Energy Landscape and Metastability of Curie–Weiss–Potts Model

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Abstract
In this paper, we thoroughly analyze the energy landscape of the Curie–Weiss–Potts model, which is a ferromagnetic spin system consisting of \( q \geq 3 \) spins defined on complete graphs. In particular, for the Curie–Weiss–Potts model with \( q \geq 3 \) spins and zero external field, we completely characterize all critical temperatures and phase transitions in view of the global structure of the energy landscape. We observe that there are three critical temperatures and four different regimes for \( q < 5 \), whereas there are four critical temperatures and five different regimes for \( q \geq 5 \). Our analysis extends the investigations performed in (Costeniuc et al in J Math Phys 46:063301, 2005); they provide the precise characterization of the second critical temperatures for all \( q \geq 3 \) and in (Landim and Seo in J Stat Phys 165:693–726, 2016), which provides a complete analysis of the energy landscape for \( q = 3 \). Based on our precise analysis of the energy landscape, we also perform a quantitative investigation of the metastable behavior of the heat-bath Glauber dynamics associated with the Curie–Weiss–Potts model.

Keywords Metastability · Potts model · Energy landscape · Phase transition

1 Introduction

The Potts model is a well-known mathematical model suitable for studying ferromagnetic spin system consisting of \( q \geq 3 \) spins. We refer to [1] a comprehensive review on the Potts model. In the present work, we focus on the Potts model defined on large complete graphs without an external field to understand the associated energy landscape as well as the metastable behavior of the heat-bath Glauber dynamics to the highly precise level. This special case of the Potts model defined on complete graphs is called a Curie–Weiss–Potts model and investigated in various studies; e.g., [2–11] and references therein. We note that the rigorous mathematical definition of the Curie–Weiss–Potts model is presented in the next section.

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1.1 The Curie–Weiss Model

The Ising case of the Curie–Weiss–Potts model, i.e., the corresponding spin system consisting only of $q = 2$ spins, is the famous Curie–Weiss model. It is well-known that the Curie–Weiss model without an external field exhibits a phase transition at the critical (inverse) temperature $\beta_c > 0$. It is mainly because the number of global minima of the potential function associated with the empirical magnetization is one for the high temperature regime $\beta \leq \beta_c$ while it becomes two for the low temperature regime $\beta > \beta_c$, where $\beta > 0$ represents the inverse temperature (cf. [12, Chapter 9] for more detail). It is also well-known that such a phase transition for the structure of the energy landscape is closely related to the mixing property of the associated heat-bath Glauber dynamics. In [13], it has been shown that the Glauber dynamics exhibits the so-called cut-off phenomenon which is a signature of the fast mixing for the high-temperature regime (i.e., $\beta < \beta_c$) and the metastability for the low-temperature regime (i.e., $\beta > \beta_c$). The metastability for the low-temperature regime has been more deeply investigated in [14].

1.2 The Curie–Weiss–Potts Model with $q = 3$

The picture for the Curie–Weiss model explained above has been fully extended to the Curie–Weiss–Potts model consisting of $q = 3$ spins. The complete description of the energy landscape has been obtained recently in [8, 9], where three critical temperatures $0 < \beta_1 < \beta_2 < \beta_3 = 3$ are characterized. More precisely, it has been shown that the potential function associated with the empirical magnetization (which will be explained in detail in Sect. 2.3) has

- the unique global minimum for $\beta \in (0, \beta_1)$,
- one global minimum and three local minima for $\beta \in (\beta_1, \beta_2)$,
- three global minima and one local minimum for $\beta \in (\beta_2, \beta_3)$, and
- three global minima for $\beta \in (\beta_3, \infty)$.

The articles [8, 9] also analyzed the associated saddle structure. Based on this analysis, [9] discussed the quantitative feature of the metastable behavior of the heat-bath Glauber dynamics in view of the Eyring–Kramers formula and Markov chain model reduction (cf. [15–17]) for all the low-temperature regime $\beta > \beta_1$. Because of the abrupt change in the structure of the potential function at $\beta = \beta_2$ and $\beta = \beta_3$, the metastable behaviors of the Glauber dynamics in three low-temperature regimes $(\beta_1, \beta_2)$, $(\beta_2, \beta_3)$, and $(\beta_3, \infty)$ turned out to be both quantitatively and qualitatively different. For the high-temperature regime $(0, \beta_1)$, the cut-off phenomenon has been verified in [5] for all $q \geq 3$. Adjoining all these works completes the picture for the Curie–Weiss–Potts model with $q = 3$ spins.

1.3 The Curie–Weiss–Potts Model with $q \geq 4$

Compared to the Curie–Weiss–Potts model with $q = 2$ or 3 spins, the analysis of the case with $q \geq 4$ spins is not completed so far. In many literature, two critical temperatures $\beta_1(q) < \beta_2(q)$ for the Curie–Weiss–Potts model with $q \geq 4$ spins are observed and the phase transitions near these critical temperatures have been analyzed. For instance, in [5], the phase transition from the fast mixing (the cut-off phenomenon) to the slow mixing (due to the appearance of new local minima) at $\beta = \beta_1(q)$ has been confirmed. In [7], it has been
observed that the limiting distributions of the empirical magnetization exhibits the abrupt change at $\beta = \beta_2(q)$. In [4], the phase transition around $\beta_2(q)$ also has been studied in view of the equivalence and non-equivalence of ensembles.

These studies focus on the phase transitions involved with the local and the global minima of the potential function. However, in order to investigate the metastable behavior whose main objective is to analyze the transitions between neighborhoods of local minima (i.e., the metastable states), the precise understanding of the saddle structure is also required. To the best of our knowledge, the analysis of the saddle structure as well as the metastable behavior of the heat-bath Glauber dynamics for $q \geq 4$ has not been analyzed yet.

1.4 Main Contribution of the Article

The main result of the present work is to provide the complete description of the energy landscape including the saddle structure and to analyze dynamical features of the Glauber dynamics based on it for the Curie–Weiss–Potts models with $q \geq 4$ spins.

First, we observe that for $q = 4$, as in the case of $q = 3$, the potential function has three critical temperatures

$$0 < \beta_1(4) < \beta_2(4) < \beta_3(4) = 4,$$

and moreover the associated metastable behavior is quite similar to that of the case $q = 3$. On the other hand, for $q \geq 5$, we will deduce that there are four critical temperatures

$$0 < \beta_1(q) < \beta_2(q) < \beta_3(q) < \beta_4(q) = q,$$

where two critical temperatures $\beta_1(q)$ and $\beta_2(q)$ play essentially the same role with $\beta_1(3)$ and $\beta_2(3)$ (and hence $\beta_1(4)$ and $\beta_2(4)$), respectively. Surprisingly, our work reveals that the role of the third critical temperature $\beta_3(q)$ for $q \leq 4$ is divided into the third and fourth critical temperatures $\beta_3(q)$ and $\beta_4(q)$ for $q \geq 5$. More precisely, for $q \leq 4$, the change in the saddle gates between global minima and the disappearance of the local minimum representing the chaotic configuration happen simultaneously at $\beta = \beta_3(q) = q$; however, for $q \geq 5$, the change of saddle gates happens at $\beta = \beta_3(q) < q$ and the disappearance of the chaotic local minimum occurs at $\beta = \beta_4(q) = q$. Hence, for $q \geq 5$, we observe another type of metastable behavior at $\beta \in [\beta_3(q), \beta_4(q))$ compared to the case $q \leq 4$.

**Remark** We can also consider the Curie–Weiss–Potts model under an external field. For such models with $q = 3$ spins, the energy landscape has been completely analyzed in [9, Sections 5, 6]. We expect similar results but rigorous demonstration seems to be very complicated for general $q \geq 4$; hence we leave it for future research. We also remark that the Curie–Weiss–Potts model with an random external field has been studied in [10, Section 5].

1.5 Other Studies on the Potts Model

Although the present work focuses on the Potts model on complete graphs, we also note that the Ising and Potts models on the lattice are widely studied as well. For instance, we refer to [12] and the references therein for the phase transition, to [18–20] for the cut-off phenomenon in the high-temperature regime, and to [21–31] for the metastability in the low-temperature regime. In addition, we refer to [32, 33] for the Potts model in many spins or large dimensions and to [34, 35] for the study of metastability of the Ising model on random graphs.
2 Model

In this section, we introduce the formal definition of the Curie–Weiss–Potts model, which will be analyzed in the present work. Fix an integer \( q \geq 3 \) and let \( S = \{1, \ldots, q\} \) be the set of spins.

2.1 Curie–Weiss–Potts Model

For a positive integer \( N \), let us denote by \( K_N = \{1, \ldots, N\} \) the set of sites. Let \( \Omega_N = S^{K_N} \) be the configuration space of spins on \( K_N \). Each configuration is represented as \( \sigma = (\sigma_1, \ldots, \sigma_N) \in \Omega_N \) where \( \sigma_v \in S \) denotes a spin at site \( v \in K_N \). Let \( h = (h_1, \ldots, h_q) \in \mathbb{R}^q \) be the external magnetic field. The Hamiltonian associated to the Curie–Weiss–Potts model with the external field \( h \) is given by

\[
H_N(\sigma) = -\frac{1}{2N} \sum_{1 \leq u, v \leq N} 1(\sigma_u = \sigma_v) - \sum_{v=1}^{N} \sum_{j=1}^{q} h_j 1(\sigma_v = j) ; \sigma \in \Omega_N,
\]

where \( 1 \) denotes the usual indicator function. Then, the Gibbs measure associated to the Hamiltonian at the (inverse) temperature \( \beta > 0 \) is given by

\[
\mu_\beta^N(\sigma) = \frac{1}{Z_N(\beta)} e^{-\beta H_N(\sigma)} ; \sigma \in \Omega_N,
\]

where \( Z_N(\beta) = \sum_{\sigma \in \Omega_N} e^{-\beta H_N(\sigma)} \) is the partition function. The measure \( \mu_\beta^N(\cdot) \) denotes the Curie–Weiss–Potts measure on \( \Omega_N \) at the inverse temperature \( \beta \).

2.2 Heat-Bath Glauber Dynamics

Now, we define a heat-bath Glauber dynamics associated with the Curie–Weiss–Potts measure \( \mu_\beta^N(\cdot) \). For \( \sigma \in \Omega_N \), \( v \in K_N \), and \( k \in S \), denote by \( \sigma^{v,k} \) the configuration whose spin \( \sigma_v \) at site \( v \) is flipped to \( k \), i.e.,

\[
(\sigma^{v,k})_u = \begin{cases} 
\sigma_u & u \neq v, \\
k & u = v .
\end{cases}
\]

Then, we will consider a heat-bath Glauber dynamics associated with generator \( \mathcal{L}_N \) which acts on \( f : \Omega_N \to \mathbb{R} \) as

\[
(\mathcal{L}_N f)(\sigma) = \frac{1}{N} \sum_{v=1}^{N} \sum_{k=1}^{q} c_{v,k}(\sigma)[f(\sigma^{v,k}) - f(\sigma)],
\]

where

\[
c_{v,k}(\sigma) = \exp \left\{ -\frac{\beta}{2} [H_N(\sigma^{v,k}) - H_N(\sigma)] \right\} .
\]

It can be observed that this dynamics is reversible with respect to the Curie–Weiss–Potts measure \( \mu_\beta^N(\cdot) \). Henceforth, denote by \( \sigma(t) = \sigma^{K_N}(t) = (\sigma_1(t), \ldots, \sigma_N(t)) \) the continuous time Markov process associated with the generator \( \mathcal{L}_N \).

\footnote{We write \( K_N \) to emphasize that our model is on the complete graph.}
2.3 Empirical Magnetization

For each spin $k \in S$, denote by $r^k_N(\sigma)$ the proportion of spin $k$ of configuration $\sigma \in \Omega_N$, i.e.,

$$r^k_N(\sigma) := \frac{1}{N} \sum_{v=1}^{N} \mathbf{1}(\sigma_v = k),$$

and define the proportional vector $r_N(\sigma)$ as

$$r_N(\sigma) := (r_1^1(\sigma), \ldots, r_{q-1}^{q-1}(\sigma)),$$

which represents the empirical magnetization of the configuration $\sigma$ containing the macroscopic information of $\sigma$.

Define $\Xi_1$ as

$$\Xi_1 = \{x = (x_1, \ldots, x_{q-1}) \in (\mathbb{R}_\geq 0)^{q-1} : x_1 + \cdots + x_{q-1} \leq 1\},$$

and then define a discretization of $\Xi$ as

$$\Xi_N = \Xi \cap (\mathbb{Z}/N)^{q-1}.$$

With this notation, we immediately have $r_N(\sigma) \in \Xi_N$ for $\sigma \in \Omega_N$.

For the Markov process $(\sigma(t))_{t \geq 0}$, we write $r_N(\cdot) = r_N(\sigma(\cdot))$ which is a stochastic process on $\Xi_N$ expressing the evolution of the empirical magnetization. Since the model is defined on the complete graph $K_N$, we obtain the following proposition.

**Proposition 2.1** The process $(r_N(t))_{t \geq 0}$ is a continuous time Markov chain on $\Xi_N$ whose invariant measure is given by

$$\nu_\beta^N(\cdot) := \mu_\beta^N(r^{-1}_N(\cdot)) ; \ x \in \Xi_N,$$

where $r^{-1}_N(\cdot)$ denotes the set $\{\sigma \in \Omega_N : r_N(\sigma) = x\}$. Furthermore, $r_N(\cdot)$ is reversible with respect to $\nu_\beta^N$.

The proof of this proposition including jump rates is given in Sect. 5.1. Let $P^N_x, \beta$ be the law of the Markov chain $r_N(\cdot)$ starting at $x \in \Xi_N$ and let $E^N_x, \beta$ be the corresponding expectation.

2.4 More on the Measure $\nu_\beta^N(\cdot)$

For $y \in \Xi$, let $\hat{y} = (y_1, \ldots, y_q, y_q) \in \mathbb{R}^q$ where $y_q = 1 - (y_1 + \cdots + y_{q-1})$. Then, the Hamiltonian $H_N$ can be written as

$$H_N(\sigma) = NH(r_N(\sigma)) ; \ \sigma \in \Omega_N,$$

where

$$H(x) = -\frac{1}{2} |\hat{x}|^2 - h \cdot \hat{x} ; \ x \in \Xi .$$

Therefore, by Proposition 2.1, the invariant measure $\nu_\beta^N(\cdot)$ of the process $r_N(t)$ on $\Xi_N$ can be written as

$$\nu_\beta^N(x) = \sum_{\sigma : r_N(\sigma) = x} \frac{1}{Z_N(\beta)} \exp\{-\beta H_N(\sigma)\}.$$
\[
\begin{align*}
&= \left( \frac{N}{(N \chi_1) \cdots (N \chi_q)} \right) \frac{1}{Z_N(\beta)} \exp\{-\beta N H(x)\} \\
&= \frac{1}{(2\pi N)^{(q-1)/2} Z_N(\beta)} \exp\{-\beta N F_{\beta, N}(x)\},
\end{align*}
\]
where, by Stirling’s formula, we can write
\[
F_{\beta, N}(x) = F_\beta(x) + \frac{1}{N} G_{\beta, N}(x),
\]
where
\[
F_\beta(x) = H(x) + \frac{1}{\beta} S(x) \quad \text{and} \quad G_{\beta, N}(x) = \frac{\log(x_1 \cdots x_q)}{2\beta} + O(N^{-1}).
\]

In this equation, \(H(\cdot)\) is the energy functional defined in (2.2) and \(S(\cdot)\) is the entropy functional defined by
\[
S(x) = \sum_{i=1}^{q} x_i \log(x_i),
\]
and \(G_{\beta, N}(x)\) converges to \(\log(x_1 \cdots x_q)/(2\beta)\) uniformly on every compact subsets of \(\text{int } \Xi\).

### 2.5 Main Objectives of the Article

Now, we can express the main purpose of the current article in a more concrete manner. In this article, we consider the Curie–Weiss–Potts model when there is no external magnetic field; i.e., \(h = 0\). Therefore, from now on, we assume \(h = 0\). Under this assumption, the first objective is to analyze the function \(F_{\beta}(\cdot)\) expressing the energy landscape of the empirical magnetization of the Curie–Weiss–Potts model. This result will be explained in Sect. 3. The second concern is to investigate the metastable behavior of the process \(r_N(\cdot)\) in the low-temperature regime. This will be explained in Sect. 4. Latter part of the article is devoted to proofs of these results.

### 3 Main Result for Energy Landscape

In view of Proposition 2.1, (2.3), and (2.4), the structure of the invariant measure \(\nu_{\beta}^N (\cdot)\) of the process \(r_N(\cdot)\) is essentially captured by the potential function \(F_{\beta}(\cdot)\); hence, the investigation of \(F_{\beta}(\cdot)\) is crucial in the analysis of the energy landscape and the metastable behavior of \(r_N(\cdot)\). In this section, we explain our detailed analysis of the function \(F_{\beta}(\cdot)\).

Note that the function \(F_{\beta}(\cdot) = H(\cdot) + \beta^{-1} S(\cdot)\) express the competition between the energy and the entropy represented by \(H(\cdot)\) and \(S(\cdot)\), respectively. Since there is a \(\beta^{-1}\) factor in front of the entropy functional, we can expect that the entropy dominates the competition when \(\beta\) is small (i.e., the temperature is high). Since entropy is uniquely minimized at the equally distributed configuration \((1/q, \ldots, 1/q) \in \Xi\), we can expect that the potential \(F_{\beta}(\cdot)\) also has the unique minimum when \(\beta\) is small. On the other hand, if \(\beta\) is large enough (i.e., the temperature is low), the energy \(H(\cdot)\) with \(q\) minima dominates the system, and therefore, we can expect that the potential \(F_{\beta}\) also has \(q\) global minima. In this section we provide the complete characterization of the complicated pattern of transition from this high-temperature regime to low-temperature regime in a precise level.
In Sect. 3.1, we define several points that will be shown to be critical points. In Sect. 3.2, we introduce several critical values of (inverse) temperature $\beta$. In Sect. 3.3, we summarize the results on the energy landscape $F_{\beta}(\cdot)$. In Sect. 3.4, as a by-product of these results, we compute the mean-field free energy.

### 3.1 Critical Points of $F_{\beta}(\cdot)$

Let us first investigate critical points of $F_{\beta}(\cdot)$. We recall that

$$F_{\beta}(x) = -\frac{1}{2} \sum_{k=1}^{q} x_k^2 + \frac{1}{\beta} \sum_{k=1}^{q} x_k \log x_k ; \ x \in \Xi .$$

**Notation 3.1** We have following notations for convenience.

1. Since there is no risk of confusion, we will write the point $x = (x_1, \ldots, x_{q-1}) \in \Xi$ as $x = (x_1, \ldots, x_{q-1}, x_q) \in \mathbb{R}^q$ where $x_q = 1 - x_1 - \cdots - x_{q-1}$.
2. Let $\{e_1, \ldots, e_{q-1}\}$ be the orthonormal basis of $\mathbb{R}^{q-1}$ and $e_q = 0 \in \mathbb{R}^{q-1}$. According to the convention above, the vectors $e_1, \ldots, e_q$ can be regarded as an orthonormal basis of $\mathbb{R}^q$.

Now, we explain the candidates for the critical points of $F_{\beta}(\cdot)$ playing important role in the analysis of the energy landscape. The first candidate is

$$p := (1/q, \ldots, 1/q) \in \Xi ,$$

which represents the state where the spins are equally distributed.

In order to introduce the other candidates, we fix $i \in \mathbb{N} \cap [1, q/2]$ and let $j = q - i$. Define $g_i : (0, 1/j) \to \mathbb{R}$ as

$$g_i(t) := \frac{i}{1 - qt} \log \left( \frac{1 - jt}{it} \right) ,$$

where we set $g_i(1/q) = q$ so that $g_i$ becomes a continuous function on $(0, 1/j)$. We refer to Fig. 1 for an illustration of graph of $g_i$. Then, it will be verified by Lemma 6.1 in Sect. 6.1 (and we can expect from the graph illustrated in Fig. 1) that $g_i(t) = \beta$ has at most two solutions. We denote by $u_i(\beta) \leq v_i(\beta)$ these solutions, provided that they exist. If there is only one solution, we let $u_i(\beta) = v_i(\beta)$ be this solution.

For $k \in S$, let

$$u^k_1 = u^k_1(\beta) := \left( u_1(\beta), \ldots, 1 - (q - 1)u_1(\beta), \ldots, u_1(\beta) \right) \in \Xi .$$

**Fig. 1** Graph of $g_2(t)$ for $q = 10$
Proposition 3.2 A saddle point is a critical point at which the Hessian has only one negative eigenvalue.

Remark 3.3 The set $U_2$ is not defined for $q = 3$ since the set $U_1$ is defined only when $i \leq q/2$. This will be explained in Sect. 6.1.

The proof of this proposition is an immediate consequence of Proposition 6.3 in Sect. 6.1. Henceforth, we write $\beta_i = \beta_i(q)$, $1 \leq i \leq 3$, since there is no risk of confusion.

### 3.2 Critical Temperatures

In this subsection, we introduce critical temperatures

$$0 < \beta_1(q) < \beta_2(q) < \beta_3(q) \leq q,$$

at which the phase transitions in the energy landscape occur. The precise definition of these critical temperatures are given in (6.9) of Sect. 6.2. Henceforth, we write $\beta_i = \beta_i(q)$, $1 \leq i \leq 3$, since there is no risk of confusion.
To describe the role of these critical temperatures, we regard $\beta$ as increasing from 0 to $\infty$. Figure 2 shows the role of $p$, $U_1$, $V_1$, and $U_2$ according to inverse temperature. Sect. 6 will prove this figure.

At $\beta = \beta_1$, the dynamics exhibits phase transition from fast mixing to slow mixing, and this is proven in [5]. Furthermore, the behavior of the dynamics changes from cutoff phenomenon to metastability. This phase transition is due to the appearance of new local minima $U_1$ of $F_\beta(\cdot)$ other than $p$ at $\beta = \beta_1$. At $\beta = \beta_2$, the ground states of dynamics change from $p$ to elements of $U_1$, as observed in [4, Theorem 3.1(b)]. To explain the role of critical temperatures $\beta_3$ and $q$, we have to divide the explanation into several cases. Let us first assume that $q \geq 4$ so that $\beta_3 < q$. At $\beta = \beta_3$, the saddle gates among the ground states in $U_1$ is changed from $V_1$ to $U_2$ (since the heights $F_\beta(v_1)$ and $F_\beta(u_2)$ are reversed at this point) and at $\beta = q$, the local minimum $p$ becomes a local maximum. On the other hand, for $q \leq 4$, we have $\beta_3 = q$. At $\beta = \beta_3$, the change of the saddle gates and the disappearance of the local minimum $p$ occur simultaneously. We refer to [9] for the detailed description when $q = 3$.

### 3.3 Stable and Metastable Sets

We define some metastable sets based on the results explained earlier. If $q \geq 4$, define $H_\beta$ as (cf. (3.5))

$$H_\beta = \begin{cases} F_\beta(v_1), & \beta \in (\beta_1, \beta_3), \\ F_\beta(u_2), & \beta \in [\beta_3, \infty). \end{cases}$$

When $q = 3$, we set $H_\beta = F_\beta(v_1)$ for all $\beta > \beta_1$ (cf. Remark 3.3). It will be verified in Lemma 6.7 and (6.9) that $H_\beta$ is the height of the lowest saddle points.

Let $\hat{S} := S \cup \{o\}$ and $u_o := p$. Let $\mathcal{W}_k = \mathcal{W}_k(\beta)$, $k \in S$, be the connected component of $\{F_\beta < H_\beta\}$ containing $u_k$, and let $\mathcal{W}_o = \mathcal{W}_o(\beta)$ be the connected component of $\{F_\beta < F_\beta(v_1)\}$ containing $u_o$. For $k, l \in \hat{S}$, let $\Sigma_{k,l} := \Sigma_{k,l}(\beta) := \overline{\mathcal{W}_k \cap \mathcal{W}_l}$ be a set of saddle gates of height $H_\beta$ between $u_k$ and $u_l$.

Now, we can state the main result on energy landscape and the proofs of theorems in this section will be presented in Sect. 9. The first result holds for all $q \geq 3$.

**Theorem 3.4** For $q \geq 3$, the following hold.

1. If $\beta \leq \beta_1$, there is no critical point other than $p$, which is the global minimum.

---

3 We define the set $\mathcal{W}_k$, $k \in S$, and $\mathcal{W}_o$ as the empty set if the set $\{F_\beta < H_\beta\}$ does not contain $u_k$ and $\{F_\beta < F_\beta(v_1)\}$ does not contain $u_o$ respectively.
2. For $\beta \in (\beta_1, q)$, we have $\mathcal{W}_0 \neq \emptyset$ and for $\beta \in [q, \infty)$, we have $\mathcal{W}_0 = \emptyset$.

3. Let $\mathcal{M}_\beta$ be a set of local minima of $F_\beta$. Then, we have

$$
\mathcal{M}_\beta = \begin{cases} 
\{p\} & \beta \in (0, \beta_1), \\
\{p\} \cup U_1 & \beta \in (\beta_1, q), \\
U_1 & \beta \in [q, \infty).
\end{cases}
$$

4. Let $\mathcal{M}_\beta^\ast$ be a set of global minima of $F_\beta$. Then, we have

$$
\mathcal{M}_\beta^\ast = \begin{cases} 
\{p\} & \beta \in (0, \beta_2), \\
\{p\} \cup U_1 & \beta = \beta_2, \\
U_1 & \beta \in (\beta_2, \infty).
\end{cases}
$$

Since there is only one minimum if $\beta \leq \beta_1$, we now consider $\beta > \beta_1$. Before we write the main result on metastable sets, we would like to emphasize that [9, Proposition 4.4] proved the case when $q = 3$, while the proof for the case $q \geq 4$ is the main novel content of the current article. We first consider the case $q \leq 4$. See Fig. 3 for the visualization of the following and above theorem.

**Theorem 3.5** For $q \leq 4$, the following hold.

1. $\beta_3 = q$.
2. For $\beta \in (\beta_1, q)$, the sets $\mathcal{W}_k$, $k \in \tilde{S}$, are nonempty and disjoint. For $k, l \in S$, $\Sigma_{k,l} = \emptyset$ and for $k \in S$, $\Sigma_{\alpha,k} = \{v^\alpha_k\}$.
3. For $\beta = q$, we have $\mathcal{W}_0 = \emptyset$. The sets $\mathcal{W}_k$, $k \in S$, are nonempty and disjoint. For $k, l \in S$, $\Sigma_{k,l} = \{p\}$.
4. For $\beta \in (q, \infty)$, we have $\mathcal{W}_0 = \emptyset$. The sets $\mathcal{W}_k$, $k \in S$, are nonempty and disjoint. For $k, l \in S$,

$$
\Sigma_{k,l} = \begin{cases} 
\{v^m_m\}, & \text{where } m \in S \setminus \{k, l\}, \text{ if } q = 3, \\
\{u^k_{k,l}\}, & \text{if } q = 4.
\end{cases}
$$

\(^4\) This figures are excerpt from [9, Fig. 4]
Next, we consider the case \( q \geq 5 \). Note that the crucial difference compared to the previous theorem lies in the third and fifth statements. See Figs. 4 and 5 for the visualization of the following theorem and Theorem 3.4.

**Theorem 3.6** For \( q \geq 5 \), the following hold.

1. \( \beta_3 < q \).
2. For \( \beta \in (\beta_1, \beta_3) \), the sets \( W_k, k \in \hat{S} \), are nonempty and disjoint. For \( k, l \in S, \Sigma_{k,l} = \emptyset \) and for \( k \in S, \Sigma_{o,k} = \{v_1^k\} \)
3. For \( \beta = \beta_3 \), the sets \( W_k, k \in \hat{S} \), are nonempty and disjoint. For \( k, l \in S, \Sigma_{k,l} = \{u_2^{k,l}\} \) and for \( k \in S, \Sigma_{o,k} = \emptyset \).
4. For \( \beta \in (\beta_3, \infty) \), the sets \( W_k, k \in S \), are nonempty and disjoint. For \( k, l \in S, \Sigma_{k,l} = \{u_2^{k,l}\} \) and for \( k \in S, \Sigma_{o,k} = \emptyset \).
5. For \( \beta \in (\beta_3, q) \), we have \( F_{\beta}(v_1) > H_\beta \). Furthermore, the set \( \{F_{\beta} < F_{\beta}(v_1)\} \) has only two connected components, the well \( W_o \) and the other containing \( U_1 \). The saddle points between them are \( V_1 \).

### 3.4 Mean-Field Free Energy

In this subsection, we compute the mean-field free energy of the Curie–Weiss–Potts model defined by

\[
\psi(\beta) := -\lim_{N \to \infty} \frac{1}{\beta N} \log Z_N(\beta) .
\]

It is well known that the Curie–Weiss model with \( q = 2 \) spins exhibits the second-order phase transition at the unique critical temperature \( \beta = \beta_c \), while the Curie–Weiss–Potts model with \( q \geq 3 \) spins exhibits the first-order phase transition at \( \beta = \beta_2 \) (cf. [4, 7, 36]). We now reconfirm this folklore by computing the free energy explicitly. This computation is based on the following observation (cf. [7, display (2.4)]):

\[
\lim_{N \to \infty} \frac{1}{\beta N} \log Z_N(\beta) = \sup_{x \in \Xi} \{-F_{\beta}(x)\} .
\]

We give a rigorous proof in Appendix B.

Now, let us assume that \( q \geq 3 \) so that by (3.7), (3.8), and Theorems 3.4, we can deduce that

\[
\psi(\beta) = \begin{cases} 
F_{\beta}(p) & \text{if } \beta \leq \beta_2 , \\
F_{\beta}(u_1) & \text{if } \beta > \beta_2 .
\end{cases}
\]

**Corollary 3.7** We have that

\[
\psi'(\beta) = \begin{cases} 
-\frac{1}{\beta^2} S(p) & \text{if } \beta < \beta_2 , \\
-\frac{1}{\beta^2} S(u_1) & \text{if } \beta > \beta_2 .
\end{cases}
\]

In particular, the Curie–Weiss–Potts model with \( q \geq 3 \) exhibits the first-order phase transition at \( \beta = \beta_2 \).

**Proof** Let \( c(\beta) \in \Xi \) be a critical point of \( F_{\beta}(-) \). Then, since \( F_{\beta} = H + \beta^{-1} S \), we have

\[
\frac{d}{d\beta} F_{\beta}(c(\beta)) = \nabla F_{\beta}(c(\beta)) \cdot \dot{c}(\beta) - \frac{1}{\beta^2} S(c(\beta)) .
\]

Since \( \nabla F_{\beta}(c(\beta)) = 0 \), we get (3.10) from (3.9). Since \( S \) attains its unique local minimum at \( p \) and \( u_1 \neq p \), \( \psi'(-) \) is discontinuous at \( \beta = \beta_2 \).
Fig. 4 Illustration of energy landscape of $F_\beta$ when $q = 5$. The first four figures are $\{F_\beta \leq H_\beta\}$ and the last figure is $\{F_\beta \leq F_\beta(v_1)\}$. The star-shaped vertices and circles represent saddle points and local minima, respectively. The empty circles are shallower minima. Each arrow represents a path from one shallower minimum to another deeper minimum passing through a saddle point.
Fig. 5  Illustration of energy landscape of $F_\beta$ when $q = 5$ and $\beta = \beta_3$. The figures are $\{F_\beta \leq H_\beta\}$. The star-shaped vertices and circles represent saddle points and local minima, respectively. The empty circles are shallower minima. Each arrow represents a path from one shallower minimum to another deeper minimum passing through a saddle point. Note that when $\beta = \beta_3$, $U_2$ and $V_1$ exist simultaneously. The first two figures are illustrations of saddle structures of $V_1$ and $U_2$, respectively. The last figures is a combination of the previous two figures.

4 Main Result for Metastability

In this section, we analyze the metastable behavior of $r_N(\cdot)$ based on the analysis of the energy landscape carried out in the previous section and the general results obtained by [37]. As inverse temperature $\beta$ varies, the behavior of this dynamics changes both qualitatively and quantitatively thanks to the structural phase transitions explained in the previous section.

Since the invariant measure $\nu_N^\beta$ is exponentially concentrated in neighborhoods of ground states, the corresponding Markov process $r_N(\cdot)$ stays most of the time at these neighborhoods. The abrupt transitions between such stable states are the metastable behavior of the process $r_N(\cdot)$ and one of the natural ways of describing these hopping dynamics among the neighborhoods of the ground states is the Markov chain model reduction. A comprehensive understanding of such approaches can be obtained from [15–17].

When the dynamics starts from a local minimum which is not a global minimum, we have to estimate the mean of the transition time to the global minimum in order to quantitatively...
understand the metastable behavior. This estimation is known as the Eyring–Kramers formula. In this section we provide the Markov chain model reduction and Eyring–Kramers formula for the metastable process $p_N(t)$.

Such a metastable behavior is observed only when there are multiple local minima; and hence we cannot expect metastable behavior at the high-temperature regime $\beta \leq \beta_1$ for which $p$ is the unique local (and global) minimum. Hence, we assume $\beta > \beta_1$ in this section.

## 4.1 Some Preliminaries

In this subsection, we introduce several notions crucial to the description of the metastable behavior.

### 4.1.1 Some Constants

We first define the so-called Eyring–Kramers constants which play fundamental role in the quantitative analysis of metastability. Recall the definition of $\{e_1, \ldots, e_q\}$ from Notation 3.1. Define $(q-1) \times (q-1)$ matrices $A_{i,j}$, $i, j \in S$, and $A(x)$ as

$$A_{i,j} = (e_j - e_i)(e_j - e_i)^\dagger \quad \text{and} \quad A(x) = \sum_{1 \leq i < j \leq q} w_{i,j}(x)A_{i,j}.$$ 

As we will see in Sect. 5.3, these constants are related to the drift of empirical magnetization as a consequence of spin update from $i$ to $j$ or $j$ to $i$. Since $A_{i,j}$, $i, j \in S$, are positive definite, $A(x)$ satisfies [37, display (A.1)] and hence, by [37, Lemma A.1], for all $k, l \in S$, the matrices $(\nabla^2 F_\beta(u_{k,l}^2))A(u_{k,l}^2)$ and $(\nabla^2 F_\beta(v_1^k))A(v_1^k)$ have the unique negative eigenvalue which will be denoted respectively by $-\mu_{k,l} = -\mu_{k,l}(\beta)$ and $-\mu_{o,k} = -\mu_{o,k}(\beta)$.

Now, let us define the Eyring–Kramers constants corresponding to our model as

$$\omega_{k,l} = \omega_{k,l}(\beta) := \frac{\mu_{k,l}(\beta)}{\sqrt{-\det[(\nabla^2 F_\beta)(u_{k,l}^2)]}} e^{-\beta G_\beta(u_{k,l}^2)}, \quad k, l \in S,$$  

$$\omega_{o,k} = \omega_{o,k}(\beta) := \frac{\mu_{o,k}(\beta)}{\sqrt{-\det[(\nabla^2 F_\beta)(v_1^k)]}} e^{-\beta G_\beta(v_1^k)}, \quad k \in S. \quad (4.2)$$

By symmetry, we have $\omega_{k,l} = \omega_{k',l'}$ for all $k, l \in S$ and $k', l' \in S$ and $\omega_{o,k} = \omega_{o,k'}$ for all $k, k' \in S$. Hence, let us write $\omega_o = \omega_{o,1}$ and $\omega_1 = \omega_{1,2}$. Next, define

$$v_k = v_k(\beta) := \frac{\exp(-\beta G_\beta(u_1^k))}{\sqrt{\beta^2 \det[(\nabla^2 F_\beta)(u_1^k)]}}, \quad k \in S, \quad (4.3)$$

$$v_o = v_o(\beta) := \frac{\exp(-\beta G_\beta(p))}{\sqrt{\beta^2 \det[(\nabla^2 F_\beta)(p)]}}. \quad (4.4)$$

As explained in [37, display (2.8)], the constants $v_k$, $k \in S$, and $v_o$ are the normalized asymptotic mass of the neighborhood of $u_1^k$ and $p$, respectively. By the symmetry, we also obtain $v_1 = \cdots = v_q$. 

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4.1.2 Time Scales

The constant $H_\beta$ defined in (3.6) denotes the height of the lowest saddle points. Let $\theta_k = \theta_k(\beta)$, $k \in \hat{S}$, be the depth of well $\mathcal{W}_k(\beta)$, i.e.,

$$
\begin{cases}
\theta_1 = \cdots = \theta_q = \beta[H_\beta - F_\beta(u_1)], \\
\theta_o = \beta[F_\beta(v_1) - F_\beta(p)].
\end{cases}
$$

Then, $e^{N\theta_1}$ and $e^{N\theta_o}$ represent the time scales on which $r_N(\cdot)$ exhibits metastability. For $\beta \geq q$, the constant $\theta_o$ is meaningless since $\mathcal{W}_o = \emptyset$.

4.1.3 Order Process and Markov Chain Model Reduction

Let $\delta = \delta(\beta) > 0$ be a small enough number such that $\delta < \min(\theta_o, \theta_1)$. If $\beta \geq q$, since $\theta_o$ is not defined, let $\delta = (1/2)\theta_1$. For $k \in S$, define

$$
\mathcal{W}_k^\delta = \mathcal{W}_k \cap \{ x \in \Xi : F_\beta(x) < H_\beta - \delta \},
$$

$$
\mathcal{W}_o^\delta = \mathcal{W}_o \cap \{ x \in \Xi : F_\beta(x) < F_\beta(v_1) - \delta \}.
$$

For $k \in \hat{S}$, define $\mathcal{E}_N^k = \mathcal{E}_N^k(\beta)$ as

$$
\mathcal{E}_N^k = \mathcal{W}_k^\delta \cap \Xi_N.
$$

This set $\mathcal{E}_N^k$ is called the metastable set, provided that it is not an empty set. For $A \subset \hat{S}$, we write

$$
\mathcal{E}_N^A = \bigcup_{k \in A} \mathcal{E}_N^k.
$$

Let $T$ be $S$, $\hat{S}$, or $\{o, S\}$. Denote by $\Psi_N = \Psi_N^\beta : \Xi_N \to T \cup \{N\}$ the projection map given by

$$
\Psi_N(x) = \sum_{k \in T} k1\{x \in \mathcal{E}_N^k\} + N1\{x \in \Xi_N \setminus \mathcal{E}_N^T\}.
$$

Let us define the so-called order process by $X_N(t) = \Psi_N(r_N(t))$ which represents the index of metastable set at which the process $r_N(\cdot)$ is staying.

**Definition 4.1** (Markov chain model reduction) Let $X(\cdot)$ be a continuous time Markov chain on $T$. We say that the metastable behavior of the process $r_N(\cdot)$ is described by a Markov Process $X(\cdot)$ in the time scale $\theta_N$ if, for all $k \in T$ and for all sequence $(x_N)_{N \geq 1}$ such that $x_N \in \mathcal{E}_N^k$ for all $N \geq 1$, the finite dimensional marginals of the process $X_N(\theta_N \cdot)$ under $\mathbb{P}_N^{\beta}$ converges to that of the Markov chain $X(\cdot)$ starting at $k$ as $N \to \infty$.

In the previous definition, it is clear that the Markov chain $X(\cdot)$ describes the inter-valley dynamics of the process $r_N(\cdot)$ accelerated by a factor of $\theta_N$.

4.2 Metastability Results for $q \leq 4$

We can now state the main result for the metastable behavior. First, we consider the case $q \leq 4$ whose result is essentially the same as that in [9,Section 4.3] where only the case $q = 3$ was considered.

We define limiting Markov chains when $q \leq 4$. 

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Definition Let $q \leq 4$ and $i \in \{ (1, 2), (2), (2, 3), (3, \infty), (4) \}$. Let $Y_q^i(\cdot)$ be a Markov chain on $T$ with jump rate $r_q^i : T \times T \to \mathbb{R}$ given by

1. $r_q^{(1,2)}(k, l) = 1[l = o] \frac{\omega_o}{v_i} \cdot T = \mathcal{S}$.
2. $r_q^{(2)}(k, l) = 1[l = o] \frac{\omega_o}{v_i} + 1[k = o] \frac{\omega_o}{v_o} \cdot T = \mathcal{S}$.
3. $r_q^{(2,3)}(k, l) = \frac{\omega_o}{v_i} \cdot T = S$.
4. $r_q^{(3,\infty)}(k, l) = \begin{cases} \frac{\omega_o}{v_i} \cdot q = 3, T = S. \\ \frac{\omega_o}{v_i} \cdot q = 4, T = S. \end{cases}$
5. $r_q^{(4)}(k, l) = 1[k = o] \frac{\omega_o}{v_o} \cdot T = \mathcal{S}$.

The following theorem is the metastability result for $q \leq 4$. We remark that the case when $q = 3$ is proven in [9, Section 4.3].

**Theorem 4.2** Let $q \leq 4$. Then, the metastability behavior of the process $r_N(\cdot)$ is described by (cf. Definition 4.1)

1. $\beta \in (\beta_1, \beta_2)$: the process $Y_q^{(1,2)}(\cdot)$ in the time scale $2\pi N e^{\beta} t$.
2. $\beta = \beta_2$: the process $Y_q^{(2)}(\cdot)$ in the time scale $2\pi N e^{\beta} t$.
3. $\beta \in (\beta_2, q)$: the process $Y_q^{(2,3)}(\cdot)$ in the time scale $2\pi N e^{\beta} t$ and by the process $Y_q^{(4)}(\cdot)$ in the time scale $2\pi N e^{\beta} t$.
4. $\beta \in (q, \infty)$: the process $Y_q^{(3,\infty)}(\cdot)$ in the time scale $2\pi N e^{\beta} t$.

The proof follows from Theorems 3.4 and 3.5, Proposition 5.3, and [37, Theorem 2.2, Remark 2.10, 2.11].

**Remark 4.3** As mentioned in [9], we cannot investigate the case $\beta = \beta_3 = q$ with the current method since $p$ is a degenerate saddle point.

**Remark 4.4** The qualitative feature of the metastable behavior of $r_N(\cdot)$ is essentially same for $q = 3$ and $q = 4$. The only difference is that the saddle points between metastable sets are defined in different ways; however, when $\beta > \beta_3$, the points in $V_1$ for $q = 3$ and $U_2$ for $q = 4$ play the same role since all the points belonging to these sets represent states in which most sites are aligned to two spins equally.

### 4.3 Metastability Results for $q \geq 5$

As in the previous subsection, we start by defining limiting Markov chains. Note that there are two different Markov chains.

**Definition** Let $q \geq 5$ and $i \in \{ (1, 2), (2), (2, 3), (3, \infty), (4), (5) \}$. Let $Y_q^i(\cdot)$ be a Markov chain on $T$ with jump rate $r_q^i : T \times T \to \mathbb{R}$ with jump rate $r_q^i : T \times T \to \mathbb{R}$ given by

1. $r_q^{(1,2)}(k, l) = 1[l = o] \frac{\omega_o}{v_i} \cdot T = \mathcal{S}$.
2. $r_q^{(2)}(k, l) = 1[l = o] \frac{\omega_o}{v_i} + 1[k = o] \frac{\omega_o}{v_o} \cdot T = \mathcal{S}$.
3. $r_q^{(2,3)}(k, l) = \frac{\omega_o}{v_i} \cdot T = S$.
4. $r_q^{(3)}(k, l) = \frac{1}{v_i} \left( \frac{\omega_o}{q} + \omega_1 \right) \cdot T = S$.

---

5 Here, $(1, 2), (2, 3), (3, \infty)$ are single element of the given set.
Now, we present the metastability result for $q \geq 5$. The new metastable behaviors are observed when $\beta = \beta_3$ and $\beta \in (\beta_3, q)$.

**Theorem 4.5** Let $q \geq 5$. Then, the metastable behavior of the process $r_N(\cdot)$ is described by

1. $\beta \in (\beta_1, \beta_2)$: the process $Y_q^{(1,2)}(\cdot)$ in the time scale $2\pi N e^{\theta_1}$.
2. $\beta = \beta_2$: the process $Y_q^{(2)}(\cdot)$ in the time scale $2\pi N e^{\theta_1}$.
3. $\beta \in (\beta_2, \beta_3)$: the process $Y_q^{(2,3)}(\cdot)$ in the time scale $2\pi N e^{\theta_1}$ and by the process $Y_q^{(4)}(\cdot)$ in the time scale $2\pi N e^{\theta_o}$.
4. $\beta = \beta_3$: the process $Y_q^{(3)}(\cdot)$ in the time scale $2\pi N e^{\theta_1}$ and by the process $Y_q^{(4)}(\cdot)$ in the time scale $2\pi N e^{\theta_o}$.
5. $\beta \in (\beta_3, q)$: the process $Y_q^{(3,\infty)}(\cdot)$ in the time scale $2\pi N e^{\theta_1}$ and by the process $Y_q^{(5)}(\cdot)$ in the time scale $2\pi N e^{\theta_o}$.
6. $\beta \in [q, \infty)$: the process $Y_q^{(3,\infty)}(\cdot)$ in the time scale $2\pi N e^{\theta_1}$.

The proof follows from Theorems 3.4 and 3.6, Proposition 5.3, and [37,Theorem 2.2, Remarks 2.10, 2.11].

**Remark 4.6** Notably, in contrast to the case $q \leq 4$, we can describe the metastable behavior for all $\beta \in (\beta_1, \infty)$ since the saddle points are nondegenerate when $\beta = \beta_3$.

We can now provide a more intuitive explanation of Theorem 4.5. See Fig. 6 also for the description of metastable behavior. Note that if $\beta_2 < \beta < q$, there are two time scales.

- $Y_q^{(1,2)}$: If $\beta_1 < \beta < \beta_2$, in the time scale $2\pi N e^{\theta_1}$, $r_N(\cdot)$ starting from $E_S^N$, reaches $E_o^N$ and stays there forever. When it goes from $E_k^N$, $k \in S$, to $E_o^N$, it visits the neighborhood of $v_1^k$.

---

Fig. 6 Figure about metastability when $q = 5$
• $Y_q^{(2)}$: If $\beta = \beta_2$, in the time scale $2\pi Ne^\theta_1$, the process $r_N(\cdot)$ goes around each well in $E^S_N$. However, when $r_N(\cdot)$ starting from $E^l_N, k \in S$, goes to $E^l_N, l \in S \setminus \{k\}$, it must pass through $E^o_N$ and as in the case $\beta \in (\beta_1, \beta_2)$, it visits the neighborhood of $v_1^k$ and then the neighborhood of $v_1$.

• $Y_q^{(2,3)}$: If $\beta_2 < \beta < \beta_3$, in the time scale $2\pi Ne^\theta_1$, the process $r_N(\cdot)$ starting from $E^S_N$ travels $E^S_N$, however, it stays in $E^o_N$ in negligible time. Furthermore, when $r_N(\cdot)$ goes from $E^k, k \in S$, to $E^l, l \in S \setminus \{k\}$, it must visit $E^o_N$.

• $Y_q^{(3)}$: If $\beta = \beta_3$, in the time scale $2\pi Ne^\theta_1$, the process $r_N(\cdot)$ starting from $E^S_N$ travels $E^S_N$, however, it stays in $E^o_N$ in negligible time. Furthermore, there are two ways in which $r_N(\cdot)$ goes from $E^k, k \in S$, to $E^l, l \in S \setminus \{k\}$. First, it goes to $E^l_N$ directly and must pass through the neighborhood of $u_{1}^{k,l}$. Second, it visits $E^o_N$ and stays there for a negligible period of time.

• $Y_q^{(3,\infty)}$: If $\beta > \beta_3$, in the time scale $2\pi Ne^\theta_1$, the process $r_N(\cdot)$ starting from $E^S_N$ travels $E^S_N$ without visiting $E^o_N$. As in the case $\beta = \beta_3$, it must pass through the neighborhood of $u_{1}^{k,l}, k, l \in S$, when it goes from $E^k_N$ to $E^l_N$.

• $Y_q^{(4)}$: If $\beta_2 < \beta \leq \beta_3$, in the second time scale $2\pi Ne^\theta_2$, the process $r_N(\cdot)$ starting from $E^o_N$, goes to $E^k_N, k \in S$, and stays there forever. As $Y_q^{(1,2)}, Y_q^{(2)}$, and $Y_q^{(2,3)}$, it passes through the neighborhood of $v_1^k$ when it moves to $E^o_N$ from $E^k_N$.

• $Y_q^{(5)}$: If $\beta_3 < \beta < q$, in the second time scale $2\pi Ne^\theta_2$, the process $r_N(\cdot)$ starting from $E^o_N$, goes to $E^k_N$ and stays there forever. This dynamics is similar to $Y_q^{(4)}$; however, $E^k_N, k \in S$, are not distinguishable.

### 4.4 Eyring–Kramers Formulae

In this subsection, we present the Eyring–Kramers formula with regard to metastable behavior.

Before we state the result, we introduce some notations. Let $[x]_N$ be the nearest point in $\mathbb{Z}_N$ of $x \in \mathbb{Z}$. If there are more than one such point, one of them is chosen arbitrarily. For $\mathcal{A} \subset \mathbb{Z}$, define $[\mathcal{A}]_N$ as

$$[\mathcal{A}]_N = \{[x]_N : x \in \mathcal{A}\}.$$ 

Denote by $H_\mathcal{A}$ the hitting time of the set $[\mathcal{A}]_N$ by the process $r_N(\cdot)$:

$$H_\mathcal{A} = \inf\{t > 0 : r_N(t) \in [\mathcal{A}]_N\}.$$ 

If $\mathcal{A} = \{x\}$, we simply write $H_\mathcal{A} = H_x$.

We have the following theorem.

**Theorem 4.7** Let $q \geq 3$. We have the following.

1. For $\beta_1 < \beta \leq \beta_2$ and $k \in S$, we have

$$E^N_{u_1^{k}}[H_p] = [1 + o_N(1)] \frac{v_1}{\omega_o} 2\pi N \exp(N\theta_1).$$

2. For $\beta_2 \leq \beta < q$, we have

$$E^N_p[H_{\mathcal{A}}} = [1 + o_N(1)] \frac{v_0}{q\omega_o} 2\pi N \exp(N\theta_0).$$
(3) For $\beta > \beta_3$ and $k \in S$, we have
\[
E_{u_i}^{N, \beta} [H_{U(t)} | u_1] = [1 + o_N(1)] \frac{v_1}{(q - 1)\omega_1} 2\pi N \exp \left( N\theta_1 \right).
\]

The proof follows from Theorems 3.4–3.6, Proposition 5.3, and [37, Theorem 2.5, Remarks 2.10, 2.11].

Because of the Eyring-Kramers formula, we can derive the large-deviation-type estimates on spectral gap and mixing time. To explain this more concretely, let $\lambda_N$ be the spectral gap of the process $r_N(\cdot)$ [which will be defined explicitly in (5.2)], and define the mixing time as
\[
t_{\text{mix}}^N = t_{\text{mix}}^N(\delta) := \inf \left\{ t > 0 : \sup_{x \in \Xi_N} \left\| P^t(x, \cdot) - v_N^\beta \right\|_{TV} < \delta \right\}; \quad \delta \in (0, 1),
\]
where $P^t(x, \cdot)$ is a distribution of $r_N(t)$ with initial condition $r_N(0) = x$ and $\| \cdot \|_{TV}$ denotes the total variation distance defined by
\[
\|\mu - v\|_{TV} := \frac{1}{2} \sum_{x \in \Xi_N} |\mu(x) - v(x)|
\]
for any two probability measures $\mu$ and $v$ on $\Xi_N$. Then, by the arguments in [10, 38], we can observe that
\[
\lim_{N \to \infty} \frac{1}{N} \log t_{\text{mix}}^N = \lim_{N \to \infty} \frac{1}{N} \log \frac{1}{\lambda_N} = \max \{\theta_0, \theta_1\}.
\]
Note that the Eyring-Kramers type estimate on the spectral gap cannot follow immediately from the results of [10, 38] since there are several valleys with same depth.

## 5 Preliminary Analysis on Potential and Generator

In this section, we conduct several preliminary analyses. In Sect. 5.1, we prove Proposition 2.1. In particular, we compute the jump rates of Markov chain $r_N(\cdot)$. In Sect. 5.2, we decompose the generator $\mathcal{L}_N$ into several simple generators $\mathcal{L}_{N, i}, x \in \Xi_N, i, j \in S$. Via this decomposition of $\mathcal{L}_N$, we can handle $\mathcal{L}_N$ using the method developed in [37] since our model is a special case of [37, Remarks 2.10, 2.11]; this correspondence will be explained in Sect. 5.3.

### 5.1 Dynamics of Proportion Vector

We prove Proposition 2.1 in this section.

**Proof of Proposition 2.1** Let $e_j^N := \frac{1}{N} e_j, j \in S$ (cf. Notation 3.1). Fix configurations $\sigma, \tau \in \Omega_N$ such that $r_N(\sigma) = r_N(\tau)$ and let
\[
x = (x_1, \ldots, x_{q-1}) = r_N(\sigma) = r_N(\tau) \in \Xi_N.
\]
For some sites $u_1, u_2, v_1, v_2 \in K_N$ such that $\sigma_{u_1} = \sigma_{v_1} = \tau_{u_2} = \tau_{v_2}$, let $i = \sigma_{v_1}$. Then, the Markovity of the process $r_N(t)$ can be inferred from the identity

\[ \frac{\partial}{\partial t} E_{\sigma}^{N, \beta} [H_{U(t)}] = \frac{1}{2} \sum_{i \in \Xi_N} \frac{\partial^2}{\partial x_i^2} E_{\sigma}^{N, \beta} [H_{U(t)}] \chi_i(x) \left( u_i - v_i \right). \]
Define a jump rate \( \tilde{R}_{i,j} \) for \( j \neq i \). Hence, \( r_N(\cdot) \) is a Markov chain.

Since there are \( N x_i \) sites whose spins are \( i \), the jump rate \( R_N(\cdot, \cdot) \) of \( r_N(\cdot) \) can be written as

\[
R_N(x, x + e_j^N - e_i^N) = \frac{N x_i}{N} \exp \left\{ -\frac{N \beta}{2} [H(x + e_j^N - e_i^N) - H(x)] \right\} .
\]

Hence, the generator \( \mathcal{L}_N \) of \( r_N(\cdot) \) is given as

\[
\mathcal{L}_N f(x) = \sum_{i, j \in S} R_N(x, x + e_j^N - e_i^N) \left[ f(x + e_j^N - e_i^N) - f(x) \right] ,
\]

for \( f : \Xi_N \to \mathbb{R} \).

Finally, this dynamics is reversible with respect to \( \nu_\beta^N \) since we have the following detailed balance condition

\[
\nu_\beta^N(x) R_N(x, x + e_j^N - e_i^N) = \nu_\beta^N(x + e_j^N - e_i^N) R_N(x + e_j^N - e_i^N, x) ,
\]

so that \( \nu_\beta^N \) is the invariant measure.

### 5.2 Cyclic Decomposition

For \( 1 \leq i < j \leq q \), let \( \gamma^i,j_N \) be the cycle \( (e_0^N, e_j^N - e_i^N, e_0^N) \) of length 2 on \((\mathbb{Z}/N)^q\) and let \( (\gamma^i,j_N)_x = x + \gamma^i,j_N \). Define \( \widehat{\Sigma}^i,j_N \) as

\[
\widehat{\Sigma}^i,j_N = \{ x \in \Xi_N : (\gamma^i,j_N)_x \subset \Xi_N \} = \{ x \in \Xi_N : x_j \leq 1 - N^{-1}, x_i \geq N^{-1} \} .
\]

Define a jump rate \( \widehat{R}^i,j_N \) associated with this cycle as

\[
\begin{align*}
\widehat{R}^i,j_{N,0}(x) &= \exp \left\{ -N \beta [F_{\beta,N}^i(x) - F_{\beta,N}(x)] \right\} , \\
\widehat{R}^i,j_{N,1}(x) &= \exp \left\{ -N \beta [F_{\beta,N}^i(x) - F_{\beta,N}(x + e_j^N - e_i^N)] \right\} ,
\end{align*}
\]

where

\[
F_{\beta,N}^i(x) = \frac{1}{2} [F_{\beta,N}(x) + F_{\beta,N}(x + e_j^N - e_i^N)] .
\]

Let \( \mathcal{L}^i,j_N \), \( x \in \widehat{\Sigma}_N \), be a generator acting on \( f : \Xi_N \to \mathbb{R} \) as

\[
(\mathcal{L}^i,j_N f)(y) = \begin{cases} 
\widehat{R}^i,j_{N,0}(x) \left[ f(x + e_j^N - e_i^N) - f(x) \right] & y = x , \\
\widehat{R}^i,j_{N,1}(x) \left[ f(x) - f(x + e_j^N - e_i^N) \right] & y = x + e_j^N - e_i^N , \\
0 & \text{otherwise} .
\end{cases}
\]

Here, \( \mathcal{L}^i,j_N \) can be regarded as a generator of a Markov chain on the cycle \( (\gamma^i,j_N)_x \).
Let
\[ w^{i,j}(x) := \sqrt{x_ix_j}, \quad \text{and} \quad w^{i,j}_N(x) := \sqrt{x_i(x_j + \frac{1}{N})}. \]
By (2.3), we can write
\[ \exp[-\beta N[F_{\beta, N}(x) - H(x)]] = (2\pi N)^{(q-1)/2}\left(\frac{N}{(N_1) \cdots (N_q)}\right). \]
By elementary computations, we obtain
\[ R_N(x, x + e^N_i - e^N_j) = R_N(x, x + e^N_i - e^N_j), \]
so that
\[ R_N(x, x + e^N_i - e^N_j)(f(x + e^N_i - e^N_j)) = w^{i,j}_N(x) \mathcal{L}^{i,j}_N f(x) \]
\[ R_N(x, x + e^N_i - e^N_j)(f(x) - f(x)) = w^{i,j}_N(x) \mathcal{L}^{i,j}_N f(x). \]
Hence, by (5.3), we can write
\[ \mathcal{L}_N f(x) = \sum_{1 \leq i < j \leq q} [w^{i,j}_N(x) \mathcal{L}^{i,j}_N x + w^{i,j}_N(x + e^N_i - e^N_j) \mathcal{L}^{i,j}_N e^N_i - e^N_j] f(x) \]
\[ = \sum_{1 \leq i < j \leq q} \sum_{y \in \mathbb{Z}^N} w^{i,j}_N(y) \mathcal{L}^{i,j}_N y f(x). \]
Since \( w^{i,j}_N \) converges uniformly to \( w^{i,j} \) and is uniformly Lipschitz on every compact subset of \( \text{int} \mathbb{Z} \), our model is a special case of [37, Remarks 2.10, 2.11] provided that several technical requirements are verified. These requirements will be verified in the next subsection.

**Remark 5.1** [37, Section 2] assumes that for \( y^{i,j}_N = (z_0, z_1), z_1 - z_0 \) generates \( \mathbb{Z}^{q-1} \); however, this requirement is needed to make \( r_N(\cdot) \) be irreducible. Since \( (y^{i,j}_N)_{1 \leq i < j \leq q} \) generate \( \mathbb{Z}^{q-1} \), we do not need this assumption.

### 5.3 Requirements for \( F_{\beta, N} \) and \( \mathcal{L}_N \)

In this subsection, we verify that our model is a special case of [37, Remarks 2.10, 2.11].

First, we give some properties of \( F_{\beta}(\cdot) \) and \( G_{\beta, N}(\cdot) \). By the following proposition, \( F_{\beta}(\cdot) \) and \( G_{\beta, N}(\cdot) \) fulfill the requirements in the first paragraph of [37, Section 2].

**Proposition 5.2** The functions \( F_{\beta}(\cdot) \) and \( G_{\beta, N}(\cdot) \) satisfy the following properties.

1. \( F_{\beta} \) is twice-differentiable and there is no critical points at \( \partial \mathbb{Z} \). For all \( x \in \partial \mathbb{Z}, \nabla F_{\beta}(x) \cdot n(x) > 0. \)
2. The second partial derivatives of \( F_{\beta}(\cdot) \) are Lipschitz-continuous on every compact subset of \( \text{int} \mathbb{Z} \).
3. On each compact subset of \( \text{int} \mathbb{Z} \), \( G_{\beta, N}(\cdot) \) is uniformly Lipschitz and converges uniformly to \( G_{\beta}(x) := (1/2\beta) \log(x_1 \cdots x_q) \) as \( N \to \infty. \)
4. There are finitely many critical points of \( F_{\beta}(\cdot) \).

**Proof** (1)–(3) are straightforward. By Lemma 6.2 in Sect. 6.1, there are finitely many critical points of \( F_{\beta}(\cdot) \).
Next, fix one of saddle points \( s \). Note that \( \nabla^2 F_\beta(s) \) has a unique negative eigenvalue. As in [37,Section 4.3], define \( (\mathcal{L}^{i,j}_N)^s \) as

\[
(\mathcal{L}^{i,j}_N)^s f(x) = \frac{1}{N^2} (e_j - e_i)^\top \nabla^2 f(x) (e_j - e_i) - \frac{1}{N} \lambda_{i,j} \nabla^2 F(s)(x - s) \cdot \nabla f(x).
\]

Denote by \( -\lambda^q_1, \lambda^q_2, \ldots, \lambda^q_{q-1} \) the eigenvalues of \( \nabla^2 F_\beta(s) \) where \( \lambda^q_i > 0 \) for all \( i = 1, \ldots, q-1 \), and by \( a^1_s, a^2_s, \ldots, a^{q-1}_s \) the corresponding eigenvectors. Let \( \epsilon_N := N^{-2/5} \ll N^{-1} \) so that \( \epsilon_N \) satisfies [37, displays (4.7), (4.8)]. Define a neighborhood of \( s \) as

\[
C^s_N := \left\{ s + \sum_{k=1}^{q-1} x_k a^k_s : |x_1| \leq \epsilon_N, |x_k| \leq \sqrt{\frac{2\beta^2}{\lambda_k}} \epsilon_N, 2 \leq k \leq q - 1 \right\} \cap \mathbb{R}^N.
\]

Then, by the next proposition, definitions (4.1)–(4.4) are consistent with [37, Remarks 2.10, 2.11].

**Proposition 5.3** For a smooth function \( f : \mathbb{R} \rightarrow \mathbb{R} \), we have uniformly on \( C^s_N \),

\[
\mathcal{L}_N f = \left[ 1 + O(\epsilon_N) \right] \sum_{1 \leq i < j \leq q} w^{i,j}(s)(\mathcal{L}^{i,j}_N)^s f(x).
\]

**Proof** Since \( |x - s| = O(\epsilon_N) \), by (5.3) and the second order Taylor expansion on \( C^s_N \), we have

\[
\sum_{y \in \mathbb{R}^N} \mathcal{L}^{i,j}_{N,y} f(x) = \left[ 1 + O(\epsilon_N) \right](\mathcal{L}^{i,j}_N)^s f(x).
\]

Hence, on \( C^s_N \), since \( w^{i,j}_N(x) = [1 + O(N^{-1})]w^{i,j}(x) = [1 + O(\epsilon_N)]w^{i,j}(s) \), we have

\[
\mathcal{L}_N f(x) = \sum_{1 \leq i < j \leq q} \sum_{y \in \mathbb{R}^N} w^{i,j}_N(y) \mathcal{L}^{i,j}_{N,y} f(x)
= \left[ 1 + O(\epsilon_N) \right] \sum_{1 \leq i < j \leq q} w^{i,j}(s) \sum_{y \in \mathbb{R}^N} \mathcal{L}^{i,j}_{N,y} f(x)
= \left[ 1 + O(\epsilon_N) \right] \sum_{1 \leq i < j \leq q} w^{i,j}(s)(\mathcal{L}^{i,j}_N)^s f(x).
\]

6 Investigation of Critical Points and Temperatures

This section is devoted to the investigation of critical points and temperatures including their definitions. We will provide a preliminary analysis of the critical points in Sect. 6.1 and of the critical temperatures in Sect. 6.2.

6.1 Classification of Critical Points

We recall that

\[
F_\beta(x) = -\frac{1}{2} \sum_{k=1}^{q} x_k^2 + \frac{1}{\beta} \sum_{k=1}^{q} x_k \log x_k,
\]
and that $x_q = 1 - (x_1 + \cdots + x_{q-1})$. For $1 \leq k \leq q-1$,
\[
\frac{\partial}{\partial x_k} F_\beta(x) = -(x_k - x_q) + \frac{1}{\beta} (\log x_k - \log x_q).
\]
If $\frac{\partial}{\partial x_k} F_\beta(x) = 0$, we must have $x_k - \frac{1}{\beta} \log x_k = x_q - \frac{1}{\beta} \log x_q$. Hence,
\[
\nabla F_\beta(x) = 0 \text{ if and only if } x_k - \frac{1}{\beta} \log x_k, \quad 1 \leq k \leq q,
\]
are the same. \hfill (6.1)

By (6.1), $p = (1/q, \ldots, 1/q)$ is a critical point.

By elementary computation, we can check that the equation $t - \frac{1}{\beta} \log t = c$ has at most two positive real solutions for fixed $\beta$, $c > 0$. Hence, if $(x_1, \ldots, x_q)$ is a critical point, $x_k$’s can have at most 2 values by (6.1). Hereafter, we assume $c$ is a critical point and
\[
c = (t, \ldots, t, \frac{1}{q} - jt \frac{1}{i}, \ldots, \frac{1}{q} - jt \frac{1}{i})
\]
where $j$ is the number of $t$’s and $i = q - j$. Observe that by symmetry, each permutation of coordinates of $c$ has the same properties. Without loss of generality, we may assume $1 \leq i \leq q/2 \leq j \leq q - 1$ and $t \neq 1/q$.

The point $p$ will be analyzed separately.

By (6.1), we obtain
\[
t - \frac{1}{\beta} \log t = \frac{1 - \frac{qj}{i}}{i} - \frac{1}{\beta} \log \left(\frac{1 - \frac{qj}{i}}{i}\right),
\]
which implies
\[
\beta = \frac{i}{1 - qt} \log \left(\frac{1 - \frac{qj}{i}}{i}\right) = g_i(t). \quad (6.2)
\]

**Lemma 6.1** Fix $q \geq 3$, $1 \leq i \leq q/2$ and $j = q - i$. Then, the function $g_i : (0, 1/j) \to \mathbb{R}$ has the unique minimum, say $m_i$. Furthermore, if $\beta > g_i(m_i)$, $\beta = g_i(t)$ has two solutions.

**Proof** Define $h_i : (0, 1/j) \to \mathbb{R}$ as
\[
h_i(t) := \log \frac{1 - \frac{qj}{i}}{i} + \frac{qt - 1}{qt(1 - j)} \quad (6.3)
\]
By elementary computation, we obtain
\[
g_i'(t) = \frac{qj}{(1 - qt)^2} h_i(t) \quad \text{and} \quad h_i'(t) = \frac{(qt - 1)(2jt - 1)}{q(1 - j)^2 t^2}. \quad (6.4)
\]
There are two cases, where $i < q/2$ and $i = q/2$. By elementary computation, we can show that the graphs of $g_i$, $h_i$, $h_i'$ are given by Fig. 7, which completes the proof.

For $1 \leq i \leq q/2$, let
\[
\beta_{x,i} = \beta_{x,i}(q) := g_i(m_i), \quad (6.5)
\]
where $m_i$ is the unique minimum of $g_i(\cdot)$ given in the above lemma.

---

6 Recall Notation 3.1.

7 As $g_i(\cdot)$; the function $h_i(\cdot)$ can be continuously extended to $(1, 1/j)$. 
If $\beta \geq \beta_{s,i}$, there are one or two solutions of $\beta = g_i(t)$ which will be denoted by $u_i = u_i(\beta), v_i = v_i(\beta)$ where $u_i \leq v_i$. Let

$$U_i = U_i(\beta) = \{\text{permutations of } (u_i, \ldots, u_i, (1 - ju_i)/i, \ldots, (1 - ju_i)/i)\},$$

$$V_i = V_i(\beta) = \{\text{permutations of } (v_i, \ldots, v_i, (1 - jv_i)/i, \ldots, (1 - jv_i)/i)\},$$

for $\beta \geq \beta_{s,i}$. We have the following candidates of the critical points of $F_\beta$.

**Lemma 6.2** A critical point of $F_\beta$ is exactly one of the following cases.

1. $p = (1/q, \ldots, 1/q)$.
2. For $1 \leq i \leq q/2$ and $\beta \in (\beta_{s,i}, \infty)$, elements of $U_i$.
3. For $1 \leq i \leq q/2$ and $\beta \in (\beta_{s,i}, \infty) \setminus \{q\}$, elements of $V_i$.
4. For $1 \leq i < q/2$ and $\beta = \beta_{s,i}$, elements of $U_i = V_i$.

**Proof** By part (1) of Proposition 5.2, points in $\partial \Xi$ cannot be critical points. Then, the proof follows from (6.1) and Lemma 6.1.

Finally, we have the following results for critical points. The proof for $q = 3$ is given in [9, Proposition 4.2].

**Proposition 6.3** The minima and saddle points of $F_\beta$ for $q = 3, q = 4$, and $q \geq 5$ are given by Tables 1, 2, and 3, respectively.

Section 7 proves the above proposition. Until now, we classified all minima and saddle points for all $q \geq 3$.  

Fig. 7 Graphs of $g_i(t), h_i(t)$, and $h'_i(t)$ when $q = 10$
### Table 1  Classification of critical points when $q = 3$

| $p$                | $U_1(\beta)$             | $V_1(\beta)$             |
|--------------------|---------------------------|---------------------------|
| $\beta \in (0, \beta_{s,1})$ | The only minimum         |                           |
| $\beta = \beta_{s,1}$          | The only minimum         | Degenerate                |
| $\beta \in (\beta_{s,1}, q)$   | Local minimum             | Local minima              |
| $\beta = q$               | Degenerate                | Local minima              |
| $\beta \in (q, \infty)$    | Local maximum             | Local minima              |

### Table 2  Classification of critical points when $q = 4$

| $p$                | $U_1(\beta)$             | $V_1(\beta)$             | $U_2(\beta) = V_2(\beta)$ |
|--------------------|---------------------------|---------------------------|-----------------------------|
| $\beta \in (0, \beta_{s,1})$ | The only minimum         |                           |                             |
| $\beta = \beta_{s,1}$          | The only minimum         | Degenerate                | Degenerate                  |
| $\beta \in (\beta_{s,1}, q)$   | Local minimum             | Local minima              | Saddle points               |
| $\beta = q$               | Degenerate                | Local minima              | Degenerate                  |
| $\beta \in (q, \infty)$    | Local maximum             | Local minima              | Index $\geq 2$              |

### Table 3  Classification of critical points when $q = 5$

| $p$                | $U_1(\beta)$             | $V_1(\beta)$             | $U_2(\beta)$ |
|--------------------|---------------------------|---------------------------|--------------|
| $\beta \in (0, \beta_{s,1})$ | The only minimum         |                           |              |
| $\beta = \beta_{s,1}$          | The only minimum         | Degenerate                |              |
| $\beta \in (\beta_{s,1}, \beta_{s,2})$ | Local minimum       | Local minima              | Saddle points |
| $\beta = \beta_{s,2}$          | Local minimum             | Local minima              | Saddle points | Degenerate       |
| $\beta \in (\beta_{s,2}, q)$   | Local minimum             | Local minima              | Saddle points | Saddle points    |
| $\beta = q$               | Degenerate                | Local minima              | Degenerate    |
| $\beta \in (q, \infty)$    | Local maximum             | Local minima              | Index $\geq 2$ | Saddle points    |

### 6.2 Definition of Critical Temperatures

In the previous subsection, we defined several temperatures $\beta_{s,i}, 1 \leq i \leq q/2$. In this subsection, we prove several properties of such temperatures and moreover introduce new temperatures. Then, we select the critical temperatures at which phase transitions occur.

The first lemma is about the order of $\beta_{s,i}$.

**Lemma 6.4** We have $\beta_{s,1} < \beta_{s,2} < \cdots < \beta_{s,\lfloor q/2 \rfloor}$. If $q$ is even, we have $\beta_{s,q/2} = q$ and otherwise, $\beta_{s, \lfloor q/2 \rfloor} < q$.

**Proof** In this proof, we regard $i$ as a real number and claim that $g_i(t)$ increases as $i \in [1, q]$ increases for fixed $t < 1/q$. By elementary computation, we obtain

$$\frac{d}{di} g_i(t) = \frac{1}{1 - qt} \left( \log \frac{1 - jt}{it} + \frac{it}{1 - jt} - 1 \right).$$

By the inequality $x - 1 > \log x$, we can conclude that $\frac{d}{dt} g_i(t) > 0$. Hence, $g_i(t) < g_{i+1}(t)$ if $t < 1/q$. 

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Hereafter, let \( i \in \mathbb{Z} \). Suppose \( i < q/2 - 1 \). Since \( m_i, m_{i+1} < 1/q \), we obtain
\[
\beta_{s,i} = g_i(m_i) \leq g_i(m_{i+1}) < g_i(m_{i+1}+1) = \beta_{s,i+1},
\]
by the above claim. The first inequality holds since \( m_i \) is a minimum of \( g_i \). If \( i = q/2 - 1 \), since \( m_i < 1/q = m_{i+1} \), we obtain
\[
\beta_{s,i} = g_i(m_i) < g_i(m_{i+1}) = q = \beta_{s,q/2}.
\]
If \( i < q/2 \), we have \( m_i < 1/q \) so that \( \beta_{s,i} < g_i(1/q) = q \). This with the above argument prove the second assertion.

**Remark** In particular, by the above lemma, we have \( \beta_{s,1} < \beta_{s,2} = q \) for \( q = 4 \) and \( \beta_{s,1} < \beta_{s,2} < q \) for \( q \geq 5 \).

The relative order of heights of critical points changes with changes in \( \beta \), and the phase transition is owing to this fact. We will explain when and how this order is changed. Since the proofs are technical, they are postponed to Sect. 8.

6.2.1 Order of Heights of \( \mathcal{U}_1 \)

Define \( \beta_c \) as
\[
\beta_c(q) := \frac{2(q - 1)}{q - 2} \log(q - 1), \tag{6.6}
\]
which is introduced in [4, display (3.3)]. Then, we obtain the following.

**Lemma 6.5** For \( q \geq 3 \), we have \( \beta_{s,1} < \beta_c \) and for \( q \geq 4 \), we have \( \beta_{s,1} < \beta_c < \beta_{s,2} \).

The proof of the lemma is given in Sect. 8.1. The following lemma is an important property of \( \beta_c \).

**Lemma 6.6** Let \( q \geq 3 \). Then, we have
\[

\begin{align*}
F_\beta(p) &< F_\beta(u_1) & \text{if } \beta \in (\beta_{s,1}, \beta_c), \\
F_\beta(p) &= F_\beta(u_1) & \text{if } \beta = \beta_c, \\
F_\beta(p) &> F_\beta(u_1) & \text{if } \beta \in (\beta_c, \infty).
\end{align*}
\tag{6.7}
\]

This result is the same as [4, Theorem 3.1(b)]. The proof is provided in [4, Appendices A, B] via convex-duality.

We may assume that \( \beta \) increases from a very small positive number. Observe that the elements of \( \mathcal{U}_1 \) and \( \mathcal{V}_1 \) simultaneously appear when \( \beta = \beta_{s,1} \) and the elements of \( \mathcal{U}_2 \) appear when \( \beta = \beta_{s,2} \). By the above two lemmas, before the appearance of critical points in \( \mathcal{U}_2 \), the heights of \( p \) and \( u_1 \) are reversed.

6.2.2 Order of Heights of \( \mathcal{V}_1 \) and \( \mathcal{U}_2 \)

We have the following lemma about the heights of \( u_2 \) and \( v_1 \). The critical temperature \( \beta_m \) given in the following lemma is the crucial development of this article.

**Lemma 6.7** Let \( q \geq 5 \). We have a critical temperature \( \beta_m \in (\beta_{s,2}, q) \) such that
\[

\begin{align*}
F_\beta(v_1) &< F_\beta(u_2) & \text{if } \beta_{s,2} \leq \beta < \beta_m, \\
F_\beta(v_1) &= F_\beta(u_2) & \text{if } \beta = \beta_m, \\
F_\beta(v_1) &> F_\beta(u_2) & \text{if } \beta_m < \beta \leq q.
\end{align*}
\tag{6.8}
\]

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The proof of the lemma is given in Sect. 8.2.
Up to this point, we have obtained four critical values
\[ 0 < \beta_{s, 1} < \beta_c < \beta_{s, 2} < \beta_m < q , \]
when \( q \geq 5 \). If \( q = 4 \), we have \( \beta_{s, 2} = q \), else if \( q = 3 \), \( \beta_{s, 2} \) is not defined. Thus, if \( q \leq 4 \), define \( \beta_m = q \) so that
\[ 0 < \beta_{s, 1} < \beta_c < \beta_m = q . \]

We conclude this section with the definition of the critical temperatures at which the phase transitions occur. We can now define critical temperatures \( \beta_1, \beta_2, \beta_3 \) appearing in Sect. 3.2. The critical temperatures are given by
\[
\beta_1(q) := \beta_{s, 1}(q), \quad \beta_2(q) := \beta_c(q), \quad \beta_3(q) := \beta_m(q).
\]  
(6.9)

7 Critical Points of \( F_\beta \)

In this section, we prove Proposition 6.3 for \( q \geq 4 \). For the case \( q = 3 \), we refer to [9] and we will only highlight the difference.

7.1 Eigenvalues of Hessian of \( F_\beta \) at Critical Points

First, we investigate \( p = (1/q, \ldots, 1/q) \), which is always a critical point for all \( \beta > 0 \). The following lemma proves the property of \( p \).

**Lemma 7.1** The point \( p \) is a local minimum of \( F_\beta \) if \( \beta < q \), a local maximum of \( F_\beta \) if \( \beta > q \), and a degenerate critical point when \( \beta = q \).

**Proof** Let \( \mathbb{1} = (1, \ldots, 1) \) be a \((q - 1) \times 1\) matrix. By elementary computation, we obtain
\[
\nabla^2 F_\beta(p) = \frac{q - \beta}{\beta} \left( \text{diag}(1, \ldots, 1) + \mathbb{1}\mathbb{1}^\top \right)
\]
whose eigenvalues are \((q - \beta)/\beta\) with multiplicity \( q - 2 \) and \( q(q - \beta)/\beta\) with 1. This completes the proof.

Now, for \( i \in [1, q/2] \cap \mathbb{N}, j = q - i, \) and \( \beta = g_i(t) \), define \( a \in \mathbb{R} \) and \( b \in \mathbb{R} \) as
\[
a = a(i, t) = -1 + 1/\beta t, \quad b = b(i, t) = -1 + i/\beta(1 - jt) .
\]  
(7.1)

We have the following lemma about eigenvalues of Hessian of \( F_\beta \) at critical points.

**Lemma 7.2** Let \( i \in [1, q/2] \cap \mathbb{N} \) and \( j = q - i \). Moreover, let \( t \in (0, 1/\beta) \) and \( \beta = g_i(t) \). Then, \( c = (t, \ldots, t, (1 - jt)/i, \ldots, (1 - jt)/i) \) is a critical point of \( F_\beta \) and eigenvalues of \( \nabla^2 F_\beta(c) \) constitute one of the following cases.

1. If \( i \geq 2 \), all eigenvalues of \( \nabla^2 F_\beta(c) \) are \( a, b \) with multiplicative \( j - 1, i - 2 \), respectively, and the roots of \( \lambda^2 - (a + qb)\lambda + b(ia + jb) \).
2. If \( i = 1 \), all eigenvalues of \( \nabla^2 F_\beta(c) \) are \( a \) with multiplicative \( j - 1 \) and \( a + (q - 1)b \) with multiplicative 1.
Proof By Lemma 6.2, \( c \) is a critical point of \( F_\beta \) since \( \beta = g_i(t) \). By elementary computation, we have

\[
\frac{\partial^2}{\partial x_k^2} F_\beta(x) = -1 + \frac{1}{\beta x_k} + \left( -1 + \frac{1}{\beta x_q} \right),
\]

\[
\frac{\partial^2}{\partial x_k \partial x_l} F_\beta(x) = -1 + \frac{1}{\beta x_q},
\]

so that

\[
\frac{\partial^2}{\partial x_k \partial x_l} F_\beta(c) = \begin{cases} 
-1 + \frac{1}{\beta t} + (-1 + \frac{i}{\beta (1 - j/2)}) & \text{if } 1 \leq k = l \leq j \\
2(-1 + \frac{i}{\beta (1 - j/2)}) & \text{if } j + 1 \leq k = l \leq q - 1 \\
-1 + \frac{i}{\beta (1 - j/2)} & \text{if } k \neq l 
\end{cases}
\]

Then, we can write \( \nabla^2 F_\beta(c) \) as

\[
\nabla^2 F_\beta(c) = \mathbb{D} + b \mathbb{1}^\dagger,
\]

where

\[
\mathbb{D} = \text{diag}(\ldots, a, \ldots, b, \ldots, b). \]

Let \( \mathbb{I} = \mathbb{I}_{q-1} \) be a \((q-1)\)-identity matrix. By the formula

\[
\det(A + vw^\dagger) = \det(A(1 + v^\dagger A^{-1} w) ,
\]

we can write

\[
\det(\nabla^2 F_\beta(c) - \lambda \mathbb{I}) = \det(\mathbb{D} - \lambda \mathbb{I} + b \mathbb{1}^\dagger) = (a - \lambda)^j (b - \lambda)^{j-1} \left[ 1 + b \left( \frac{j}{a - \lambda} + \frac{i - 1}{b - \lambda} \right) \right].
\]

Hence, we obtain

\[
\det(\nabla^2 F_\beta(c) - \lambda \mathbb{I}) = \begin{cases} 
(a - \lambda)^{j-1} (b - \lambda)^{j-2} (\lambda^2 - (a + qb)\lambda + b(i a + j b)) & \text{if } i \geq 2 \\
(a - \lambda)^{j-1} (a + j b - \lambda) = (a - \lambda)^{q-2} (a + (q - 1) b - \lambda) & \text{if } i = 1
\end{cases}
\]

The proof of the lemma arises directly from this explicit computation of characteristic polynomial of Hessian of \( F_\beta(c) \).

We have the following lemma about the sign of the eigenvalues of \( \nabla^2 F_\beta(c) \). Recall the definition of \( m_i \) from Lemma 6.1.

**Lemma 7.3** Let \( i \in [1, q/2] \cap \mathbb{N} \) and \( j = q - i \). Moreover, let \( t \in (0, 1/j) \) and \( \beta = g_i(t) \). Then, we have the following table regarding the sign of each value. If \( i = q/2 \), we ignore \( t = m_i \) and \( t \in (m_i, 1/q) \).

|             | \( t \in (0, m_i) \) | \( t = m_i \) | \( t \in (m_i, 1/q) \) | \( t = 1/q \) | \( t \in (1/q, 1/j) \) |
|-------------|---------------------|--------------|---------------------|-------------|---------------------|
| \( a \)     | +                   | +            | +                   | 0           | -                   |
| \( b \)     | -                   | -            | -                   | 0           | +                   |
| \( ia + jb \)| +                   | 0            | -                   | 0           | +                   |
| \( b(ia + jb) \)| -                   | 0            | +                   | 0           | +                   |
**Proof** First, suppose that $t < 1/q$. Then,

$$a > 0 \iff \frac{1}{t} > \beta = \frac{i}{1 - qt} \log \left(\frac{1 - j t}{i t}\right) \iff \frac{1 - q t}{i t} > \log \left(\frac{1 - j t}{i t}\right).$$

By substituting $x = (1 - j t)/(i t)$, one can deduce that $a > 0$ is equivalent to $t \neq 1/q$ which implies $a > 0$. Moreover, by the same argument above, we have $b < 0$. In the same manner, if $t > 1/q$, we obtain $a < 0$ and $b > 0$.

Now, we investigate the sign of $ia + jb$. We write

$$ia + jb = -i + \frac{i}{\beta t} - j + \frac{ij}{\beta (1 - j t)} = -q + \frac{i}{\beta t (1 - j t)}.$$

By elementary computation, $ia + jb = 0$ if $t = 1/q$. Hence, $ia + jb > 0$ if and only if

$$\frac{i}{qt(1 - j t)} > \beta = \frac{i}{1 - qt} \log \left(\frac{1 - j t}{i t}\right).$$

First, assume $t < 1/q$. Then, $ia + jb > 0$ if and only if

$$h_i(t) = \log \left(\frac{1 - j t}{i t}\right) + \frac{qt - 1}{qt(1 - j t)} < 0.$$

By investigating the graph of $h_i$ (cf. Fig. 7), the above inequality holds if and only if $t < m_i$. Second, assume $t > 1/q$. Then, $ia + jb > 0$ if and only if $h_i(t) > 0$ if and only if $t > 1/q$. Hence, $ia + jb > 0$ if and only if $t < m_i$ or $t > 1/q$.

The case when $t = 1/q$ can be proven by the argument in the first paragraph of this proof. If $t = m_i$, then $ia + jb = 0$ since $h_i(m_i) = 0$. The above argument can prove the case when $i = q/2$ since $m_{q/2} = 1/q$.

Now, we study the critical points more deeply. We note that the Morse index of a critical point is the number of negative eigenvalues of the Hessian at that point.

### 7.2 Critical Points of Morse Index 0 or 1

When we consider critical points in $\mathcal{U}_i$ or $\mathcal{V}_i$, we assume that $\beta > \beta_{s,i}$ since when $\beta = \beta_{s,i}$, the elements of $\mathcal{U}_i = \mathcal{V}_i$ are degenerate. The case when $\beta = \beta_{s,i}$ is treated in Sect. 7.4.

By the Morse theory, critical points with more than 2 negative eigenvalues can be neither saddle points nor minima. Hence, the critical points with only positive eigenvalues or only one negative eigenvalue and $q - 2$ positive eigenvalues are relevant to the landscape of $F_\beta$. We select these critical points in this subsection.

As in (7.1), for $i \in [1, q/2] \cap \mathbb{N}$, $j = q - i$, and $\beta > \beta_{s,i}$, when we consider $u_i \in \mathcal{U}_i$, let

$$a = a(u_i) := -1 + \frac{1}{\beta u_i}, \quad b = b(u_i) := -1 + \frac{1}{\beta (1 - j u_i)},$$

and when we consider $v_i \in \mathcal{V}_i$, let

$$a = a(v_i) := -1 + \frac{1}{\beta v_i}, \quad b = b(v_i) := -1 + \frac{1}{\beta (1 - j v_i)}.$$

**Lemma 7.4** Let $q \geq 4$. If $\beta > \beta_{s,1}$, $\mathcal{U}_1$ is a set of local minima. If $\beta > \beta_{s,2}$, $\mathcal{U}_2$ is a set of saddle points. If $\beta_{s,1} < \beta < q$, $\mathcal{V}_1$ is a set of saddle points else if $\beta > q$, each point in $\mathcal{V}_1$ has at least two negative eigenvalues.
Proof Consider \( u_1 \in \mathcal{U}_1 \). Eigenvalues of \( \nabla^2 F_\beta(u_1) \) are \( a \) with multiplicative \( q - 2 \) and \( a + (q - 1)b \) with multiplicative \( 1 \). By Lemma 7.3, if \( \beta > \beta_{s,1} \), then since \( u_1 < m_1 < 1/q \), we obtain \( a', a + (q - 1)b > 0 \); hence, \( u_1 \) is a local minimum.

Next, consider \( v_1 \in \mathcal{V}_1 \). Eigenvalues of \( \nabla^2 F_\beta(v_1) \) are \( a \) with multiplicative \( q - 2 \) and \( a + (q - 1)b \) with multiplicative \( 1 \). By Lemma 7.3, if \( \beta_{s,1} < \beta < q \), then since \( m_1 < v_1 < 1/q \), we obtain \( a > 0 \) and \( a + (q - 1)b < 0 \); hence, it is a saddle point. If \( \beta > q \), then since \( v_1 > 1/q \), we obtain \( a < 0 \) and \( a + (q - 1)b > 0 \) so that \( v_1 \) has more than two negative eigenvalues.

Finally, let \( i \geq 2 \), \( j = q - i \), and \( \beta > \beta_{s,i} \). In this case, \( u_i \) has eigenvalues \( a, b \) with multiplicative \( j - 1, i - 2 \) and the roots of \( \lambda^2 - (a + q b)\lambda + b(i a + j b) \). Since \( u_i < m_i \leq 1/q \) for all \( i \) and \( \beta > \beta_{s,i} \), by Lemma 7.3, \( a > 0 \), \( b < 0 \), and \( b(i a + j b) < 0 \) so that it has \( j \) positive eigenvalues and \( i - 1 \) negative eigenvalues. Hence, \( u_2 \) is a saddle point.

Remark 7.5 For \( q = 3 \), by the same argument, \( \nabla^2 F_\beta(v_1) \) has only one negative eigenvalue and two positive eigenvalues for \( \beta \in (\beta_{s,1}, \infty) \backslash \{q\} \).

7.3 Critical Points of Morse Index Larger than 1

In this subsection, we eliminate unneeded critical points.

Lemma 7.6 Let \( q \geq 5 \). For \( i \in [3, q/2] \cap \mathbb{N} \) and \( \beta > \beta_{s,i} \), each point in \( \mathcal{U}_i \) has at least two negative eigenvalues. And for \( i \in [2, q/2] \cap \mathbb{N} \) and \( \beta \in (\beta_{s,i}, \infty) \backslash \{q\} \), each point in \( \mathcal{V}_i \) has at least two negative eigenvalues.

Proof By the proof of Lemma 7.4, \( u_i \) for \( i \geq 3 \) has at least two negative eigenvalues. Now, let \( i \geq 2, j = q - i \), and \( \beta \in (\beta_{s,i}, \infty) \backslash \{q\} \). In this case, each points in \( \mathcal{V}_i \) has eigenvalues \( a, b \) with multiplicative \( j - 1, i - 2 \), and the roots of \( \lambda^2 - (a + q b)\lambda + b(i a + j b) \). If \( \beta_{s,i} < \beta < q \), then \( v_i < 1/q \) so that \( a > 0 \), \( b < 0 \), and \( b(i a + j b) > 0 \). In this case,

\[
a + q b = i a + j b + (1 - i)a + (q - j)b < i a + j b < 0 ,
\]

so that the two roots of \( \lambda^2 - (a + q b)\lambda + b(i a + j b) \) are negative. Hence, it has \( j - 1 \) positive eigenvalues and \( i \) negative eigenvalues. If \( \beta > q \), then \( v_i > 1/q \) so that \( a < 0 \), and points in \( \mathcal{V}_i \) have at least \( j - 1 \) negative eigenvalues, where \( j - 1 \geq 2 \) since \( q \geq 5 \).

Lemma 7.7 Let \( q = 4 \) and \( \beta \geq q \). Then, we have \( \mathcal{V}_2 = \mathcal{U}_2 \).

Proof Observe that \( \beta_{s,2} = q \). If \( \beta = q \), \( \mathcal{V}_2 = \mathcal{U}_2 \) since there is only one solution \( m_2 \) to \( q = g_2(t) \). Suppose \( \beta > q \). By elementary computation, we obtain

\[
g_2\left(\frac{1}{4} - t\right) = g_2\left(\frac{1}{4} + t\right) \text{ for } t \in \left[0, \frac{1}{4}\right],
\]

so that \( v_2 = (1/2) - u_2 \). Hence, \( \mathcal{V}_2 = (u_2, u_2, v_2, v_2) \) is a permutation of \( u_2 \), that is, each element of \( \mathcal{V}_2 \) is one of the elements of \( \mathcal{U}_2 \) so that \( \mathcal{V}_2 = \mathcal{U}_2 \).

By lemmas in this subsection, \( \mathcal{U}_i, i \geq 3 \), and \( \mathcal{V}_i, i \geq 2 \), are not of interest.

7.4 At Critical Temperature

In this subsection, we investigate the critical points at the critical temperatures, that is, at \( \beta = \beta_{s,i} \) or \( \beta = q \). The point \( u_i = v_i \) is degenerate when \( \beta = \beta_{s,i} \) and the point \( p = v_i \) is degenerate when \( \beta = q \) by Lemmas 7.2 and 7.3.
Lemma 7.8 If \( i \leq q/2 \) and \( \beta = \beta_{s,i} \), the point \( u_i = v_i \) is not a local minimum. If \( \beta = q \), the point \( p = v_i \) is not a local minimum.

**Proof** Fix \( 1 \leq i \leq j \leq q - 1 \) such that \( i + j = q \) and define \( \ell_i : [0, 1/j] \to \Xi \) as

\[
\ell_i(s) = \left(s, \ldots, s, \frac{1 - js}{i}, \ldots, \frac{1 - js}{i} \right).
\]

We therefore obtain

\[
F_\beta(\ell_i(s)) = -\frac{1}{2j} \left[js^2 + i \left( \frac{1 - js}{i} \right) \right] + \frac{1}{\beta} \left [ js \log s + (1 - js) \log \left( \frac{1 - js}{i} \right) \right ]
\]

\[
= -\frac{1}{2i} \left(jqs^2 - 2js + 1 \right) + \frac{1}{\beta} \left[ (1 - js)(1 - q^3) \frac{\ell_i(s)}{i} + \log s \right].
\]

By (6.3) and (6.4), we have

\[
\frac{d}{ds} F_\beta(\ell_i(s)) = \frac{j}{i} (1 - q^3) + \frac{j}{\beta_i} (q^3 - 1) g_i(s) = \frac{j}{\beta_i} (1 - q^3)(\beta - g_i(s)).
\]

We claim that \( F_{\beta_{s,i}}(\ell_i(m_i)) \) and \( F_q(\ell_i(1/q)) \) are not the local minima of \( F_{\beta_{s,i}}(\ell_i(s)) \) and \( F_q(\ell_i(s)) \), respectively, and this completes the proof.

For the first claim, assume \( i < j \), and note that \( m_i < 1/q \). Then, \( 1 - q^3 > 0 \) and \( \beta_{s,i} = g_i(s) < 0 \) if \( s \) is in a neighborhood of \( m_i \) and \( s \neq m_i \). In this case, \( \frac{d}{ds} F_{\beta_{s,i}}(\ell_i(s)) < 0 \) near \( m_i \) so that \( u_i = v_i \) is not a local minimum. If \( i = j, \beta_{s,i} = q \) so that \( p = v_i \) is not a local minimum.

Even though \( u_i, i \geq 3 \), is not a saddle point if \( \beta > \beta_{s,i} \), we cannot exclude the possibility that \( u_i \) is a saddle point when \( \beta = \beta_{s,i} \); however, by the next two lemmas, \( U_i(\beta_{s,i}), i \geq 3 \), are irrelevant to the landscape of \( F_\beta \).

**Lemma 7.9** Let \( q \geq 8 \) and \( i \geq 4 \). Then, if \( \beta = \beta_{s,i} \), \( u_i = v_i \) is not a saddle point.

**Proof** By Lemma 7.2, \(-1 + 1 \left[ \beta_{s,i} \{- ju_i(\beta_{s,i})\} \right] \) is an eigenvalue of \( \nabla F_{\beta_{s,i}} \) at \( u_i \) with a multiple of at least two. Hence, by Lemma 7.3, it has at least two negative eigenvalues.

**Lemma 7.10** Let \( q \geq 6 \). We have \( F_{\beta_{s,3}}(u_3) > F_{\beta_{s,3}}(u_2) \). Furthermore, if \( q \geq 7 \), we have \( F_{\beta_{s,3}}(u_3) > F_{\beta_{s,3}}(v_1) \). Hence, \( u_3 \) cannot be a saddle point lower than \( u_2 \) or \( v_1 \).

The proof is presented in Sect. 8.3. We remark that if \( q = 6 \), we have \( \beta_{s,3} = q \) so that \( v_1(\beta_{s,3}) = p \) and the second assertion is not needed.

**8 Analysis of Energy Landscape**

In this section, we prove lemmas introduced in Sect. 6.2 and Lemma 7.10. To prove these lemmas, we need numerical computation given in Appendix 11.
8.1 Proof of Lemma 6.5

Lemma 8.1 If \( q \geq 4 \), we have \( v_1(\beta_{s,2}) > \frac{1}{2(q-1)} \).

Proof Fix \( \beta = \beta_{s,2} \) and write \( v_1 = v_1(\beta_{s,2}) \) for convenience. Since \( \beta_{s,2} = g_2(m_2) = g_1(v_1) \), we have

\[
\frac{2}{1 - qm_2} \log \frac{1 - (q - 2)m_2}{2m_2} = \frac{1}{1 - qv_1} \log \frac{1 - (q - 1)v_1}{v_1} \quad (8.1)
\]

Let

\[
v_1^* = \frac{1}{2q} + \frac{m_2}{2}, \quad \text{so that} \quad \frac{1}{1 - qv_1^*} = \frac{2}{1 - qm_2}. \quad (8.2)
\]

We claim that \( g_1(v_1^*) \leq g_1(v_1) \), that is, by (8.1),

\[
\frac{1}{1 - qv_1^*} \log \frac{1 - (q - 1)v_1^*}{v_1^*} \leq \frac{2}{1 - qm_2} \log \frac{1 - (q - 2)m_2}{2m_2}.
\]

By (8.2), the above inequality is equivalent to

\[
\frac{1 - (q - 1)v_1^*}{v_1^*} \leq \frac{1 - (q - 2)m_2}{2m_2}.
\]

By plugging \( v_1^* \) given in (8.2) into this inequality, it becomes \( q^2m_2 - 2qm_2 + 1 \geq 0 \). Hence, since \( g_1 \) is increasing at \( v_1 \), we obtain \( v_1^* \leq v_1 \).

Finally, we claim that

\[
v_1^* = \frac{1 + qm_2}{2q} > \frac{1}{2(q-1)}, \quad \text{i.e.,} \quad m_2 > \frac{1}{q(q-1)}.
\]

According to Fig. 7, we can show this by

\[
h_2\left(\frac{1}{q(q-1)}\right) = \log \frac{q^2 - 2q + 2}{2} - \frac{q(q-1)(q-2)}{q^2 - 2q + 2} < 0.
\]

This holds if \( q = 4 \) or \( q = 5 \) by elementary computation. Now, assume \( q \geq 6 \). Therefore, we obtain

\[
\log \frac{q^2 - 2q + 2}{2} < \log q^2 = 2 \log q < q - 2 < \frac{q(q-1)(q-2)}{q^2 - 2q + 2},
\]

which completes the proof.

We can prove Lemma 6.5 by the aforementioned lemma.

Proof of Lemma 6.5 Since \( \beta_c = g_1(\frac{1}{q(q-1)}) = g_1(\frac{1}{2(q-1)}) \), we have \( \beta_{s,1} < \beta_c \). By Lemma 8.1, since \( g_1(t) \) is increasing on \( (m_1, 1/(q-1)) \) and \( m_1 < 1/(2q - 2) \), we obtain

\[
\beta_{s,2} = g_1(v_1) > g_1\left(\frac{1}{2(q-1)}\right) = \beta_c.
\]
8.2 Proof of Lemma 6.7

We first introduce two lemmas.

Lemma 8.2 Let $q \geq 5$. When $\beta = \beta_s, 2$, we have $F_{\beta_s, 2}(v_1) < F_{\beta_s, 2}(u_2)$ and when $\beta = q$, we have $F_q(v_1) = F_q(p) > F_q(u_2)$.

The proof of the above lemma is given in Sect. 8.3.

Lemma 8.3 Let $q \geq 5$. $\beta \frac{d}{d\beta}[F_\beta(u_2) - F_\beta(v_1)]$ decreases as $\beta$ increases in $(\beta_s, 2, q)$.

Proof For $t = t(\beta)$, which satisfies $\beta = g_i(t)$, let $c_i = c_i(\beta) = (t, \ldots, t, \frac{1 - j t}{it}, \ldots, \frac{1 - j t}{it})$. (8.3)

Since $c_i$ is a critical point, by the proof of Corollary 3.7, we have

$$\frac{d}{d\beta}F_\beta(c_i) = -\frac{1}{\beta^2}S(c_i).$$

Define a function $k_i : (0, 1) \to \mathbb{R}$ as

$$k_i(t) := (1 - j t) \log \frac{1 - j t}{it} + \log t.$$  

(8.4)

By elementary computations, we obtain $S(c_i) = k_i(t)$ so that we have

$$\frac{d}{d\beta}F_\beta(c_i) = -\frac{1}{\beta^2}k_i(t).$$  

(8.5)

Now, by (8.5), we obtain

$$\beta^2 \frac{d}{d\beta}[F_\beta(u_2) - F_\beta(v_1)] = k_1(v_1(\beta)) - k_2(u_2(\beta)).$$  

(8.6)

Observe that the value $u_2(\beta)$ decreases and the value $v_1(\beta)$ increases as $\beta$ increases. By elementary computation, for $t \in (0, 1/q)$, we obtain

$$k_i(t) = -j \log \frac{1 - j t}{it} + (1 - j t) \left(\frac{-j}{1 - j t} - \frac{1}{t}\right) + \frac{1}{t} = -j \log \frac{1 - j t}{it} < 0,$$

(8.7)

so that $k_i(t)$ decreasing on $(0, 1/q)$. Hence, (8.6) decreases as $\beta$ increases in $(\beta_s, 2, q)$.

We can now prove Lemma 6.7.

Proof of Lemma 6.7 By Lemma 8.2, there is $\beta_0 \in (\beta_s, 2, q)$, such that $\frac{d}{d\beta}[F_\beta(u_2) - F_\beta(v_1)] < 0$. Hence, by Lemma 8.3, we can deduce that there is only one critical value $\beta_m \in (\beta_s, 2, q)$, such that

$$F_{\beta_m}(u_2) = F_{\beta_m}(v_1).$$  

(8.8)

8.3 Proofs of Lemmas 7.10 and 8.2

Before we go further, we conduct some computations. Recall the definition of $m_2$ from Lemma 6.1. Since $\beta_{s, i} = g_i(m_i) = \frac{i}{1 - q m_i} \log \frac{1 - j m_i}{i m_i}$ and $m_i$ is the minimum of $g_i$, we have

$$0 = h_i(m_i) = \log \frac{1 - j m_i}{i m_i} + \frac{q m_i - 1}{q m_i(1 - j m_i)}.$$
\[
\frac{1 - qm_i}{i} \beta_{s,i} - \frac{1 - qm_i}{qm_i(1 - jm_i)},
\]
so that
\[
qm_j^2 - qm_i = qm_i(jm_i - 1) = - \frac{i}{\beta_{s,i}}. \tag{8.9}
\]
For \(c_i\) defined in (8.3), since \(S(c_i) = k_i(t)\) and \(\beta = g_i(t)\), we can write
\[
F_\beta(c_i) = \frac{1}{2i} \left[ j^2 t^2 - 2qt + 1 \right] + \frac{1}{\beta} \log t. \tag{8.10}
\]
Hence, by (8.9) and \(\beta_{s,i} = g_i(m_i)\), we have
\[
F_{\beta_{s,i}}(u_i) = \frac{1 - qm_i}{2i} + \frac{1}{\beta_{s,i}} \left( \log m_i - \frac{1}{2} \right) \tag{8.11}
\]
By (8.9) again, we obtain
\[
F_{\beta_{s,i}}(u_i) = -\frac{1}{2\beta_{s,i}} \log(qe\beta_{s,i}). \tag{8.12}
\]
Now, we introduce two technical lemmas required in the proof of Lemmas 7.10 and 8.2.

**Lemma 8.4** For \(q \geq 6500\), we have
\[
\frac{1}{\beta_{s,2}} \left( \log qm_2 - \frac{1}{2} \right) > \frac{(q - 1)}{8q} (qm_2)^2 - \frac{1}{4} m_2 + \frac{-q^2 + 4q + 1}{8q(q - 1)}. \]
The proof is given in Sect. 10.

**Lemma 8.5** Let \(q \geq 5\). Define \(f_c(\beta) = -\frac{1}{2\beta} \log(qe\beta)\) and
\[
\Phi(\beta) = \frac{d}{d\beta} [f_c(\beta) - F_\beta(u_2)].
\]
Then, we have \(\Phi(\beta) > 0\) for \(\beta > \beta_{s,2}\).

**Proof** We have
\[
\frac{d}{d\beta} f_c(\beta) = \frac{1}{2\beta^2} \log qe\beta - \frac{1}{2\beta} \frac{1}{\beta} = \frac{1}{2\beta^2} \log q\beta.
\]
By (8.5), we obtain
\[
\beta^2 \frac{d}{d\beta} [f_c(\beta) - F_\beta(u_2)] = \frac{1}{2} [\log q\beta + 2k_2(u_2)].
\]
By (8.7), the above expression is increasing function of \(\beta\) since \(u_2\) decreases as \(\beta\) increases. Hence, it is sufficient to show \(\Phi(\beta_{s,2}) > 0\). First, let \(q \geq 55 > e^4\). By (8.7)
\[
\log q\beta + 2k_2(u_2) > \log q\beta_{s,2} + 2k_2(\frac{1}{2j}) = \log q\beta_{s,2} + \log \frac{2j - j}{i} + 2 \log \frac{1}{2j} = \log q\beta_{s,2} + \frac{1}{4ij}.
\]

where we use \( u_2 < 1/(2j) \) for the inequality. Since \( \beta_{s, 2} > \beta_c > 2 \log q \), we obtain

\[
\frac{q \beta_{s, 2}}{4ij} > \frac{2q \log q}{8(q - 2)} > \frac{q}{q - 2}.
\]

Finally, for \( 5 \leq q \leq 54 \), by Proposition A.1, we have \( \Phi(\beta_{s, 2}) > 0. \)

By the above lemmas, Lemma 8.2 can be proven.

**Proof of Lemma 8.2** By Proposition A.1 given in Appendix, we can check that \( F_{\beta_{s, 2}}(u_2) > F_{\beta_{s, 2}}(v_1) \) holds for \( 5 \leq q \leq 6500 \). Now, suppose that \( q > 6500 \). By (8.10) and (8.11), we can write

\[
F_{\beta_{s, 2}}(u_2) = -\frac{1}{4} q m_2 + \frac{1}{4} + \frac{1}{\beta_{s, 2}} \left( \log m_2 - \frac{1}{2} \right),
\]

\[
F_{\beta_{s, 2}}(v_1) = \frac{1}{2} \left[ q(q - 1) \left( \frac{m_2 + 1}{2q} - \frac{1}{q - 1} \right)^2 - \frac{1}{q - 1} \right] + \frac{1}{\beta_{s, 2}} \log v_1.
\]

By the proof of Lemma 8.1, we have

\[
\frac{q m_2 + 1}{2q} = v_1^* \leq v_1 < \frac{1}{q},
\]

so that

\[
F_{\beta_{s, 2}}(v_1) < \frac{1}{2} \left[ q(q - 1) \left( \frac{m_2 + 1}{2q} - \frac{1}{q - 1} \right)^2 - \frac{1}{q - 1} \right] - \frac{1}{\beta_{s, 2}} \log q.
\]

Hence, the lemma can be proven if we can prove

\[
-\frac{1}{4} q m_2 + \frac{1}{4} + \frac{1}{\beta_{s, 2}} \left( \log m_2 - \frac{1}{2} \right) \geq \frac{1}{2} \left[ q(q - 1) \left( \frac{m_2 + 1}{2q} - \frac{1}{q - 1} \right)^2 - \frac{1}{q - 1} \right] - \frac{1}{\beta_{s, 2}} \log q
\]

\[
= \frac{1}{8} q(q - 1)(m_2)^2 - \frac{1}{4} (q + 1)m_2 + \frac{(q + 1)^2}{8q(q - 1)} - \frac{1}{\beta_{s, 2}} \log q.
\]

This is the content of Lemma 8.4. Finally, by Lemma 8.5, we obtain \( F_q(p) - F_q(u_2) = f_c(q) - F_q(u_2) > 0 \) since \( f_c(\beta_{s, 2}) = F_{\beta_{s, 2}}(u_2) \).

Now, we prove Lemma 7.10.

**Proof of Lemma 7.10** Since the proof for \( F_{\beta_{s, 3}}(u_3) > F_{\beta_{s, 3}}(v_1) \) is exactly the same as the proof of Lemma 8.2 including numerical verification, we omit it. By (8.12), we can write

\[
F_{\beta_{s, 3}}(u_3) = f_c(\beta_{s, 3}).
\]

Hence, by Lemma 8.5 and by Proposition A.1, we have

\[
F_{\beta_{s, 3}}(u_3) = f_c(\beta_{s, 3}) > F_{\beta_{s, 3}}(u_2).
\]

### 9 Characterization of Metastable Sets

In this section, we prove Theorems 3.4-3.6. First, we prove Theorem 3.4.
**Proof of Theorem 3.4** The first assertion is immediate from Lemmas 6.2 and 6.4. The third assertion is proven by Proposition 6.3 and Lemma 7.8. The fourth assertion is Lemma 6.6.

Now, it remains to show the second assertion. For \( \beta \in (\beta_1, \beta_2] \), since \( p \) is the global minimum and \( v_1 \) is a saddle point, we have \( F_\beta(p) < F_\beta(v_1) \) so that \( \mathcal{W}_0 \neq \emptyset \). By the same argument in the proof of Lemma 8.3, we have

\[
\frac{d}{d\beta} [F_\beta(v_1) - F_\beta(p)] = -\frac{1}{\beta^2} [k_1(v_1(\beta)) + \log q].
\]

By 8.7, \( k_1(\cdot) \) is decreasing on \((0, 1/q)\) and increasing on \((1/q, 1/(q-1))\). Since \( k_1(1/q) = -\log q \), we have \( k_1(v_1(\beta)) + \log q > 0 \) for \( \beta \in (\beta_1, q) \) so that

\[
\frac{d}{d\beta} [F_\beta(v_1) - F_\beta(p)] < 0.
\]

Since \( v_1 = p \) when \( \beta = q \), we have \( F_\beta(v_1) > F_\beta(p) \) for \( \beta < q \) and \( F_\beta(v_1) < F_\beta(p) \) for \( \beta > q \).

### 9.1 Proof of Theorem 3.6

Before we go further, we recall the height between two points. Let \( a, b \in \text{int } \mathbb{S} \), and let \( \Gamma_{a,b} \) be a set of all \( C^1 \)-path \( \gamma : [0, 1] \to \text{int } \mathbb{S} \), such that \( \gamma(0) = a \) and \( \gamma(1) = b \). Then, we can define the height \( \gamma(a, b) \) between \( a \) and \( b \) as \( \gamma(a, b) = \inf_{y \in \Gamma_{a,b}} \sup_{0 \leq t \leq 1} F_\beta(\gamma(t)) \). We prove Theorem 3.6 in several steps.

**Lemma 9.1** Let \( q \geq 4 \). If \( \beta > \beta_m \), the sets \( \mathcal{W}_i(\beta), i \in S \), are different. In particular, they are nonempty.

**Proof** Since the elements of \( \mathcal{U}_1 \) are the lowest minima, we have \( F_\beta(u_1^1) < H_\beta \) so that \( \mathcal{W}_i \)'s are nonempty. Without loss of generality, suppose \( \mathcal{W}_1 = \mathcal{W}_2 \). Since \( u_1^1, u_1^2 \in \mathcal{W}_1 \) and \( \mathcal{W}_1 \) is connected, there is a \( C^1 \)-path \( \gamma : [0, 1] \to \mathcal{W}_1 \), such that \( \gamma(0) = u_1^1, \gamma(1) = u_1^2 \). Therefore, we have \( F_\beta(\gamma(t)) < H_\beta \) for \( 0 \leq t \leq 1 \), so that

\[
F_\beta(u_1^1) < \gamma(u_1^1, u_1^2) < H_\beta.
\]

Then, there is a saddle point \( \sigma(u_1^1, u_1^2) \), such that \( F_\beta(\sigma(u_1^1, u_1^2)) = \gamma(u_1^1, u_1^2) \). However, by Proposition 6.3, the values of saddle points are greater than or equal to \( H_\beta \). This is contradiction. Hence, \( \mathcal{W}_i \)'s are different.

**Lemma 9.2** Let \( q \geq 4 \). If \( \beta > q \), the set \( \Sigma_{i,j} \) is singleton for all \( i, j \in S \).

**Proof** First, we claim that \( \Sigma_{i,j} \)'s are not empty. Suppose one of \( \Sigma_{i,j} \)'s is empty. Then, by symmetry, all of them are empty. We will derive a contradiction from this.

Let us fix \( 1 \leq k < l \leq q \). Since \( u_{2,k,l} \) is a saddle point, there is a unit eigenvector \( w \) that corresponds to the unique negative eigenvalue of \( \nabla^2 F_\beta(u_{2,k,l}) \). There exists \( \eta > 0 \), such that \( F_\beta(u_{2,k,l} + t w) < H_\beta \) for all \( 0 < |t| < \eta \). Now, consider the path \( y(t) \) described by the ordinary differential equation

\[
\dot{y}(t) = -\nabla F_\beta(y(t)), \quad y(0) = u_{2,k,l} + \eta w.
\]

(9.1)

Then, \( y(t) \) converges to a critical point whose height is less than \( H_\beta \) as \( t \to \infty \). If this convergent point is not a local minimum, we can find an eigenvector \( w_1 \) corresponding to a negative eigenvalue of the Hessian of \( F_\beta \) at that point. Then, by the same argument defining
the path \((9.1)\), the next path converges to another critical point whose height is lower than that of the previous critical point. Finally, this path converges to a local minimum. Since there is no local minimum other than \(U_1\), \(y(t)\) converges to some elements of \(U_1\), say \(u^0\). Since \(W_i\)’s are different, \(y(\cdot)\) converges to only one minimum. By the same argument, the similar path starting at \(u^{k,l}_2 - \eta u\) converges to some \(u_1\), say \(u^m_1\). If \(n \neq m\), \(u^{k,l}_2 \in \Sigma_{n,m}\) so that \(\Sigma_{n,m}\) is not empty. So, we have \(m = n\). In this case, we obtain \(u^{k,l}_2 \in W_1\) and \(u^{k,l}_2 \notin \bar{W}_a\) for all \(a \neq n\). See Fig. 8 for the visualization these paths.

By symmetry, since \(U_2\) has \(q(q - 1)/2\) elements and the number of \(W_i\) is \(q\), there are \((q - 1)/2\) elements in \(U_2\) corresponding to each \(W_i\), that is, \(|W_i| = (q - 1)/2\), where \(|A|\) is the number of elements of set \(A\). If \(u^{1,a}_2 \in \bar{W}_1\), for some \(2 \leq a \leq q\), we obtain \(u^{1,a}_2 \in \bar{W}_a\) by symmetry, and therefore \(\Sigma_{1,a} = \bar{W}_1 \cap \bar{W}_a \neq \emptyset\). Hence, we have \(u^{1,a}_2 \notin \bar{W}_1\).

If \(u^{a,b}_2 \in \bar{W}_1\) for some \(1 < a, b\), since \(q \geq 4\) and by symmetry, \(u^{a,b}_2 \in \bar{W}_m\) for some \(m \neq 2, a, b\), and this contradicts the assumption that \(\Sigma_{1,m} = \bar{W}_1 \cap \bar{W}_m = \emptyset\). Hence, all of \(\Sigma_i, j\)’s are nonempty.

Observe that the elements of \(\Sigma_i, j\) are saddle points and \(F_\beta(x) = H_\beta\) for all \(x \in \Sigma_i, j\). Hence, by Proposition 6.3, \(\Sigma_i, j \subset U_2\). Since \(\nabla^2 F_\beta(u_2)\)’s are nondegenerate and have only one negative eigenvalue, each element of \(U_2\) connects only two wells, i.e., \(\Sigma_i, j \cap \Sigma_k, l = \emptyset\) if \(i, j \neq k, l\). Therefore, since \(U_2\) has \(q(q - 1)/2\) elements, \(\Sigma_i, j\) has at most one point so that we obtain \(|\Sigma_i, j| = 1\).

We can now prove Theorem 3.6.

**Proof of Theorem 3.6** The first assertion follows from the definition of critical temperatures (6.9) and Lemma 6.7.

Let \(\beta > q\). By Lemma 9.2, to prove \(\Sigma_{i, j} = \{u^{i, j}_2\}\), without loss of generality, it is sufficient to show that \(\Sigma_{1, 2} \neq \{u^{1,4}_2\}\) and \(\Sigma_{1, 2} \neq \{u^{3,4}_2\}\). First, suppose \(\Sigma_{1, 2} = \{u^{1,4}_2\}\). Then, by symmetry, we obtain \(u^{1,4}_2 \in \Sigma_{1, 3}\), which contradicts to \(\Sigma_{1, 2} \cap \Sigma_{1, 3} = \emptyset\). Second, suppose \(\Sigma_{1, 2} = \{u^{3,4}_2\}\) so that by symmetry, we have \(\Sigma_{1, 5} = \{u^{3,4}_2\}\) which is also contradiction. Hence, we obtain \(\Sigma_{1, 2} = \{u^{1,2}_2\}\).

Since \(F_\beta\) is continuous in \(\beta\), the values \(H_\beta\) and \(\mathcal{F}(u^i_1(\beta), u^j_1(\beta)), i, j \in S\), are continuous in \(\beta\). Note that \(\mathcal{F}(u^i_1(\beta), u^j_1(\beta)) = F_\beta(u_2) = H_\beta\) for \(\beta \geq q\) since there is no saddle point other than \(U_2\). Since \(F_\beta(v_1) > H_\beta\) if \(\beta > \beta_m = \beta_3\) and there is no saddle point other than the elements of \(U_2 \cup V_1\), by continuity, we obtain

\[
\mathcal{F}(u^i_1(\beta), u^j_1(\beta)) = H_\beta \text{ if } \beta \geq \beta_3.
\]
Hence, \( u_{2}^{i,j} \) is a saddle point between \( u_{1}^{i} \) and \( u_{1}^{j} \) and \( \Sigma_{i,j} = \{ u_{2}^{i,j} \} \) if \( \beta > \beta_{3} \). Coupled with Lemma 9.1, the fourth assertion holds except that \( \Sigma_{\sigma,i} = \emptyset \).

If \( \beta \geq q \), \( \mathcal{W}_{0} = \emptyset \). Let \( \beta_{3} \leq \beta < q \). Without loss of generality, suppose that \( \Sigma_{\sigma,1} = \overline{\mathcal{W}_{0} \cap \mathcal{W}_{1}} \neq \emptyset \). Let \( \mathbf{a} \in \overline{\mathcal{W}_{0} \cap \mathcal{W}_{1}} \). Note that \( \mathbf{a} \in \mathcal{W}_{0} \) since \( F_{\beta}(\mathbf{a}) \leq H_{\beta} < F_{\beta}(\mathbf{v}_{1}) \). Since \( \mathbf{a} \in \mathcal{W}_{1} \), \( \mathbf{a} \) is connected to \( u_{1}^{1} \) in \( \{ \mathbf{x} : F_{\beta}(\mathbf{x}) \leq H_{\beta} \} \). In addition, since \( H_{\beta} < F_{\beta}(\mathbf{v}_{1}) \) and \( \mathbf{a} \in \mathcal{W}_{0}, \mathcal{W}_{0} \) must contain \( u_{1}^{1} \). We, therefore, obtain \( \mathcal{y}(\mathbf{p}, u_{1}^{1}(\beta)) < F_{\beta}(\mathbf{v}_{1}) \) so that \( \mathcal{y}(u_{1}^{1}(\beta)) = H_{\beta} \). By continuity, we get

\[
\mathcal{y}(\mathbf{p}, u_{1}^{1}(\beta)) = H_{\beta} \text{ for } \beta_{3} \leq \beta < q,
\]

so that \( F_{\beta}(\mathbf{p}) \leq H_{\beta} \). However, it is in contradiction to \( F_{q}(\mathbf{p}) = F_{q}(\mathbf{v}_{1}) > H_{q} \). Hence, we obtain \( \Sigma_{\sigma,i} = \emptyset \) for \( i \in S \).

By the same argument and symmetry, the second assertion can be proven for \( \beta \in (\beta_{s,1}, \beta_{s,2}) \). By continuity argument, we can extend these to \( \beta \in (\beta_{1}, \beta_{3}) \).

The third assertion holds because of the first and fourth assertions, symmetry, and continuity. Finally, the fifth assertion can be proven by the same argument.

### 9.2 Proof of Theorem 3.5

If \( q = 4 \), \( \Sigma_{1,2} \neq \{ u_{2}^{3,4} \} \) cannot be proven by symmetry argument. Hence, we directly prove the Theorem 3.5.

**Proof of Theorem 3.5** By Lemma 6.7 and (6.9), we obtain the first assertion.

Consider \( \mathcal{K}_{i,j} = \{ \mathbf{x} \in \Xi : x_{i} = x_{j} = \max\{x_{1}, \ldots, x_{4}\} \} \). It can be observed that these six planes divide \( \Xi \) into four pieces, and each plane contains one element of \( U_{4} \) and \( u_{2}^{i,j} \in \mathcal{K}_{i,j} \). We claim that \( H_{\beta} = F_{\beta}(u_{2}^{i,j}) < F_{\beta}(\mathbf{x}) \) for all \( \mathbf{x} \in \mathcal{K}_{i,j} \) if \( \beta > q \). Note that \( \mathbf{p} \) is not local minimum if \( \beta \geq q \).

Let \( \tilde{F}_{\beta}(\mathbf{x}) \) be a restriction of \( F_{\beta} \) to \( \mathcal{K}_{3,4} \) and let \( \mathcal{K}_{3,4}^{0} = \{ \mathbf{x} \in \mathcal{K}_{3,4} : x_{3} = x_{4} > x_{1}, x_{2} \} \). Since \( x_{3} = x_{4} = \frac{1}{2}(1 - x_{1} - x_{2}) \),

\[
\frac{\partial}{\partial x_{i}} \tilde{F}_{\beta}(\mathbf{x}) = -x_{i} + \frac{1}{\beta} \log x_{i} + x_{3} = \frac{1}{\beta} \log x_{3},
\]

so that if \( \mathbf{x} \in \mathcal{K}_{3,4} \) is a critical point, we have

\[
-x_{1} + \frac{1}{\beta} \log x_{1} = -x_{2} + \frac{1}{\beta} \log x_{2} = -x_{3} + \frac{1}{\beta} \log x_{3}.
\]

Since \( x_{3} = x_{4} > x_{1}, x_{2} \), if \( \beta \geq q \), the critical points in \( \mathcal{K}_{3,4}^{0} \) are \( u_{2}^{3,4}, v_{2}^{1,2} \). From the proof Lemma 7.7, we obtain \( u_{2}^{3,4} = v_{2}^{1,2} = (u_{2}, u_{2}, v_{2}, v_{2}) \).

Let \( a = -1 + \frac{1}{\beta u_{2}} \) and \( b = -1 + \frac{1}{\beta v_{2}} \). We therefore obtain

\[
\nabla^{2} \tilde{F}_{\beta}(u_{2}^{3,4}) = \begin{pmatrix} a + \frac{1}{2}b & \frac{1}{2}b \\ \frac{1}{2}b & a + \frac{1}{2}b \end{pmatrix}.
\]

The eigenvalues of \( \nabla^{2} \tilde{F}_{\beta}(u_{2}^{3,4}) \) are \( a \) and \( a + b \). By Lemma 7.3, \( a, b > 0 \) so that \( u_{2}^{3,4} \) is a local minimum in \( \mathcal{K}_{3,4}^{0} \). Since this is the unique critical point, \( u_{2}^{3,4} \) is the unique minimum in \( \mathcal{K}_{3,4}^{0} \). Since \( \mathcal{K}_{3,4} \) is a closure of \( \mathcal{K}_{3,4}^{0} \) and there is no critical point in \( \mathcal{K}_{3,4}^{0} \setminus \{ u_{2}^{3,4} \} \), \( u_{2}^{3,4} \) is the unique minimum in \( \mathcal{K}_{3,4} \). Hence, \( \mathcal{W}_{i} \)’s are different if \( \beta > q \).

Let \( \beta > q \). By the definition of \( \mathcal{K}_{i,j} \), we obtain \( \overline{\mathcal{W}_{k} \cap \mathcal{K}_{i,j}} = \emptyset \) if \( k \neq i, j \) so that \( \Sigma_{i,j} \subset \mathcal{K}_{i,j} \). By Lemma 9.2, \( \Sigma_{i,j} \) are not empty. It can be observed \( F_{\beta}(\mathbf{x}) = H_{\beta} \) and
\[ \nabla F_\beta(x) = 0 \] if \( x \in \Sigma_{i,j} \). Since \( \Sigma_{i,j} \subset K_{i,j} \), we have \( \Sigma_{i,j} = \{u_i^j\} \), thus the fourth assertion is proved.

For the third assertion, note that \( F_q(x) = H_q \) for all \( x \in \Sigma_{i,j} \) and \( p \) is the only point in \( K_{i,j} \), such that \( F_q(x) = H_q \). Moreover, we obtain \( F_q(x) > H_q = F_q(p) \) if \( x \in K_{i,j} \), and finally we can conclude \( F_q(x) > H_q = F_q(p) \) if \( x \in K_{i,j} \) using elementary calculus. Hence, \( W_i \)’s are different if \( \beta = q \).

For the second assertion, we can use the symmetry argument and the proofs are the same as the proof of Theorem 3.6.

10 Proof of Lemma 8.4

This section is devoted to the proof of Lemma 8.4. In Sect. 10.1, we provide an auxiliary lemma to prove Lemma 10.1. In Sect. 10.2, we prove this auxiliary lemma. So far, we have fixed an integer \( q \geq 3 \); however, in this section, we consider \( q \) as a real number and several variables as functions of \( q \). For example, \( m_2 = m_2(q) \), \( j(q) = q - 2 \), and \( \beta_{s,2} = \beta_{s,2}(q) \).

10.1 Proof of Lemma 8.4

Lemma 10.1 The function \( f_\star \) of \( q \) is defined as

\[
 f_\star(q) = \frac{1}{\beta_{s,2}} \left( \log q m_2 - \frac{1}{2} \right) - \frac{1}{8} (q m_2)^2 + \frac{1}{4} m_2 + \frac{251}{2002}. \tag{10.1}
\]

Then, if \( q > e^8 \), \( f_\star'(q) = \frac{d}{dq} f_\star(q) > 0 \).

Proof of Lemma 8.4 By Proposition A.1, we obtain \( f_\star(6500) > 0 \). We observe that \( \frac{(q-1)}{8q} < 1 \) and \( -\frac{q^2+4q+1}{8q(q-1)} < -\frac{251}{2002} \) if \( q > 1000 \). Hence, Lemma 10.1 proves Lemma 8.4.

10.2 Proof of Lemma 10.1

Let \( s_2 = s_2(q) = q m_2 \). In the first lemma, we compute \( m_2' = (d/dq)m_2 \), \( s_2' = (d/dq)s_2 \), and \( \beta_{s,2}' = (d/dq)\beta_{s,2} \).

Lemma 10.2 We have

\[
m_2' = \frac{d}{dq} m_2 = -\frac{m_2(1 - jm_2 - q jm_2')}{q(1 - 2 jm_2)},
\]

\[
s_2' = \frac{d}{dq} s_2 = -\frac{js_2^2(1 - s_2)}{q(q - 2 js_2)},
\]

\[
\beta_{s,2}' = \frac{d}{dq} \beta_{s,2} = \frac{1}{1 - s_2} \left( \beta_{s,2} s_2' - 2 \frac{-s_2 + s_2^2 + q s_2'}{(q - js_2)s_2} \right).
\]

Proof We observe that \( \beta_{s,2} = g_2(m_2) = \frac{2}{1 - q m_2} \log \left( \frac{1 - jm_2}{2 m_2} \right) = \frac{2}{q m_2(1 - jm_2)} \), so that

\[
\log(1 - jm_2) - \log 2 m_2 = \frac{2}{q} \left( \frac{1}{2 m_2} - \frac{1}{1 - jm_2} \right).
\]
By differentiating this equation in $q$, we get
\[ \frac{-m_2 - jm_2'}{1 - jm_2} - \frac{m_2'}{m_2} = -\frac{2}{q^2} \left( \frac{1}{2m_2} - \frac{1}{1 - jm_2} \right) + \frac{2}{q} \left( -\frac{m_2'}{2m_2^2} + \frac{-m_2 - jm_2'}{(1 - jm_2)^2} \right). \]

By elementary computation, we can write
\[ m_2' = -\frac{m_2(1 - jm_2 - qjm_2^2)}{q(1 - 2jm_2)}. \]

Let $s_2 = qm_2$. Then,
\[ s_2' = m_2 + qm_2' = -\frac{js_2^2(1 - s_2)}{q(q - 2js_2)}. \]

Next, we compute $\beta'_s$. Note that
\[ \beta_s = \frac{2}{1 - s_2} \log \frac{q - js_2}{2s_2}, \]
so that
\[ \beta'_s = \frac{2s_2'}{(1 - s_2)^2} \log \frac{q - js_2}{2s_2} + \frac{2}{1 - s_2} \left( \frac{1 - s_2 - js_2'}{q - js_2} - \frac{s_2'}{s_2} \right) \]
\[ = \frac{1}{1 - s_2} \left( \beta_s s_2' - 2 - s_2 + s_2^2 + q s_2' \right). \]

The next lemma provides the bound of $m_2(q)$.

**Lemma 10.3** Let $q > e^8$. We have
\[ \frac{1}{2q \log q} < m_2(q) < \frac{1}{q \log q}. \]

**Proof** It can be observed that $h_2(m_2) = 0$ and $h_2(t) > 0$ if $m_2 < t < 1/q$. We claim that
\[ h_2(a) = \log \frac{1 - ja}{2a} + \frac{qa - 1}{qa(1 - ja)} > 0, \]
where $a = 1/q \log q$. The above inequality can be written as
\[ \log \frac{q \log q - j}{2} > \left( \frac{q \log q - q}{q \log q - j} \right) \log q. \]
Since the right-hand side is smaller than $\log q$, it suffices to show that
\[ \log q + \log \frac{\log q - 1 + 2/q}{2} > \log q, \]
which is true if $q > e^3$. Hence, $m_2 < 1/q \log q$. Next, we have $m_2 > (1/2q) \log q$ since
\[ \log \left( q \log q - \frac{j}{2} \right) - 2 \left\{ \frac{q \log q - q/2}{(q \log q - j/2)} \right\} \log q < 0, \]
which is true if $q > e^{8}$. In the next two lemmas, we prove that some quantities are positive.
Lemma 10.4 Let \( q > e^8 \). We have
\[ m_2' - s_2s_2' > 0. \]

Proof We have
\[
m_2' - s_2s_2' = -\frac{m_2(1 - jm_2 - jqm_2^2)}{q(1 - 2jm_2)} + \frac{js_3^3(1 - s_2)}{q(q - 2js_2)}
= \frac{s_3(-1 + jm_2 + jq(q + 1)m_2^2 - jq^3m_2^3)}{q(q - 2js_2)}.
\]
It suffices to show that
\[ jq(q + 1)m_2^2 - jq^3m_2^3 - 1 > 0. \]
Since \( \frac{1}{2q \log q} < m_2 < \frac{1}{q \log q} \), we obtain
\[
jq(q + 1)m_2^2 - jq^3m_2^3 - 1 > \frac{jq(q + 1)}{4q^2(\log q)^2} - \frac{jq^3}{q^3(\log q)^3} - 1
= \frac{1}{q(\log q)^3}[(q + 1)(q - 2) - 4q(q - 2) - q(\log q)^3]
> \frac{1}{q(\log q)^3}[2(q + 1)(q - 2) - q(q - 2) - q(\log q)^3]
= \frac{1}{q(\log q)^3}[q^2 - q(\log q)^3 - 4] > 0.
\]
In the second and third inequalities, we use \( q > e^8 \). Hence, \( m_2' - s_2s_2' > 0 \). \( \square \)

Lemma 10.5 Let \( q > e^8 \). We have
\[
\left( \frac{1}{2} - \log s_2 \right) \beta_{s,2}' + \beta_{s,2} \frac{s_2'}{s_2} > 0.
\] (10.5)

Proof Let \( A(q) = \frac{1}{2} - \log s_2 \). From Lemma 10.3, we obtain
\[ \frac{5}{2} < \frac{1}{2} + \log 8 < \frac{1}{2} + \log \log q < A(q) < \frac{1}{2} + \log(2 \log q), \]
and
\[
A(q) \beta_{s,2}' + \beta_{s,2} \frac{s_2'}{s_2} = \frac{s_2'}{1 - s_2} \left[ A(q) \beta_{s,2} - \frac{2q}{q - 2} \frac{A(q)}{s_2^2} \right] + \frac{s_2'}{1 - s_2} \left[ \frac{1 - s_2}{s_2} \beta_{s,2} \right]
= \frac{s_2'}{1 - s_2} \left[ \beta_{s,2} \left( \frac{1}{s_2} + A(q) - 1 \right) - \frac{2q}{q - 2} \frac{A(q)}{s_2} \right].
\]
Hence, since \( s_2' < 0 \), it suffices to show that
\[
\left( \frac{2q}{q - 2} \right) \frac{A(q)}{s_2^2} > \beta_{s,2} \left( \frac{1}{s_2} + A(q) - 1 \right) = \frac{\beta_{s,2}}{s_2} \left[ 1 + (A(q) - 1)s_2 \right],
\]
i.e.,
\[
\beta_{s,2} < \frac{1}{1 + (A(q) - 1)s_2} \cdot \frac{2q}{q - 2} \cdot \frac{A(q)}{s_2}.
\]
Since, $s_2 < 1/\log q$, the right-hand side is greater than
\[
\frac{1}{1 + (A(q) - 1)s_2} \cdot \frac{2q A(q)}{q - 2} \log q > \frac{1}{5} \left( \frac{5q}{q - 2} \right) \log q
\]
and
\[
\beta_{s, 2} < g_2(1/q \log q) = \frac{2 \log q}{\log q - 1} \log \left( \frac{q \log q - (q - 2)}{2} \right) < \frac{5}{2} \log(q \log q) < \frac{15}{4} \log q ,
\]
where the last inequality is equivalent to $1/2 > \log(\log q) / \log q$ which is true for $q > e^8$.

Hence, it is enough to show that
\[
\beta_{s, 2} < g_2(1/q \log q) < \frac{1}{3}.
\]

Now, we return to $f^\star(q)$. We have
\[
f^\star(q) = \frac{1}{\beta_{s, 2}} \left( \log q m_2 - 1 + \frac{1}{2} \right) - \frac{1}{8} (q m_2)^2 + \frac{1}{4} m_2 + \frac{251}{2002}.
\]
so that
\[
f_{\beta_{s, 2}}^\star(q) = \frac{1}{\beta_{s, 2}^2} \left( \log s_2 - \frac{1}{2} \right) - \frac{1}{8} (s_2)^2 + \frac{1}{4} m_2 + \frac{251}{2002}.
\]
so that
\[
f_{\beta_{s, 2}}^\star(q) = \frac{\beta_{s, 2}^\prime}{\beta_{s, 2}^2} \left( \log s_2 - \frac{1}{2} \right) + \frac{1}{\beta_{s, 2}} \left( \frac{s_2^\prime}{s_2} \right) + \frac{1}{4} (m_2^2 - s_2 s_2^\prime).
\]
Finally, Lemmas 10.4 and 10.5 prove Lemma 10.1.
11 Appendix A: Some Numerical Computations

Recall the definition (10.1) of $f_*(-)$. In this section, we verify several inequalities numerically. Our purpose is the following proposition. The proof is presented at the end of this section.

**Proposition A.1** The following hold.

1. For $5 \leq q \leq 6500$, we have $F_{\beta_{s,2}}(u_2) > F_{\beta_{s,2}}(v_1)$.
2. For $6 \leq q \leq 54$, we have $\frac{d}{d\beta}(f_*(-))\bigg|_{\beta=\beta_{s,2}} > 0$.
3. $f_*(-)(6500) > 0$.

11.1 Bounds of $\beta_{s,2}$, $m_2$ and $v_1$.

We will obtain the bounds of $\beta_{s,2}$, $m_2$, and $v_1$. Fix $q \geq 5$ and let $j = q - 2$. By gradient descent method, we obtain the following.

**Algorithm A.2** We define $\beta_{s,2}^u$ and $\beta_{s,2}^l$ in the following way.

1. $t_0 \leftarrow 1 / (2q - 4)$.
2. While $g_2'(t_i) > 10^{-6}$, let $t_{i+1} \leftarrow t_i - g_2'(t_i)/(300q^2)$.
3. If $g_2'(t_i) \leq 10^{-6}$, let $m_2^* \leftarrow t_i$.

Let $\beta_{s,2}^u := g_2(m_2^*) + (36/q)|g_2'(m_2^*)|$ and $\beta_{s,2}^l := g_2(m_2^*) - (36/q)|g_2'(m_2^*)|$.

We record $m_2^*$ in the above algorithm and let

$$
\rho_m := \frac{g_2'(m_2^*)}{q}.
$$

**Algorithm A.3** We define $m_2^u$ and $m_2^l$ in the following way.

1. If $h_2(m_2^*) \geq 0$, let $m_2^u := m_2^* + \rho_m$.
   (a) $t_0 \leftarrow m_2^*$.
   (b) While $h_2(t_i) \geq 0$, let $t_{i+1} \leftarrow t_i - \rho_m$.
   (c) If $h_2(t_i) < 0$, let $m_2^l := t_i - \rho_m$.

2. If $h_2(m_2^*) < 0$, let $m_2^l := m_2^* - \rho_m$.
   (a) $t_0 \leftarrow m_2^*$.
   (b) While $h_2(t_i) \leq 0$, let $t_{i+1} \leftarrow t_i + \rho_m$.
   (c) If $h_2(t_i) > 0$, let $m_2^u := t_i + \rho_m$.

By Newton method, we approximate $v_1$ which satisfies $g_1(v_1) = \beta_{s,2}$.

**Algorithm A.4** We define $v_1^u$ and $v_1^l$ in the following way.

1. Let $t_0 = 0.8/q$ and $t_{-1} = 0$.
   (a) While $|t_i - t_{i-1}| > 10^{-5}/q$, let $t_{i+1} \leftarrow t_i - (g_1(t_i) - \beta_{s,2}^u)/g_1(t_i)$.
   (b) If $|t_i - t_{i-1}| \leq 10^{-5}/q$, let $v_1^u := t_i$ and $\rho_v := |t_i - t_{i-1}|$.

2. If $g_1(v_1^u) > \beta_{s,2}^u$, let $v_1^u := v_1^u + \rho_v$.
3. If $g_1(v_1^u) \leq \beta_{s,2}^u$, let
   (a) $a_0 \leftarrow v_1^u$.
   (b) While $g_1(a_i) \leq \beta_{s,2}^u$, let $a_{i+1} \leftarrow a_i + \rho_v$. 
(c) If \( g_1(a_i) > \beta_{s,2}^u \), let \( v_1^u := a_i + \rho_v \).

(4) If \( g_1(v_1^u) < \beta_{s,2}^l \), let \( v_1^l := v_1^u - \rho_v \).

(5) If \( g_1(v_1^u) \geq \beta_{s,2}^l \), let

(a) \( b_0 \leftarrow v_1^l \).

(b) While \( g_1(b_i) \geq \beta_{s,2}^l \), let \( b_{i+1} \leftarrow b_i - \rho_v \).

(c) If \( g_1(b_i) < \beta_{s,2}^l \), let \( v_1^l := b_i - \rho_v \).

**Lemma A.5** We have \( \beta_{s,2}^l < \beta_s < \beta_{s,2}^u \), \( m_2^l < m_2 < m_2^u \), and \( v_1^l < v_1 < v_1^u \).

**Proof** From the Taylor’s theorem, we obtain

\[ g_2(m_2 + t) = g_2(m_2) + g_2'(m_2 + t^*) t \]

for some \( t^* \in (0, t) \) if \( t > 0 \) or \( t^* \in (t, 0) \) if \( t < 0 \). Since \( h_2 \) is increasing in the neighborhood of \( m_2 \), we obtain

\[
|g_2'(m_2 + t^*)| = \left| \frac{2q}{[1 - q(m_2 + t^*)]^2} h_2(m_2 + t^*) \right|
\leq \left| \frac{2q}{[1 - q(m_2 + t^*)]^2} h_2(m_2 + |t|) \right|
= \left( \frac{1 - q(m_2 + |t|)}{1 - q(m_2 + t^*)} \right)^2 |g_2'(m_2 + |t|)|.
\]

Since \( m_2 + t^* \), \( m_2 < 1/(2j) \), we obtain

\[
\frac{1 - q(m_2 + |t|)}{1 - q(m_2 + t^*)} \leq \frac{1}{1 - q/(2j)} \leq \frac{1}{1 - q/4} = \frac{2q - 4}{q - 4} \leq 6 ,
\]

where the last inequality is from \( q \geq 5 \). Hence, we have

\[
|g_2'(m_2 + t^*)| \leq 36 |g_2'(m_2 + |t|)| ,
\]

so that we have

\[
|\beta_s - g_2(m_2 + t)| = |g_2(m_2) - g_2(m_2 + t)| \leq |g_2'(m_2 + t^*)||t| \leq \frac{36}{q} |g_2'(m_2 + |t|)| ,
\]

which proves the first claim. In the last inequality, we use the fact that \( |t| < 1/q \).

Since \( h_2(t) > 0 \) if \( t > m_2 \) and \( h_2(t) < 0 \) if \( t < m_2 \), the second claim is true. Finally, since \( g_1 \) is increasing in the neighborhood of \( v_1 \), the third claim holds.

We finally prove Proposition A.1.

**Proof of Proposition A.1** From Lemma A.5, we obtain

\[ \beta_{s,2}^l < \beta_s < \beta_{s,2}^u \), \( m_2^l < m_2 < m_2^u \), and \( v_1^l < v_1 < v_1^u \).

By elementary computation, we have

\[
F_{\beta_{s,2}}(u_2) - F_{\beta_{s,2}}(v_1) \geq \frac{1}{4} \left[ q(q - 2) \left( m_2^u - \frac{1}{q - 2} \right)^2 - \frac{2}{q - 2} \right] + \frac{1}{\beta_{s,2}^l} \log m_2^l
- \frac{1}{2} \left[ q(q - 1) \left( v_1^l - \frac{1}{q - 1} \right)^2 - \frac{1}{q - 1} \right] - \frac{1}{\beta_{s,2}^u} \log v_1^u ,
\]

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\[ \log q \beta_s, 2 + 2k_2(m_2) \geq \log (q \beta_s, 2) + 2k_2(m_2') , \]
\[ f_*(6500) \geq \frac{1}{\beta_s, 2} \left( \log q m_2' \right) - \frac{1}{8} \left( q m_2' \right)^2 + \frac{1}{4} m_2' + \frac{251}{2002} . \]

The second inequality holds since \( k_2(\cdot) \) is decreasing according to (8.7). From the numerical computations, we find that the right-hand sides of the displayed equations are positive for \( 5 \leq q \leq 6500 \), and this completes the proof.

12 Appendix B: Proof of (3.8)

**Proof of (3.8)** Since we have

\[ Z_N(\beta) = \sum_{x \in \Xi} \frac{N!}{(N x_1)! \cdots (N x_q)!} \exp \{-\beta N H(x)\} , \]

we can use the elementary bound

\[ k \log k - k \leq \log k! \leq (k + 1) \log (k + 1) - k , \]

to obtain

\[ \sum_{x \in \Xi} \exp \left\{ -\beta N \left[ -\frac{1}{2} (x_1^2 + \cdots + x_q^2) + \frac{1}{\beta} \sum_{i=1}^q \left( x_i + \frac{1}{N} \right) \log \left( x_i + \frac{1}{N} \right) \right] - q \log N \right\} \]
\[ \leq Z_N(\beta) \leq \sum_{x \in \Xi} \exp \left\{ -\beta N F_\beta(x) + \log (N + 1) + N \log \left( 1 + \frac{1}{N} \right) \right\} . \]

Hence, by the definition of \( F_\beta (2.4) \), we can obtain

\[ \sup_{x \in \Xi} \{-F_\beta(x)\} + O\left( \frac{\log N}{N} \right) \leq \frac{1}{\beta N} \log Z_N(\beta) \leq \sup_{x \in \Xi} \{-F_\beta(x)\} + O\left( \frac{\log N}{N} \right) \]

and the proof is completed.

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