising model: (a) microcanonical entropy per spin, $S(e)/L^2$; (b) inverse microcanonical temperature, $\beta(e)$; (c) second derivative, $\gamma(E)L^2$; (d) third derivative, $\delta(E)L^4$. The dashed lines mark the positions of independent-type (green) and dependent-type (orange) signals for different system sizes.

From [Phys. Rev. E. 106, 014134 (2022)].

Equilibrium spin models are the most important starting platform for research on high-order transitions. On the one hand, such models have clear Hamiltonians, mature numerical methods, and relatively stable phase-diagram structures, making them suitable for testing new theoretical criteria. On the other hand, they are sufficiently rich to cover different primary transition types, including continuous phase transitions, first-order phase transitions, and tricritical behavior. Therefore, from the Ising and Baxter–Wu models to the Potts and Blume–Capel models, equilibrium spin models not only constitute the main testing ground for high-order-transition research, but also gradually show how high-order signals evolve from "additional phenomena" into comparable transition spectra. Along this chain of models, research on high-order transitions has progressed step by step from verifying their existence, to comparing primary phase-transition types, and then to reorganizing high-order spectra near tricritical points.

3.1 Ising and Baxter–Wu Models: Early Verification

The status of the two-dimensional Ising model in phase-transition theory needs no elaboration. It is both an important testing platform for classical continuous-phase-transition theory and a benchmark object for many later finite-system analysis methods. The 2022 study of finite-size two-dimensional Ising and Baxter–Wu models was carried out precisely against this background. That work used Wang–Landau sampling to obtain the DOS,

and, in combination with microcanonical inflection-point analysis (MIPA), systematically studied the order of finite-size pseudo-phase transitions. The results show that, for the Ising model, the order of the principal transition obtained from microcanonical analysis is consistent with that from conventional canonical analysis; more importantly, beyond the principal second-order phase transition, third-order transition signals can also be identified.

Figure 4 shows the microcanonical entropy per spin of the Ising model and the variation of its higher-order derivatives with energy. The independent-type signals on the low-temperature side correspond to local defects or local rearrangements, whereas the dependent-type signals on the high-temperature side correspond to boundary roughening or global rearrangement. As the system size increases, the peak value of γ decreases, indicating a weakening of the latent-heat effect. These features provide a benchmark for understanding the behavior of third-order signals in finite-size systems. Moreover, in the thermodynamic limit, the signals of both third-order dependent and independent transitions still persist, demonstrating the stability of third-order transitions.

In addition to the Ising model, the Baxter–Wu model provides another finite-size-system setting for verifying higher-order signals. It is defined on a triangular lattice and, at finite size, exhibits more pronounced coexistence and back-bending features. Figure 5 shows the results of microcanonical inflection-point analysis for spin-1/2 systems (left three panels) and spin-1 systems (right three panels). The peaks of $\gamma(E)$ and $\delta(E)$ clearly mark the locations of independent-type and dependent-type third-order signals. Compared with the Ising model, the independent-type and dependent-type signals in the Baxter–Wu system are closer to each other in energy space, and their peak values decrease as the system size increases, further verifying the recognizability of higher-order signals in a pseudo-first-order background.

Figure 5 Schematic illustration of microcanonical inflection-point analysis for the Baxter–Wu model: the left three panels (a–c) are for the spin-1/2 system, and the right three panels (d–f) are for the spin-1 system: (a,d) inverse microcanonical temperature $\beta(E)$; (b,e) second derivative $\gamma(E)$; (c,f) third derivative $\delta(E)$. Different colors indicate different system sizes N, and the peaks correspond to independent-type and dependent-type third-order signals. From [J. Stat. Mech. 2024, 093201 (2024)].

This phenomenon can be understood as follows: an independent-type third-order transition corresponds to the local rearrangement of a higher-order superheated state into a lower-order metastable state, whereas a dependent-type third-order transition corresponds to the evolution of a supercooled lower-order metastable state into a disordered state. Overall, these results demonstrate the universality of microcanonical higher-order signals in two-dimensional spin models and provide a theoretical foundation for subsequent analyses of complex systems.

3.2 Potts model: from continuous phase transitions to first-order phase transitions

If the Ising and Baxter–Wu models mainly completed the early verification of the existence of higher-order signals, then the Potts model pushed this question to a more systematic level of comparison. The outstanding advantage of the Potts model is that, by changing the value of q, continuous phase transitions and first-order phase transitions can be compared within the same theoretical framework. It is therefore especially well suited to answering the following question: when the nature of the primary phase transition changes, how do the hierarchy, strength, and visibility of higher-order transitions change? The 2024 work on finite-size Potts models was developed precisely around this question [34]. The article used two methods, Wang-Landau and parallel tempering, to obtain the DOS, and employed MIPA to systematically locate third-order transitions. The results obtained show that the two methods give highly consistent positions for the higher-order transitions.

The significance of the work on the Potts model lies first in making the methodology itself more robust. Unlike the Ising model, for which an exact DOS benchmark exists, the DOS of the Potts model must be obtained numerically. The article specifically compared the two commonly used methods, Wang-Landau and PT, and pointed out that the DOS obtained by the two are close to each other, thereby verifying the reliability of using WL for further MIPA. In this way, the identification of higher-order transitions is no longer merely a result under one particular algorithm, but is jointly supported by two different numerical routes.

Figure 6 Microcanonical inflection-point analysis of the two-dimensional Potts model: the three panels on the left (a–c) are for the $q = 4$ system, and the three panels on the right (d–f) are for the $q = 6$ system; (a, d) inverse microcanonical temperature $\beta(E)$; (b, e) second derivative $\gamma(E)$; (c, f) third derivative $\delta(E)$. Different colors represent different system sizes N; the peak values correspond to independent-type (green) and dependent-type (orange) third-order signals. From [J. Stat. Mech. 2024, 093201 (2024)].

More importantly, the Potts model enabled researchers, for the first time, to systematically compare third-order signals under different types of primary phase transitions. In its results, the article presented MIPA analyses for $q = 3, 4, 6, 8$, and summarized a more general odd–even order criterion: for odd

order transitions: for the independent type, the positive local minimum of a higher-order entropy derivative corresponds to it, while for the dependent type, the negative local maximum corresponds to it; for even orders, the signs are reversed. At the same time, the authors pointed out that when $q = 6$, the third-order independent and dependent transitions are very close in temperature. This is because, at finite size, the six-state Potts model has entered the first-order phase-transition regime, where $\beta(E)$ exhibits backbending; the latent heat and the approximately isothermal process bring the two third-order signals close together in temperature, although the energy states to which they correspond remain separated.

Figure 6 presents the microcanonical inflection-point analysis for the $q = 4$ system (left three columns a–c) and the $q = 6$ system (right three columns d–f). The peak values of the second derivative $\gamma(E)$ and the third derivative $\delta(E)$ clearly mark the positions of the independent-type (green) and dependent-type (orange) third-order signals. For the continuous main phase transition at $q = 4$, both the independent-type and dependent-type signals can be identified; whereas in the first-order main phase transition at $q = 6$, the independent-type signal still exists, but the dependent-type signal is no longer clear because of the backbending and latent-heat effects of the main phase transition. Curves for different system sizes N show that the amplitude and sharpness of the higher-order signals adjust with system size, but the overall trend remains consistent.

The further significance of the Potts model lies in that it connects the third-order signals identified by MIPA with geometric observables in the canonical ensemble. Studies have shown that the geometric order parameters in the Ising model cannot be directly transplanted into the multistate Potts model: a single-site cluster in a high-temperature fragmented background is not equivalent to an isolated defect in the ordered phase. Therefore, isolated spin vortices need to be redefined. The number of isolated spin vortices can stably characterize the third-order independent transition on the low-temperature side, whereas the average cluster perimeter is more suitable than cluster area for tracking the third-order dependent transition on the high-temperature side. This also suggests that dependent-type signals may rely more on whether a distinguishable boundary-rearrangement window exists near the main phase transition, while independent-type signals are closer to local rearrangements inside the ordered side. A more general geometric interpretation will be developed in the next section.

3.3 Blume–Capel Model: Tricritical Point and Higher-Order Spectral Recombination

On the basis of the preceding analyses of the Ising, Baxter–Wu, and Potts models, we further examine the Blume–Capel model in order to explore how higher-order signals evolve with changes in the type of main phase transition. The Blume–Capel model contains, within the same system, second-order phase transitions, first-order phase transitions, and tricritical points [70–72], making it an ideal object for studying higher-order signal spectral recombination [36].

In the second-order phase-transition interval (for example, $D = 1.0$), the system can simultaneously exhibit independent-type and dependent-type third-order signals. Near the tricritical point, several positive local minima may appear on the low-energy side, but some of them disappear as the system size increases; only the independent-type signal on the high-energy side remains stable. After further entering the first-order phase-transition region, only an independent-type third-order signal can be observed; the dependent-type signal disappears, while a new fourth-order independent signal appears in the high-temperature region. This indicates that higher-order signals are not fixed to the two sides of the main phase transition, but instead may be promoted in order, disappear, or rearrange as the main phase-transition mechanism changes.

This result suggests that studies of higher-order transitions should be placed in a broader spectral perspective: when a third-order dependent signal disappears, the system does not mean that it lacks higher-order structure, but may instead turn toward an additional recombination process of higher order, more distant in position, or different in mechanism. The Blume–Capel model is the first typical example that clearly demonstrates this phenomenon.

3.4 Clock Model: Higher-Order Precursors in Topological Transitions

In addition to Landau-type symmetry-breaking models, the two-dimensional six-state Clock model provides a topological testing ground for higher-order transitions. When $q \geq 5$, the system usually undergoes two Berezinskii–Kosterlitz–Thouless (BKT)–type transitions: low-temperature quasi-long-range ordered phase → intermediate critical phase → high-temperature disordered phase [73–77]. This type of transition differs from conventional first- or second-order phase transitions; its core mechanism relies on the unbinding of topological defects such as vortices.

Recent studies have used Wang–Landau sampling and MIPA to identify two main transition points in the finite-size six-state Clock model, and, combined with canonical geometric analysis, discussed fourth-order dependent transition signals [?]. The results show that these signals may provide early warnings before the main transition, indicating that higher-order signals are not limited to third order, nor are they limited to traditional Landau-type systems. In transitions driven by topological defects, higher-order dependent signals may carry information about changes in local modes of organization.

It should be noted that BKT-type transitions have exponential divergence of the correlation length, strong finite-size drift, and thermodynamic peaks that do not

···such as sharpness. Therefore, the locations and scaling of higher-order signals must be rigorously verified. At the same time, a unified framework has not yet been established for the canonical criteria and geometric interpretation of fourth-order dependent transitions. Thus, in this paper, the Clock model is more suitable as an example of the "extension of the higher-order hierarchy to topological transitions" than as a universal conclusion.

For ease of comparison, Table 3 summarizes the primary phase-transition backgrounds, higher-order signals, and principal characterization methods in several typical models. It can be seen that the form in which higher-order signals exist changes with the type of phase transition, the structure of the degrees of freedom, and the topology of the phase diagram. Meanwhile, the mutual corroboration among microscopic canonical derivatives, canonical responses, and geometric observables provides an important basis for judging the physical meaning of the signals.

Table 3 Higher-order transition signals in typical models and their characterization methods

Model	Primary phase-transition background	Higher-order signal	Main characterization quantities
Ising	Second order	Third-order independent/dependent	Entropy derivative, isolated spins, cluster quantities
Baxter–Wu	Finite-size pseudo-first-order	Third-order independent/dependent	MIPA, analysis of the backbending region
Potts	Continuous for $q \leq 4$; first-order for $q > 4$	Third-order signal changes with q	Number of isolated spins, average cluster perimeter

Model	Primary phase-transition background	Higher-order signal	Main characterization quantities
Blume–Capel	Second-order, first-order, tricritical point	Third-order dependence disappears; fourth-order independence appears	MIPA, geometric quantities, phase-diagram parameters
Clock	BKT-type topological transition	Precursor of fourth-order dependence	m_{Z_6}, average cluster perimeter

However, merely identifying where higher-order signals appear is not sufficient to explain what physical processes they correspond to. As studies of models continue to accumulate, a more critical question gradually becomes prominent: do these higher-order signals reflect the nucleation of defects, the rearrangement of boundaries, or more general changes in mesoscopic organization? This requires us to move beyond criterion-based identification toward geometric interpretation, transforming independent- and dependent-type signals into more intuitive images of structural reorganization.

4 Geometric Characterization and Structural Images of Higher-Order Transitions

Microscopic canonical derivatives and canonical cumulants can indicate the location and type of higher-order transitions, but by themselves they do not directly explain what kinds of structural changes occur inside the system. The role of geometric characterization is to convert these abstract criteria into interpretable structural images: independent-type signals on the low-temperature side usually correspond to the emergence of local defects in an ordered background, whereas dependent-type signals on the high-temperature side more often reflect cluster boundaries, interfacial complexity, and the rearrangement of fragmented structures. Starting from computational methods and geometric observables, this section summarizes the physical images of higher-order transitions.

4.1 Overview of Cluster Statistical Methods

The geometric characterization of higher-order transitions relies on stable identification of cluster structures in microscopic configurations. Unlike bulk phase averages such as heat capacity and magnetization, cluster statistics directly depict local defects, connected regions, and boundary organization in spin models, and are therefore especially suitable for explaining the structural origins of independent- and dependent-type third-order signals. In general, cluster statistical analysis includes three steps: first, equilibrium configurations are obtained by Monte Carlo methods; second, connected regions of identical spins in each configuration are labeled; finally, cluster area, perimeter, number of isolated spins, and their temperature responses are computed and compared with the locations of higher-order signals given by MIPA or canonical-cumulant criteria.

In configuration sampling, commonly used algorithms include Metropolis, Wolff, or Swendsen–Wang cluster-update algorithms [78–80]. For two-dimensional Ising and Potts models near criticality, local updates are easily affected by critical slowing down; therefore, cluster-update methods are usually more efficient. Taking the Swendsen–Wang method as an example, between neighboring lattice sites in the same spin state, bonds are placed with probability

$$p = 1 - \exp(-\beta J) \tag{4.1}$$

Fortuin–Kasteleyn bonds are placed with this probability, and the resulting random clusters are updated as a whole, thereby improving sampling efficiency near the critical region. It should be noted that the Fortuin–Kasteleyn clusters used for updating are not exactly the same as the iso-spin geometric clusters in the subsequent geometric analysis: the former serve Monte Carlo sampling, whereas the latter are used to characterize the spatial organization of configurations. Therefore, in geometric statistics it is usually necessary to relabel the iso-spin configurations obtained by sampling into clusters.

Cluster labeling is commonly performed using the Hoshen–Kopelman [81] method. For a given configuration $\{\sigma_i\}$, define a cluster C as the largest connected component consisting of nearest-neighbor-connected sites with the same spin state, namely

$$i, j \in C, \quad j \in nn(i), \quad \sigma_i = \sigma_j. \tag{4.2}$$

Here $nn(i)$ denotes the set of nearest neighbors of lattice site i. For each cluster C, its area is defined as the number of lattice sites in the cluster,

$$A(C) = \sum_{i \in C} 1, \tag{4.3}$$

and its perimeter is defined as the number of boundary edges between the cluster and external regions with different spin states:

$$P(C) = \sum_{i \in C} \sum_{j \in nn(i)} \left[1 - \delta_{\sigma_i, \sigma_j}\right]. \tag{4.4}$$

Under periodic boundary conditions, boundary edges should also be counted according to the periodic adjacency relation.

In a configuration, if there are N_{cl} geometric clusters in total, then the mean cluster area and mean cluster perimeter can be written as

$$\langle A\rangle = \frac{1}{N_{\text{cl}}}\sum_{C} A(C), \qquad \langle P\rangle = \frac{1}{N_{\text{cl}}}\sum_{C} P(C). \tag{4.5}$$

If the focus is on the boundary structure of non-singleton clusters, singleton clusters with $A(C) = 1$ may also be excluded, and one may define

$$\langle P\rangle_{A>1} = \frac{1}{N_{\text{cl}}^{A>1}}\sum_{C:A(C)>1} P(C). \tag{4.6}$$

This treatment is particularly useful in systems with a strong high-temperature fragmentation background, because a large number of singleton clusters may obscure the true boundary-reorganization signal.

The number of isolated spins is an important geometric quantity for characterizing local defects in an ordered background. In the binary Ising model, an isolated spin can be approximately understood as a singleton cluster whose spin differs from all nearest-neighbor spins; its number can be written as

$$n_{\text{iso}} = \sum_{i}\prod_{j\in nn(i)}\left[1-\delta_{\sigma_i,\sigma_j}\right]. \tag{4.7}$$

For the multi-state Potts model, singleton clusters and isolated spins in an ordered background must be distinguished more carefully. The reason is that, in the high-temperature phase, a large number of singleton clusters may simply be part of the fragmented background and do not necessarily correspond to defect nucleation in the low-temperature ordered region. Therefore, in the Potts model, the definition of isolated spins usually needs to be combined with local neighborhood states or with a resetting of the dominant-cluster background, and cannot simply copy the definition used in the Ising model.

To identify high-order structural signals, one usually considers not only the geometric quantities themselves, but also their rates of change with temperature. For example, for the mean geometric quantity $O(T_i)$ obtained on a temperature sequence T_i, a central-difference estimate may be used:

$$\left.\frac{dO}{dT}\right|_{T_i} \simeq \frac{O(T_{i+1})-O(T_{i-1})}{T_{i+1}-T_{i-1}}, \tag{4.8}$$

where O may be taken as $\langle A\rangle$, $\langle P\rangle$, n_{iso}, or the boundary density, etc. In actual calculations, to reduce numerical noise, one may first perform local polynomial fitting or smoothing of $O(T)$, and then take the derivative. Subsequently, the positions of local extrema of the geometric quantity or its derivative are compared with

MIPA compares the T_{ind} and T_{dep} that it yields, or the extremal positions of $\Xi(T)$ given by the canonical cumulant criterion. In general, the number of isolated spins is more sensitive to independent-type signals on the low-temperature side, whereas the average cluster perimeter or boundary density is more sensitive to dependent-type signals on the high-temperature side.

Figure 7 illustrates the basic definitions of cluster area, perimeter, and the number of isolated spins. The area $A(C)$ counts the number of lattice sites in a cluster; the perimeter $P(C)$ counts the number of boundary edges between the cluster and external regions with different spins; and the number of isolated spins n_{iso} is used to characterize the emergence of local defects. Through these geometric quantities, the higher-order signals identified by microcanonical or canonical criteria can be further transformed into concrete structural images.

Figure 7. Method for cluster observation. The cluster size $A(C)$ counts the number of sites in a connected equal-spin cluster; the perimeter $P(C)$ counts the number of boundary edges; and n_{iso} counts isolated spins. From [arXiv:2603.11522 (2026)].

4.2 Cluster-Geometric Statistics of the Ising and Potts Models

A comparison between the Ising model and the Potts model shows that geometric statistics are not only auxiliary tools for verifying the locations of higher-order transitions, but also key to understanding their physical mechanisms. For the two-dimensional Ising model, microcanonical inflection-point analysis shows that, in addition to the principal second-order ferromagnetic-paramagnetic transition, the system also exhibits a third-order independent transition in the low-temperature ferromagnetic phase and a third-order dependent transition in the high-temperature paramagnetic phase. The corresponding cluster analysis further indicates that the independent-type signal on the low-temperature side corresponds to the peak in the number of isolated spins, showing that the proliferation of local defects in the ordered background reaches its strongest level; whereas the dependent-type signal on the high-temperature side appears as a local minimum in the temperature derivative of the average cluster area, reflecting the fragmentation rate of clusters in the paramagnetic phase and the rearrangement of preordered structures [27].

This geometric picture has been further tested in the Potts model, but it also displays clear model dependence. Because the q-state Potts model has more than two spin orientations, the definition of an "isolated spin" in the Ising model cannot be directly transferred. A more reasonable definition is as follows: a spin has an orientation different from those of its four nearest neighbors, and the four nearest neighbors belong to the same ordered cluster; in this case, the spin is equivalent to a local defect embedded in an ordered cluster. Based on this definition, the number of isolated spins can still stably indicate the third-order independent transition on the low-temperature side. By contrast, for the third-order dependent transition on the high-temperature side, the average cluster area is no longer always sensitive in the Potts model, whereas the average cluster perimeter can more directly characterize changes in cluster boundaries and interfacial complexity, and therefore becomes a more effective geometric quantity for identifying dependent-type third-order signals [35].

Thus, the comparison between the Ising and Potts models shows that the geometric characterization of higher-order transitions should distinguish between two types of structural processes: one is the nucleation of local defects inside the ordered phase, which can be described by local-defect indicators such as the number of isolated spins; the other is the rearrangement of cluster boundaries in the disordered phase or on the critical high-temperature side, which is better characterized by the average perimeter, boundary density, and their temperature derivatives. This result also suggests that geometric statistical methods should not be simply understood as the universal application of a fixed observable, but should instead be adjusted according to the model degrees of freedom, the cluster definition, and the type of principal phase transition.

Figure 8. Schematic analysis of cluster structures in the Ising model and the Potts model: (a,c) the average cluster area $\langle A\rangle$ and average cluster perimeter $\langle P\rangle$ as functions of temperature; (b,d) their derivatives with respect to temperature, $\mathrm{d}\langle A\rangle/\mathrm{d}T$ and $\mathrm{d}\langle P\rangle/\mathrm{d}T$. Different colors denote different system sizes L, and the orange dashed line marks the location of the dependent third-order transition. The figure shows that, on the high-temperature side, the dependent-type signal corresponds to rapid rearrangement of cluster boundaries, whereas on the low-temperature side, the independent-type signal corresponds to the nucleation of local defects in an ordered background. From [arXiv:2603.11522 (2026)].

5 From Finite Macromolecules to Complex Networks: Extensions of the Idea of Higher-Order Transitions

5.1 A Finite-System Perspective in Polymer and Biomacromolecular Systems

Although research on higher-order transitions first developed a clear framework in classical spin models, its deeper motivation comes from the statistical physics of finite systems. Polymers, protein folding, peptide aggregation, and adsorption systems are not thermodynamic-limit systems in the strict sense, yet they often display cooperative behaviors resembling phase transitions, such as collapse, freezing, folding, aggregation, and adsorption. In canonical systems, such processes often appear as broad peaks, shoulder peaks, or multiple overlapping peaks, making it difficult for conventional heat capacity or structural fluctuations to provide a unique classification. Microcanonical analysis therefore has a natural advantage in soft-matter and biomacromolecular systems [?].

In studies of semiflexible polymers, the value of MIPA lies not only in locating transition points, but also in distinguishing neighboring structural transitions that are difficult to resolve using traditional canonical analysis. Related doctoral work and subsequent studies have shown that, near the collapse line of semiflexible polymers, there may exist a mixed structural region composed of hairpin-like, ring-like, and toroidal conformations, while conventional specific heat or radius-of-gyration fluctuations may not clearly indicate the transition into this intermediate phase [50, 51]. This shows that, for finite macromolecular systems with complex conformational spaces and non-sharp phase-region boundaries, the curvature of the microcanonical entropy provides a more refined capability for analyzing phase structure than a single canonical response.

Peptide aggregation systems further demonstrate the role of MIPA in multistage hierarchical transitions. The GNNQQNY heptapeptide is a classic short-peptide model in studies of amyloid aggregation. Its aggregation process contains multiple levels, from monomer conformational adjustment and oligomer formation to the stabilization of ordered aggregate structures. Using efficient microcanonical histogram analysis, one can directly estimate microcanonical quantities from energy histograms and, in combination with generalized MIPA, reveal the complete transition sequence [49]. This type of work complements studies of third-order transitions in spin models: spin models provide clear criteria and controllable phase diagrams, while macromolecular systems show that hierarchical structural reorganization in finite systems is not merely a model phenomenon, but a statistical-mechanical problem widely present in soft matter and biophysical systems.

It is therefore necessary to regard polymers and biomacromolecular systems as an important background. They remind us that the goal of research on higher-order transitions is not merely to extend the Ehrenfest classification by order, but to develop a language for describing phase behavior that is applicable to finite, heterogeneous systems with complex conformational spaces. For such systems, the so-called phase transition is often better understood as the re[[unclear: continuation not visible]]

ordering, the replacement of dominant basins in the free-energy landscape, and changes in the balance among local interactions, entropic effects, and geometric constraints. This finite-system perspective also provides a conceptual basis for subsequently applying higher-order signals to the analysis of complex networks, nonequilibrium dynamics, and absorbing-state systems.

Beyond finite macromolecular systems, complex-network and nonequilibrium-dynamics models further test the limits of applicability of the idea of higher-order transitions. The key question here is not only whether the original criteria can be transplanted into new models, but also whether, in the presence of topological heterogeneity, dynamical rules, and absorbing-state mechanisms, the hierarchical relations, optimal observables, and physical interpretations of higher-order signals remain stable.

5.2 Small-World Networks: Topological Robustness

Studies of higher-order transitions on regular lattices have tacitly assumed local neighborhoods and Euclidean geometry, whereas real complex systems often possess long-range shortcuts, degree heterogeneity, and irregular connections. Thus, a natural question is: does the temperature hierarchy and structural picture of higher-order transitions depend on regular lattices, or can they be maintained under topological perturbations? The Ising and Potts models on small-world networks provide a controlled platform for this question. Based on Watts-Strogatz networks [82], related work compared, under different rewiring probabilities, the positional relations among the principal critical point and the third-order independent-type and dependent-type signals, and found that the hierarchical relation $T_{\text{ind}} < T_c < T_{\text{dep}}$ can be tracked on both regular lattices and small-world networks [59].

This result shows that higher-order signals do not depend entirely on the local geometry of regular lattices. Network shortcuts do not simply erase the third-order hierarchy; instead, they may enhance the visibility of signals associated with boundary reorganization. The physical reason is that long-range connections alter the routes of fluctuation propagation and cluster-boundary rearrangement, making local structural perturbations more readily coupled at the network scale. Therefore, the significance of studying small-world networks is not merely to place the Ising or Potts model on another topology, but to test whether the structural picture of higher-order transitions still has explanatory power under topologically heterogeneous backgrounds.

At the same time, network systems also remind us that the optimal observables for higher-order signals change with the topological structure. In multistate Potts networks, interface-type and perimeter-type observables are usually more sensitive than bulk averages, because they more directly reflect boundary rearrangements among clusters in different states. This indicates that, when extending studies of higher-order transitions to complex networks, one cannot mechanically apply order parameters from regular lattices; rather, one needs to reselect geometrically or topologically sensitive observables according to the connection mode and degree-of-freedom structure of the network.

5.3 Majority-Vote Model: Nonequilibrium Precursors

The majority-vote model further tests whether the idea of higher-order transitions can move beyond equilibrium statistical physics [83–87]. This model generally does not satisfy detailed balance and has neither a strict free energy nor a microcanonical density of states, and therefore the original thermodynamic definitions of MIPA cannot be applied directly. However, related studies indicate that the structural hierarchies represented by independent-type and dependent-type signals can still appear in nonequilibrium dynamics and are correlated with the presence or absence of principal critical behavior [58].

In majority-vote models with noisy feedback, isolated opinion clusters can be used to characterize independent-type higher-order signals, while consensus opinion clusters and their rates of change can be used to track dependent-type signals. The results show that independent-type signals are relatively stable across multiple network and noise-level structures, reflecting the local structural loosening of the system during the initial stage of transition from ordered organization to disordering; dependent-type signals, by contrast, rely more on the principal critical behavior itself, and usually emerge clearly only when the system still has an observable collective critical transition. When the network structure becomes more decentralized and traditional finite-size analysis also has difficulty identifying the principal critical point, the dependent-type third-order signal likewise disappears.

This point is very important for interpreting precursors. It suggests that dependent-type signals are not incidental additional extrema appearing in equilibrium models, but may correspond to windows of structural reorganization near the principal critical behavior. In nonequilibrium systems, whether dependent-type signals exist can, in turn, serve as a diagnostic clue for determining whether the system still retains a clear collective critical behavior. Of course, this diagnostic significance still needs to be understood cautiously: at present it is established more in controlled models, and its role as a stable early-warning indicator in truly complex systems still requires further statistical testing and error assessment.

5.4 Bootstrap percolation: methodological extension and boundaries of applicability

Compared with the majority-vote model, bootstrap percolation touches even more directly on the boundaries of the concept of higher-order transitions. In essence, it is an irreversible absorbing-state dynamical system: the control parameter is the initial occupation probability, and the endpoint of the evolution is an absorbing state rather than a thermal equilibrium state [88]. Therefore, there is no microcanonical entropy or density of states that can be constructed directly here, nor can one strictly apply the language of transition order from equilibrium statistical physics. The relevant results should not be interpreted as strict thermodynamic higher-order transitions in the Ising or Potts sense.

Nevertheless, bootstrap percolation still has methodological value. It shows that an important idea formed in the study of higher-order transitions—namely, that boundary- and interface-related observables often reveal the hierarchy of structural reorganization more effectively than bulk density fluctuations—can be extended to absorbing-state processes without a well-defined thermodynamic potential. As the activation threshold increases, the system' s response is no longer dominated by a single bulk-density window; instead, branch splitting and multiple geometric response scales emerge. At accessible finite sizes, what truly controls the trend of geometric reorganization is often nonlocal boundary observables rather than fluctuations in the final active density.

Thus, the role of bootstrap percolation in this paper is not that of yet another higher-order transition model, but rather that of a case illustrating the limits of applicability. It demonstrates that the geometric ideas developed in higher-order transition studies can go beyond the framework of equilibrium thermodynamics and become a general perspective for analyzing structural reorganization in complex cooperative systems. At the same time, it also reminds us that strict thermodynamic classification, finite-system structural signals, and broader geometric response analysis must be distinguished, rather than simply identified with one another.

Precisely because the study of higher-order transitions has already extended from equilibrium spin models to finite macromolecules, complex networks, nonequilibrium systems, and even more general problems of structural reorganization, it inevitably exposes new conceptual tensions and methodological boundaries. What must be discussed next is no longer merely whether more higher-order signals can still be found, but in what sense these signals constitute stable, comparable, and generalizable physical phenomena.

6 Current issues and future directions

Although in recent years the study of higher-order transitions has made clear progress in theoretical criteria, model validation, geometric interpretation, and extension of scope, this direction is still under active construction. The most important current issue is no longer simply to prove the existence of higher-order signals, but to further clarify their physical boundaries, unified language, and potential applications. More specifically, what higher-order transition research must next answer is: in what sense these signals constitute stable, comparable, and generalizable physical phenomena; what their relationship is to traditional phase transitions in the thermodynamic limit; whether observables and criteria can establish a unified correspondence across different statistical levels; and to what extent they can move beyond theoretical models into complex-system analysis and applications in early-warning prediction. Around this goal, the fate of these signals in the thermodynamic limit, the universality of observables, the bridging relationship between microcanonical and canonical frameworks, rigorous standards for precursor interpretation, and how still higher-order hierarchies unfold constitute several core issues most deserving of attention at the present stage.

6.1 Theoretical boundaries: finite size, the thermodynamic limit, and unification of criteria

The first fundamental issue faced by the study of higher-order transitions is how these signals should be distinguished from finite-size effects. Because most existing results are based on finite systems, higher-order signals inevitably carry a finite-size background. The key question is not whether they possess finite-size character, but whether they correspond to structural levels that are reproducible, comparable, and have clear physical meaning.

Overall, existing studies tend to regard these signals not as mere numerical artifacts, but as real organizational rearrangement phenomena present in finite systems. The main evidence supporting this judgment includes the repeated appearance of similar hierarchical relations in different models, the consistency of results obtained by different numerical methods, and increasingly clear geometric images of defects, boundaries, and clusters. However, there is still no fully unified conclusion regarding the fate of these signals in the thermodynamic limit. Some higher-order signals may, in

after system size is increased, whereas others may be absorbed or masked by the dominant singularity of the primary phase transition. Therefore, an important future direction is to further distinguish which higher-order signals correspond to finite-system structural hierarchies with asymptotic stability, and which are more appropriately understood as transient organization processes in the vicinity of the primary phase transition.

6.2 Characterization Problems: Universality of Observables and Rigorous Foreshadowing

Another core issue in the study of higher-order transitions is whether the observables are universal. Existing results have shown clear commonalities at the level of the physical picture: the low-temperature side is closer to the nucleation of local defects and reorganization on the ordered side, whereas the high-temperature side is closer to precursor boundary rearrangement and accelerated cluster fragmentation. However, the specific most effective observables often exhibit strong model dependence.

In the Ising model, isolated spins can characterize additional reorganization on the low-temperature side very well; in the Potts model, isolated spins must be redefined, and the mean perimeter is superior to area-type quantities; in the Blume–Capel model, because of the introduction of the zero-spin degree of freedom, local clusters and high-temperature additional structures become more complex; whereas in bootstrap percolation, the most effective quantities are boundary-type quantities rather than simple bulk-density fluctuations. This indicates that current studies of higher-order transitions still lack a unified observable that can be directly compared across models, in the same way as heat capacity or magnetic susceptibility. A direction worth pursuing in the future is to define, at a more abstract level, generalized structural indicators capable of spanning different models—for example, local defect density, boundary complexity, or interfacial rearrangement rate—so that the concrete geometric quantities in different systems can be regarded as different realizations of the same structural class.

The bridging relationship between the microcanonical and canonical frameworks: with the proposal of canonical cumulant criteria, the relationship between the microcanonical and canonical descriptions has become another key issue in this field. MIPA has clear advantages in its classification language: it can identify independent and dependent higher-order transitions within a unified framework of entropy derivatives. The canonical criteria, by contrast, place greater emphasis on operability, and are especially suitable for systems in which the density of states cannot be explicitly reconstructed. Therefore, the two are more appropriately understood as complementary rather than as simple substitutes for one another.

6.3 Future Directions: Higher-Order Spectra and Data-Driven Development

Furthermore, the canonical cumulant criteria can in principle be generalized to higher orders. By reconstructing the hierarchy of microcanonical entropy derivatives in the single-saddle-point region, one can define a family of higher-order canonical diagnostic quantities. For example, the third-order case is

$$\Sigma_3(T) = \frac{\kappa_3}{\kappa_2^3}, \tag{6.1}$$

and the fourth- and fifth-order cases may formally be written as

$$\Sigma_4(T) = \frac{\kappa_2\kappa_4 - 3\kappa_3^2}{\kappa_2^5}, \tag{6.2}$$

$$\Sigma_5(T) = \frac{\kappa_2^2\kappa_5 - 10\kappa_2\kappa_3\kappa_4 + 15\kappa_3^3}{\kappa_2^7}. \tag{6.3}$$

These expressions suggest that the canonical characterization of higher-order transitions can be systematically extended to combinations of higher-order cumulants. However, as the order increases, higher-order cumulants become more sensitive to sampling noise, distribution tails, and numerical smoothing. Therefore, at present the relatively robust and operable criterion remains the third-order criterion, while fourth- and higher-order criteria still require more model studies and numerical validation.

The most mature results at present are mainly concentrated on third-order transitions, especially independent and dependent third-order transitions. The reason is that third-order signals were the first to receive relatively systematic testing and are also the easiest for which to establish a geometric picture. However, from the theoretical framework itself, higher-order transitions should not stop at third order. Results in models such as Blume–Capel have already suggested that, within appropriate parameter ranges, systems may exhibit fourth-order independent transitions, indicating that the higher-order spectrum itself reorganizes as the type of primary phase transition changes.

Therefore, issues requiring further study in the future include: whether fourth- and higher-order transitions also possess identifiable unified geometric pictures; whether they correspond to finer-grained boundary roughening, multiscale defect competition, or hierarchical splitting of local clusters; and whether, in canonical systems, there exist higher-order generalized responses or cumulant criteria analogous to those for third order. At the same time, machine-learning and data-driven methods may also bring new tools to the study of higher-order transitions. In the future, it is entirely conceivable that, from ensembles of configurations or time-

automatic learning of optimal representations of high-order structural rearrangements in temporal sequences, thereby reducing the excessive empirical dependence involved in the selection of geometric quantities. Nevertheless, this direction should still be grounded in clear physical interpretation, rather than proceeding at the cost of mechanistic understanding.

Summary of this section

Overall, research on high-order transitions has advanced from the discovery of additional signals to the stage of understanding their physical boundaries and statistical significance. The question now most deserving of attention is no longer whether high-order extrema can still be found in more models, but how to further clarify the fate of these signals in the thermodynamic limit, establish a more unified language of characterization, and assess their stability as structural precursors and observable criteria. It can be expected that future studies of high-order transitions will increasingly move from analyses of single models toward integrated development across statistical levels, dynamical backgrounds, and modes of data representation.

7 Conclusions

In general, the principal contribution of research on high-order transitions lies not merely in the discovery of additional signals of the main phase transition in a number of finite systems, but in the fact that it has prompted us to reconsider the meaning of the concept of phase transition in finite systems, complex topologies, and nonequilibrium settings. In this sense, high-order transitions may be regarded as a class of thermodynamic principles governing the rearrangement of statistical structures in finite systems: on the one hand, they reveal hierarchical organizational changes near the main transition through the microcanonical entropy derivatives, canonical fluctuation criteria, geometric statistical structures, and intrinsic microstate spectral organization; on the other hand, they provide a new analytical framework for defect nucleation, boundary rearrangement, and mesoscopic structural evolution before the formation of dominant critical behavior in complex systems.

Regarding this issue, microcanonical inflection-point analysis provides the most important theoretical foundation for the study of high-order transitions. By interpreting phase transitions as the least-sensitive inflection points and local extrema in the microcanonical entropy and its higher-order derivatives, MIPA establishes a unified classification framework for independent and dependent transitions, enabling high-order signals for the first time to move beyond the ambiguous status of additional peaks or numerical details and become hierarchical structural phenomena that can be discussed systematically. Subsequent studies in models such as Ising, Baxter–Wu, Potts, and Blume–Capel have continuously enriched this picture, showing that high-order signals are not confined to a certain class of continuous phase-transition systems, but instead exhibit different strengths, positions, and modes of spectral-system reorganization according to differences in the type of main transition, the degree of phase coexistence, and the topology of the phase diagram.

At the same time, the introduction of geometric characterizations has further shifted the study of high-order transitions from criterion-based identification toward physical interpretation. Existing results show that independent third-order transitions are closer to the nucleation and expansion of ordered-side local defects, whereas dependent third-order transitions are closer to the rearrangement of boundary precursors on the high-temperature side of the main transition. Geometric quantities such as isolated spin vortices, loop perimeter, and boundary density not only enhance the interpretability of high-order signals, but also indicate that high-order transitions are not simply thermodynamic peaks appended to the two sides of the main transition; rather, they are structural hierarchies closely related to defect generation, interface evolution, and organizational changes at intermediate scales.

Furthermore, the proposal of canonical cumulants and generalized response criteria has allowed the study of high-order transitions to develop from microcanonical principles dependent on the density of states into observable signals that can be extracted within more general fluctuation statistics. Work on complex networks, majority-vote models, and related systems shows that the most valuable part of high-order-transition research has begun to shift from the identification of extra signals in finite equilibrium systems toward a broader structural-analysis perspective for complex systems. In particular, the repeated superiority of boundary- and interface-related observables across multiple systems suggests that high-order-transition research is in fact helping us understand a more universal question: near the main transition, how complex cooperative systems often first undergo hierarchical reorganization at the levels of local constraints, boundary organization, and mesoscopic structure.

Of course, at the present stage, research on high-order transitions has not yet formed a fully closed and mature theory. Its fate in the thermodynamic limit, the unified hierarchy of observables, the bridging boundary between microcanonical and canonical frameworks, the rigorous formulation of precursor interpretations, and the manner in which higher-order spectra should be developed still require further work. What is certain, however, is that high-order-transition research is no longer merely a marginal supplement to traditional phase-transition theory; it is gradually forming a new research direction: starting from finite systems, it continually approaches a more general problem—namely, how statistical structures in complex systems reorganize hierarchically and leave observable precursor signals before macroscopic critical behavior emerges.

In this sense, research on higher-order transitions is not merely a simple modification of traditional phase-transition theory; rather, it provides a finer-scale elaboration of a set of questions concerning how transitions occur, how structures evolve, and how precursors can be characterized. As theoretical criteria, geometric pictures, and observable signatures become further unified, this direction is expected to play an increasingly important role in the statistical physics of finite systems, complex-network dynamics, and the broader analysis of complex systems.

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Progress in Higher-Order Phase Transitions in Finite Systems: Statistical Structural Reorganization, Geometric Characterization, and Critical Precursors

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Abstract: Traditional phase-transition theory is mainly based on singularities in derivatives of free energy in the thermodynamic limit. For finite systems, however, more subtle structural reorganizations and asymmetric fluctuations often accompany the main transition and are difficult to characterize using conventional low-order thermodynamic quantities alone. In recent years, microcanonical inflection-point analysis has provided a systematic framework for identifying higher-order transitions in finite systems and has revealed independent and dependent third-order transitions in models such as Ising, Baxter-Wu, Potts, and Blume-Capel systems. Furthermore, geometric observables such as isolated spins, cluster area, and perimeter provide a more intuitive structural picture, while canonical criteria based on energy cumulant ratios extend higher-order transition analysis beyond explicit density-of-states reconstruction. This review summarizes recent progress in the study of third- and higher-order phase transitions in finite systems, with emphasis on microcanonical identification, geometric characterization, complex-network and nonequilibrium extensions, and canonical criteria.

Key words: higher-order transition; microcanonical inflection-point analysis; geometric characterization; canonical criteria; finite system

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