

# Mean-Field Limits of the Quantum Potts Model

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**Abstract.** We consider the  $q$ -component quantum Potts model on a  $d$ -dimensional cubic lattice with symmetry breaking and transverse fields. The model is solved exactly in two special limiting cases: 1) the infinite lattice-dimensionality ( $d \rightarrow \infty$ ) limit and 2) the limit of infinitely-weak, long-range interactions of Kac type. In each case the resulting free energy and its first partial derivatives (order parameters) are shown to be identical to the corresponding mean-field expressions.

## 1. Introduction

The Potts model is a model of central interest in statistical mechanics as is evidenced by the recent and extensive review article by Wu [1]. Although this model is a simple generalization of the 2-component Ising model to a  $q$ -component model, it exhibits much richer critical behaviour. Of particular interest is the order of the phase transition as one varies the lattice dimension  $d$  and the number of components  $q$ , regarded as continuous parameters. Mean-field theory [2] predicts a continuous transition for  $q \leq 2$  and a first-order transition for all  $q > 2$ , independent of the lattice dimension  $d$ . However, Baxter's exact result [3] in two dimensions shows a continuous transition for  $q \leq 4$  and a first-order transition for  $q > 4$ . In general, it is now believed that there exists a critical value  $q_c(d)$ , with a non-trivial dependence on the dimension  $d$  (see Fig. 2 in [1]), such that the mean-field prediction is correct for  $q > q_c(d)$ . In addition, renormalization-group arguments [4] indicate that the mean-field predictions are correct for  $d > 4$ . It is thus known that  $q_c(2) = 4$  and  $q_c(d) = 2$  for  $d > 4$ . An obvious question is what is the value of  $q_c(d)$  for  $d = 3$ , in particular, is  $q_c(3)$  greater than or less than 3? For some time the usual series expansions [5] and renormalization-group analyses [6] gave conflicting answers, but the weight of opinion now seems to be that  $q_c(3) < 3$ , that is, in three dimensions the 3-component Potts model undergoes a first-order transition.

Recently, a new attack has been made on these problems by looking at the quantum Hamiltonian (field theory) version [7] of the Potts model. Mean-field

theory of the quantum Potts model [8] again predicts a continuous phase transition for  $q \leq 2$  and a first-order transition for  $q > 2$ , independent of the lattice dimension  $d$ . Indeed, the initial motivation for studying the quantum model was the underlying belief that  $d$ -dimensional classical models and their  $(d-1)$ -dimensional quantum Hamiltonian counterparts have the same phase diagrams and lie in the same universality class [9]. This is certainly true for the  $d=2$  Potts case, where Baxter's results [3] can be carried over [10] to the one-dimensional quantum Potts model, and is borne out in higher dimensions by approximate calculations. In particular, by using  $1/q$ -expansions for the  $(d-1)$ -dimensional quantum Potts model, Kogut and co-workers [11] have obtained the remarkable results  $q_c(3) = 2.6 \pm 0.1$  and  $q_c(d) = 2.00 \pm 0.05$  for all  $d \geq 4$ . The quantum Potts model has thus clearly emerged as a model worthy of study in its own right.

For many lattice spin systems, it is known [12–15] that mean-field theory becomes exact in certain special limiting cases. Here we shall prove analogous results for a general  $q$ -component quantum Potts model. This model includes both the classical and the usual (transverse) quantum Potts models as special cases. More specifically, we shall show that the mean-field theory of the general quantum Potts model becomes exact in the following limits: 1) the infinite lattice-dimensionality ( $d \rightarrow \infty$ ) limit and 2) the limit of infinitely weak, long-range interactions of Kac type.

We also expect that the mean-field theory becomes exact in the many-component ( $q \rightarrow \infty$ ) limit. This was proved by graphical methods in [15] for the classical Potts model. However, we are not able to prove it for the general quantum model by the methods used here. Although we shall not be concerned with the lattice gauge Potts model here, it is interesting to note that recently this model has been solved exactly [16] in the  $q \rightarrow \infty$  limit, yielding mean-field results for the thermodynamic functions.

The rest of this section is devoted to giving a precise statement of our results. For convenience, we describe the classical Potts model before introducing the full quantum model.

The Hamiltonian of the classical Potts model is

$$H = -\frac{1}{2} \sum_{j,k} J_{jk} \delta(\sigma_j, \sigma_k) - \xi \sum_j \delta(\sigma_j, 1), \quad (1.1)$$

where  $\delta(\cdot, \cdot)$  is the Kronecker delta,  $\xi \geq 0$  is an external symmetry-breaking field and the parameters  $J_{jk} = J_{kj} \geq 0$  are pair interaction strengths (with  $J_{jj} = 0$ ). For simplicity, we shall always take sums on  $j$  and  $k$  to be over the  $N = v^d$  lattice vectors in  $\mathbb{Z}^d$  of a  $d$ -dimensional cube of side  $v$ . At each lattice site  $j$ , the spin  $\sigma_j$  is restricted to one of  $q$  distinct values: in order to make contact with the quantum model, we shall assume that  $\sigma_j = 1, \omega, \omega^2, \dots, \omega^{q-1}$ , with  $\omega = \exp(2\pi i/q)$  a  $q^{\text{th}}$  root of unity. The partition function for the classical model can then be written as

$$Z_N = \sum_{\sigma_1=1}^{\omega^{q-1}} \dots \sum_{\sigma_N=1}^{\omega^{q-1}} \exp(-\beta H), \quad (1.2)$$

where  $\beta = 1/k_B T$  is the inverse temperature and the sums extend over all values of the spins.

The quantum Potts model is a generalization of the classical Potts model. The Hamiltonian we shall consider is

$$H = -\frac{1}{2}q^{-1} \sum_{j,k} \sum_{\alpha=1}^q J_{jk}(\Omega_j^\dagger \Omega_k)^\alpha - \xi q^{-1} \sum_j \sum_{\alpha=1}^q \Omega_j^\alpha - \eta q^{-1} \sum_j \sum_{\alpha=1}^q M_j^\alpha, \quad (1.3)$$

where the lattice structure and interactions are as described previously, with  $\eta \geq 0$  an additional (transverse) field. The spin operators (matrices)  $\Omega_j$  and  $M_j$  commute at different sites. At the same site, however, they do not commute but obey the  $\mathbb{Z}_q$  algebra :

$$M_j \Omega_j = \omega \Omega_j M_j, \quad M_j^\dagger \Omega_j = \omega^{-1} \Omega_j M_j^\dagger, \quad \Omega_j^q = M_j^q = I, \quad (1.4)$$

where  $I$  is the identity and the dagger denotes the Hermitian conjugate. In particular, these operators can be represented as direct products of  $N$   $q \times q$  matrices

$$\begin{aligned} \Omega_j &= I \otimes \dots \otimes I \otimes \Omega \otimes I \otimes \dots \otimes I, \\ M_j &= I \otimes \dots \otimes I \otimes M \otimes I \otimes \dots \otimes I, \end{aligned} \quad (1.5)$$

where the matrices  $\Omega$  and  $M$ , occurring in the  $j^{\text{th}}$  positions, are given by

$$\Omega = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & \omega & \dots & 0 \\ \vdots & & \ddots & \\ 0 & 0 & \dots & \omega^{q-1} \end{bmatrix}, \quad M = \begin{bmatrix} 0 & 1 & 0 & \dots \\ 0 & 0 & 1 & \dots \\ \vdots & & & \ddots \\ 1 & 0 & 0 & \dots \end{bmatrix}. \quad (1.6)$$

We shall work only in this representation, in which the  $\Omega_j$  are simultaneously diagonal. The partition function is now

$$Z_N = \text{Tr} \exp(-\beta H), \quad (1.7)$$

where  $H$  is the quantum Hamiltonian and  $\text{Tr}$  denotes the matrix trace. The free energy per spin  $\psi$  in the thermodynamic limit is given by

$$\beta \psi(\beta) = - \lim_{N \rightarrow \infty} N^{-1} \ln Z_N. \quad (1.8)$$

The quantum Potts model reduces to the classical model when the transverse field  $\eta$  is set to zero : in this case the Hamiltonian (1.3) is diagonal and the partition function (1.7) reduces to (1.2) after repeated use of the identity

$$\delta(\sigma, \sigma') = q^{-1} \sum_{\alpha=1}^q (\bar{\sigma} \sigma')^\alpha, \quad (1.9)$$

where  $\sigma$  and  $\sigma'$  are  $q^{\text{th}}$  roots of unity and the bar denotes complex conjugate. The transverse Ising model is also obtained as a special case by setting  $q=2$ . In this case  $\Omega$  and  $M$  are familiar Pauli matrices.

In the sequel we shall always assume that the interactions are ferromagnetic and translationally invariant, i.e.

$$J_{jk} = J_{kj} = J(j-k) \geq 0, \quad (1.10a)$$

and impose periodic boundary conditions so that

$$J_N = \sum_j J_{jk} \tag{1.10b}$$

does not depend on  $k$ . In addition, we shall also assume

$$J_\infty = \lim_{N \rightarrow \infty} J_N < \infty, \tag{1.10c}$$

so that the limiting free energy (1.8) exists [17].

Under these assumptions the result we prove can be stated in two parts as follows:

**Theorem.** 1) Let  $\psi_d(\beta)$  be the free energy (1.8) for the quantum Potts model (1.3) with nearest-neighbor interactions given by

$$J_{jk} = \begin{cases} J/2d & |j-k|=1 \\ 0 & \text{otherwise.} \end{cases} \tag{1.11}$$

Then

$$\lim_{d \rightarrow \infty} \psi_d(\beta) = \psi_{\text{MF}}(\beta, J), \tag{1.12}$$

where  $\psi_{\text{MF}}$  is the mean-field free energy given by

$$\begin{aligned} \psi_{\text{MF}}(\beta, J) = \min_{x \in \mathbb{R}} \{ & \frac{1}{2} q^{-1} (q-1) J x^2 - \frac{1}{2} q^{-1} (q-2) J x - \frac{1}{2} (q^{-1} J + \xi + \eta) \\ & - \beta^{-1} \ln [2 \cosh [\frac{1}{2} \beta ((Jx + \xi)^2 - 2q^{-1} (q-2) (Jx + \xi) \eta + \eta^2)^{1/2}]] \\ & + (q-2) \exp [-\frac{1}{2} \beta (Jx + \xi + \eta)] \}. \end{aligned} \tag{1.13}$$

2) Let  $\psi_\gamma(\beta)$  be the free energy (1.8) for Kac type interactions

$$J_{jk} = J(j-k) = \gamma^d \varrho(\gamma|j-k|), \quad j \neq k, \tag{1.14a}$$

where it is assumed that  $\varrho(r)$  is everywhere bounded and that

$$J = \lim_{\gamma \rightarrow 0^+} \lim_{N \rightarrow \infty} J_N = \int_{\mathbb{R}^d} \varrho(|\mathbf{r}|) d\mathbf{r} \tag{1.14b}$$

exists as a Riemann integral. Then

$$\lim_{d \rightarrow \infty} \psi_\gamma(\beta) = \psi_{\text{MF}}(\beta, J). \tag{1.15}$$

An immediate corollary to this theorem is that, in the two limits considered, the order parameters for the quantum Potts model (1.3) are also given by their corresponding mean-field expressions. To see this, we observe that the free energies  $\psi_d(\beta)$  and  $\psi_\gamma(\beta)$  are concave functions [17] of the fields  $\xi$  and  $\eta$ ; it therefore follows, by a result of Griffiths [18], that taking the limit commutes with the operation of taking the first partial derivative with respect to  $\xi$  or  $\eta$ , so that, for example

$$\lim_{d \rightarrow \infty} \frac{\partial}{\partial \xi} \psi_d(\beta) = \frac{\partial}{\partial \xi} \lim_{d \rightarrow \infty} \psi_d(\beta) = \frac{\partial}{\partial \xi} \psi_{\text{MF}}(\beta, J). \tag{1.16}$$

We shall not enter here into the details of the order parameters or phase transitions of the general mean-field model given by (1.13). Instead, we refer the reader to the discussions given in [2] for the classical Potts model ( $\eta=0$ ) and [8] for the transverse Potts model ( $\xi=0, J\eta=1$ ). It is worth pointing out, however, that for the classical Potts model ( $\eta=0$ ), the mean-field free energy (1.13) becomes

$$\psi_{\text{MF}}(\beta, J) = \min_{x \in \mathbb{R}} \left\{ \frac{1}{2} q^{-1} (q-1) J x^2 + q^{-1} J x - \frac{1}{2} q^{-1} J - \beta^{-1} \ln [e^{\beta(Jx + \xi)} + q - 1] \right\}, \tag{1.17}$$

which differs from the expression given by Mittag and Stephen [2] but can easily be shown to be equivalent using the common stationary condition

$$x = \frac{e^{\beta(Jx + \xi)} - 1}{e^{\beta(Jx + \xi)} + q - 1}. \tag{1.18}$$

To prove the theorem we shall use the methods of [12] and [14] to obtain upper and lower bounds on the free energy  $\psi(\beta)$  which coalesce in the stated limits. In Sect. 2, we use the Bogoliubov variational principle to show that the mean-field free energy always gives an upper bound. In Sect. 3, the lower bound is obtained via a functional integral representation of the Trotter approximation to the partition function.

## 2. Upper Bound on the Free Energy

In this section we shall use Bogoliubov’s variational principle [19] to show that

$$\psi(\beta) \leq \psi_{\text{MF}}(\beta, J_\infty). \tag{2.1}$$

Before proceeding, however, it is convenient to introduce a vector notation. We define the following  $(q-1)$ -dimensional vectors:

$$\begin{aligned} \mathbf{\Omega}_j &= (\Omega_j, \Omega_j^2, \dots, \Omega_j^{q-1}), \\ \mathbf{M}_j &= (M_j, M_j^2, \dots, M_j^{q-1}), \\ \mathbf{1} &= (1, 1, \dots, 1). \end{aligned} \tag{2.2}$$

Given two  $(q-1)$ -dimensional vectors  $\mathbf{A}$  and  $\mathbf{B}$ , whose elements are either scalars or  $q \times q$  matrices, we define their dot product to be the Hermitian operator

$$\mathbf{A} \cdot \mathbf{B} = \frac{1}{2} \sum_{\alpha=1}^{q-1} (A_\alpha^\dagger B_\alpha + B_\alpha^\dagger A_\alpha). \tag{2.3}$$

Note that, when  $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{q-1}$ , the dot product is just the usual real inner product in  $\mathbb{C}^{q-1}$  regarded as the vector space  $\mathbb{R}^{2(q-1)}$ .

Using this compact notation, we can decompose the Hamiltonian (1.3) as

$$H = H_0 + H_1, \tag{2.4}$$

where

$$H_0 = \frac{1}{2} q^{-1} (q-1) N J_N x^2 - N q^{-1} \left( \frac{1}{2} J_N + \xi + \eta \right) - q^{-1} (J_N x + \xi) \sum_j \mathbf{1} \cdot \mathbf{\Omega}_j - q^{-1} \eta \sum_j \mathbf{1} \cdot \mathbf{M}_j \tag{2.5}$$

$$H_1 = -\frac{1}{2}q^{-1} \sum_{j,k} J_{jk}(x\mathbf{1} - \mathbf{\Omega}_j) \cdot (x\mathbf{1} - \mathbf{\Omega}_k), \quad (2.6)$$

and  $x \in \mathbb{R}$  is arbitrary. Bogoliubov's variational principle [19] now states that

$$\text{Tr} \exp[-\beta(H_0 + H_1)] \geq \exp(-\beta \langle H_1 \rangle_0) \text{Tr} \exp(-\beta H_0), \quad (2.7)$$

where

$$\langle \dots \rangle_0 = \text{Tr}[\dots \exp(-\beta H_0)] / \text{Tr} \exp(-\beta H_0). \quad (2.8)$$

In this case we find

$$\begin{aligned} \langle H_1 \rangle_0 &= -\frac{1}{2}q^{-1} \sum_{j,k} J_{jk}(x\mathbf{1} - \langle \mathbf{\Omega}_j \rangle_0) \cdot (x\mathbf{1} - \langle \mathbf{\Omega}_k \rangle_0) \\ &= -\frac{1}{2}q^{-1}(q-1) \sum_{j,k} J_{jk}(x - \langle \Omega_j \rangle_0)(x - \langle \Omega_k \rangle_0). \end{aligned} \quad (2.9)$$

Since  $J_{jj} = 0$ , this follows because the expectation  $\langle \dots \rangle_0$  factors over the sites and

$$\langle \Omega_j \rangle_0 = \langle \Omega_j^2 \rangle_0 = \dots = \langle \Omega_j^{q-1} \rangle_0 \in \mathbb{R}. \quad (2.10)$$

To obtain the desired bound we now choose  $x$  to be a solution of

$$x = \langle \Omega_j \rangle_0. \quad (2.11)$$

Since  $\langle \Omega_j \rangle_0$  is independent of  $j$ ,  $x$  will also be independent of  $j$ . With this choice of  $x$ , we see that  $\langle H_1 \rangle_0 = 0$  and hence, from (2.7),

$$Z_N \geq \text{Tr} \exp(-\beta H_0). \quad (2.12)$$

From (1.8), (2.5), and (2.11) we therefore conclude that

$$\begin{aligned} \psi(\beta) &\leq \frac{1}{2}J_\infty q^{-1}(q-1)x^2 - q^{-1}(\frac{1}{2}J_\infty + \xi + \eta) \\ &\quad - \beta^{-1} \ln \text{Tr} \exp[\beta q^{-1}((J_\infty x + \xi)\mathbf{1} \cdot \mathbf{\Omega} + \eta\mathbf{1} \cdot \mathbf{M})], \end{aligned} \quad (2.13)$$

where  $J_\infty$  is given by (1.10c) and  $x$  is any solution of the equation

$$(q-1)x = \frac{\text{Tr}(\mathbf{1} \cdot \mathbf{\Omega}) \exp[\beta q^{-1}((J_\infty x + \xi)\mathbf{1} \cdot \mathbf{\Omega} + \eta\mathbf{1} \cdot \mathbf{M})]}{\text{Tr} \exp[\beta q^{-1}((J_\infty x + \xi)\mathbf{1} \cdot \mathbf{\Omega} + \eta\mathbf{1} \cdot \mathbf{M})]}. \quad (2.14)$$

But this equation is precisely the condition for the right side of (2.13) to be stationary with respect to variations in  $x$ . Thus it follows that (2.1) holds with

$$\begin{aligned} \psi_{\text{MF}}(\beta, J) &= \min_{x \in \mathbb{R}} \left\{ \frac{1}{2}Jq^{-1}(q-1)x^2 - q^{-1}(\frac{1}{2}J + \xi + \eta) \right. \\ &\quad \left. - \beta^{-1} \ln \text{Tr} \exp[\beta q^{-1}((Jx + \xi)\mathbf{1} \cdot \mathbf{\Omega} + \eta\mathbf{1} \cdot \mathbf{M})] \right\}. \end{aligned} \quad (2.15)$$

In Appendix A we evaluate the matrix trace which appears in (2.15). Using this result then gives the explicit expression (1.13) for the mean-field free energy  $\psi_{\text{MF}}(\beta, J)$ .

### 3. Lower Bound on the Free Energy

In this section we derive a lower bound on the free energy (1.8). We begin by writing the Hamiltonian (1.3) in vector notation as

$$H = -Nq^{-1}(\frac{1}{2}J_N + \xi + \eta) - \frac{1}{2}q^{-1} \sum_{j,k} J_{jk} \mathbf{\Omega}_j \cdot \mathbf{\Omega}_k - q^{-1} \xi \sum_j \mathbf{1} \cdot \mathbf{\Omega}_j - q^{-1} \eta \sum_j \mathbf{1} \cdot \mathbf{M}_j. \tag{3.1}$$

Let us now regard the interactions  $J_{jk}$  as the entries of a matrix  $J$ . Since  $J$  is a cyclic matrix it is readily diagonalized [20]. Defining

$$S_{jk} = N^{-1/2} \prod_{\mu=1}^d \exp(2\pi i j_{\mu} k_{\mu} / v), \tag{3.2}$$

where  $N = v^d$  and  $j_{\mu}$  denotes the components of the lattice vector  $j$ , we have

$$S^{-1}JS = \text{diag}(\lambda_j), \tag{3.3}$$

where

$$\lambda_j = \lambda \left( \frac{2\pi j_1}{v}, \frac{2\pi j_2}{v}, \dots, \frac{2\pi j_d}{v} \right), \tag{3.4}$$

and

$$\lambda(\theta) = \lambda(\theta_1, \theta_2, \dots, \theta_d) = \sum_k J(k) e^{ik \cdot \theta}. \tag{3.5}$$

To proceed with the derivation of the lower bound we wish to replace the matrix  $J$  with a suitable positive definite matrix  $K$ . This matrix has to be defined differently for the two limits considered in the theorem. For the  $\gamma \rightarrow 0+$  limit [Part 2) of the theorem], it is sufficient to set

$$K_{jk} = J_{jk} + \gamma^d \varrho(0) \delta_{jk} = \gamma^d \varrho(\gamma|j-k|), \tag{3.6}$$

where  $\varrho(0)$  is chosen sufficiently large to make  $K$  positive definite. The additional diagonal term of course will not contribute in the limit  $\gamma \rightarrow 0+$ . For the  $d \rightarrow \infty$  limit [Part 1) of the theorem], we define the cyclic matrix  $K$  by

$$K_{jk} = |J|_{jk} + \varepsilon \delta_{jk}, \quad (\varepsilon > 0), \tag{3.7}$$

where the non-negative definite matrix  $|J|$  is given by

$$|J| = S \text{diag}(|\lambda_j|) S^{-1}. \tag{3.8}$$

Since  $\sum_{j,k} (K_{jk} - J_{jk}) \mathbf{\Omega}_j \cdot \mathbf{\Omega}_k$  is a positive definite matrix, it follows immediately from the Peierls theorem [17] that

$$\begin{aligned} Z_N \leq & \exp[\beta N q^{-1}(\frac{1}{2}J_N + \xi + \eta)] \text{Tr} \exp\left[\frac{1}{2} \beta q^{-1} \sum_{j,k} K_{jk} \mathbf{\Omega}_j \cdot \mathbf{\Omega}_k \right. \\ & \left. + \beta q^{-1} \xi \sum_j \mathbf{1} \cdot \mathbf{\Omega}_j + \beta q^{-1} \eta \sum_j \mathbf{1} \cdot \mathbf{M}_j\right]. \end{aligned} \tag{3.9}$$

For Hermitian matrices  $A$  and  $B$ , a straightforward generalization of the Golden-Thompson inequality [21] states that  $\text{Tr} e^{A+B} \leq \text{Tr}(e^{A/n} e^{B/n})^n$ , for all positive integers  $n$ . By Trotter's formula [22], equality is actually achieved in the limit  $n \rightarrow \infty$ . Applying this inequality to the right side of (3.9) we obtain

$$Z_N \leq \exp[\beta N q^{-1}(\frac{1}{2}J_N + \xi + \eta)] Z_{N,n}, \tag{3.10}$$

where

$$Z_{N,n} = \text{Tr} \left[ \exp \left( \frac{1}{2} \beta q^{-1} n^{-1} \sum_{j,k} K_{jk} \boldsymbol{\Omega}_j \cdot \boldsymbol{\Omega}_k + \beta q^{-1} n^{-1} \xi \sum_j \mathbf{1} \cdot \boldsymbol{\Omega}_j \right) \exp \left( \beta q^{-1} n^{-1} \eta \sum_j \mathbf{1} \cdot \mathbf{M}_j \right) \right]^n \quad (3.11)$$

We are now in a position to use the identity

$$\exp \left( \frac{1}{2} \beta \sum_{j,k} K_{jk} \Omega_j^\dagger \Omega_k \right) = (\beta/2\pi)^N (\text{Det } K)^{-1} \int_{\mathbb{R}^{2N}} \prod_j d^2 z_j \cdot \exp \left[ -\frac{1}{2} \beta \sum_{j,k} K_{jk}^{-1} \bar{z}_j z_k + \frac{1}{2} \beta \sum_j (\bar{z}_j \Omega_j + z_j \Omega_j^\dagger) \right], \quad (3.12)$$

where  $d^2 z$  means  $d(\text{Re } z) d(\text{Im } z)$ . This identity is valid for an arbitrary set of diagonal operators  $\Omega_j$  and any real symmetric positive definite matrix  $K$ . Applying it to each such term in the product of  $2n$  ordered exponentials in (3.11) gives

$$\begin{aligned} Z_{N,n} &= (\beta/2\pi q n)^{Nn(q-1)} (\text{Det } K)^{n(1-q)} \int_{\mathbb{R}^{2Nn(q-1)}} \prod_j \prod_{t=1}^n d^2 \mathbf{z}_{jt} \\ &\cdot \exp \left[ -\frac{1}{2} \beta q^{-1} n^{-1} \sum_{j,k} \sum_{t=1}^n K_{jk}^{-1} \mathbf{z}_{jt} \cdot \mathbf{z}_{kt} \right] \\ &\cdot \text{Tr} \prod_{t=1}^n \left\{ \exp \left[ \beta q^{-1} n^{-1} \sum_j (\mathbf{z}_{jt} + \xi \mathbf{1}) \cdot \boldsymbol{\Omega}_j \right] \exp \left[ \beta q^{-1} n^{-1} \eta \sum_j \mathbf{1} \cdot \mathbf{M}_j \right] \right\}. \end{aligned} \quad (3.13)$$

Next we need to estimate the trace in (3.13). This we do in three stages. Firstly, in Appendix B, we show that, for *even*  $n$  and arbitrary  $\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_n \in \mathbb{C}^{q-1}$  and  $\eta \geq 0$ ,

$$\begin{aligned} &\left| \text{Tr} \prod_{t=1}^n [\exp(q^{-1} n^{-1} \mathbf{z}_t \cdot \boldsymbol{\Omega}) \exp(q^{-1} n^{-1} \eta \mathbf{1} \cdot \mathbf{M})] \right| \\ &\leq \prod_{t=1}^n \{ [1 + 4n^{-1} \exp(3\|\mathbf{z}_t\| + \eta)] \cdot \text{Tr} \exp[q^{-1} (\mathbf{z}_t \cdot \boldsymbol{\Omega} + \eta \mathbf{1} \cdot \mathbf{M})] \}^{1/n}. \end{aligned} \quad (3.14)$$

Secondly, in Appendix C, we show that, for  $\mathbf{z} \in \mathbb{C}^{q-1}$  and  $\eta \geq 0$ ,

$$\text{Tr} \exp(\mathbf{z} \cdot \boldsymbol{\Omega} + \eta \mathbf{1} \cdot \mathbf{M}) \leq \text{Tr} \exp[(q-1)^{-1/2} \|\mathbf{z}\| \mathbf{1} \cdot \boldsymbol{\Omega} + \eta \mathbf{1} \cdot \mathbf{M}]. \quad (3.15)$$

Lastly, in Appendix D, we prove the monotonicity property

$$\frac{\partial}{\partial x} \text{Tr} \exp(x \mathbf{1} \cdot \boldsymbol{\Omega} + \eta \mathbf{1} \cdot \mathbf{M}) \geq 0 \quad (3.16)$$

for  $x \geq 0$  and  $\eta \geq 0$ . Combining these inequalities with the triangle inequality  $\|\mathbf{z} + \xi \mathbf{1}\| \leq \|\mathbf{z}\| + (q-1)^{1/2} \xi \leq \|\mathbf{z}\| + q\xi$ , we obtain

$$\begin{aligned} &\left| \text{Tr} \prod_{t=1}^n \{ \exp[\beta q^{-1} n^{-1} (\mathbf{z}_t + \xi \mathbf{1}) \cdot \boldsymbol{\Omega}] \exp[\beta q^{-1} n^{-1} \eta \mathbf{1} \cdot \mathbf{M}] \} \right| \\ &\leq \prod_{t=1}^n \{ [1 + 4n^{-1} \exp(3\beta \|\mathbf{z}_t\| + 3\beta q \xi + \beta \eta)] \\ &\cdot \text{Tr} \exp[\beta q^{-1} ((q-1)^{-1/2} \|\mathbf{z}_t\| + \xi) \mathbf{1} \cdot \boldsymbol{\Omega} + \beta q^{-1} \eta \mathbf{1} \cdot \mathbf{M}] \}^{1/n}. \end{aligned} \quad (3.17)$$

If we now factor out the direct product over  $j$  appearing in (3.13) and apply the inequality (3.17) at each site we find

$$\begin{aligned}
Z_{N,n} &\leq (\beta/2\pi qn)^{Nn(q-1)} (\text{Det } K)^{-n(q-1)} \int_{\mathbb{R}^{2Nn(q-1)}} \prod_j \prod_{t=1}^n d^2 \mathbf{z}_{jt} \\
&\cdot \exp \left[ -\frac{1}{2} \beta q^{-1} n^{-1} \sum_{j,k} \sum_{t=1}^n (K_{jk}^{-1} - \zeta^{-1} \delta_{jk}) \mathbf{z}_{jt} \cdot \mathbf{z}_{kt} \right] \\
&\cdot \prod_j \prod_{t=1}^n \exp \left\{ -\frac{1}{2} \beta q^{-1} n^{-1} \zeta^{-1} \|\mathbf{z}_{jt}\|^2 \right. \\
&\quad \left. + n^{-1} \ln \text{Tr} \exp [\beta q^{-1} ((q-1)^{-1/2} \|\mathbf{z}_{jt}\| + \xi) \mathbf{1} \cdot \boldsymbol{\Omega} + \beta q^{-1} \eta \mathbf{1} \cdot \mathbf{M}] \right. \\
&\quad \left. + n^{-1} \ln [1 + 4n^{-1} \exp(3\beta \|\mathbf{z}_{jt}\| + 3\beta q \xi + \beta \eta)] \right\}, \tag{3.18}
\end{aligned}$$

where, in anticipation of the next step, we have added and subtracted a term in the exponent with  $\zeta > 0$  arbitrary.

To obtain the required upper bound on  $Z_{N,n}$ , our strategy now is to replace each term in the product over  $j, t$  in (3.18) by the common maximum. This maximum occurs for  $\|\mathbf{z}_{jt}\| = \|\mathbf{z}\|$  satisfying the stationary condition

$$\zeta^{-1} \|\mathbf{z}\| = F(\|\mathbf{z}\|), \tag{3.19}$$

where

$$\begin{aligned}
F(x) &= \frac{\text{Tr}(\mathbf{1} \cdot \boldsymbol{\Omega}) \exp[\beta q^{-1} ((q-1)^{-1/2} x + \xi) \mathbf{1} \cdot \boldsymbol{\Omega} + \beta q^{-1} \eta \mathbf{1} \cdot \mathbf{M}]}{(q-1)^{1/2} \text{Tr} \exp[\beta q^{-1} ((q-1)^{-1/2} x + \xi) \mathbf{1} \cdot \boldsymbol{\Omega} + \beta q^{-1} \eta \mathbf{1} \cdot \mathbf{M}]} \\
&\quad + \frac{12qn^{-1} \exp(3\beta x + 3\beta q \xi + \beta \eta)}{1 + 4n^{-1} \exp(3\beta x + 3\beta q \xi + \beta \eta)}. \tag{3.20}
\end{aligned}$$

After the maximization of the product over  $j, t$  in (3.18), we perform the remaining Gaussian integrals. Setting

$$x = (q-1)^{-1/2} \zeta^{-1} \|\mathbf{z}\|, \tag{3.21}$$

we obtain

$$\begin{aligned}
Z_{N,n} &\leq \text{Det}(I - \zeta^{-1} K)^{-n(q-1)} \\
&\cdot \max_{x \in \mathbb{R}} \{ \exp[-\frac{1}{2} \beta q^{-1} (q-1) \zeta x^2] \cdot \text{Tr} \exp[\beta q^{-1} (\zeta x + \xi) \mathbf{1} \cdot \boldsymbol{\Omega} + \beta q^{-1} \eta \mathbf{1} \cdot \mathbf{M}] \\
&\cdot [1 + 4n^{-1} \exp(3\beta (q-1)^{1/2} \zeta x + 3\beta q \xi + \beta \eta)] \}^N. \tag{3.22}
\end{aligned}$$

The manipulation leading to (3.22) clearly requires the matrix  $I - \zeta^{-1} K$  to be positive definite. This will certainly be true if we choose  $\zeta$  to be greater than the maximum eigenvalue of  $K$ , i.e., either

$$\zeta > J_N + \varepsilon \quad \text{or} \quad \zeta > J_\infty + \gamma^d q(0) \tag{3.23}$$

as appropriate. We now take the thermodynamic limit  $N \rightarrow \infty$ . From (3.9), (3.10), and (3.22), it then follows that

$$\begin{aligned}
 \psi(\beta) &= - \lim_{N \rightarrow \infty} (\beta N)^{-1} \ln Z_N \\
 &\geq \min_{x \in \mathbb{R}} \{ \frac{1}{2} q^{-1} (q-1) \zeta x^2 - q^{-1} (\frac{1}{2} J_\infty + \zeta + \eta) \\
 &\quad - \beta^{-1} \ln \text{Tr} \exp[\beta q^{-1} (\zeta x + \zeta) \mathbf{1} \cdot \mathbf{\Omega} + \beta q^{-1} \eta \mathbf{1} \cdot \mathbf{M}] \\
 &\quad - \beta^{-1} \ln [1 + 4n^{-1} \exp(3\beta(q-1)^{1/2} \zeta x + 3\beta q \zeta + \beta \eta)] \} + n(q-1) R(\beta, \zeta),
 \end{aligned} \tag{3.24}$$

where, by Szegő's theorem [23], the remainder term  $R(\beta, \zeta)$  is

$$R(\beta, \zeta) = \beta^{-1} \lim_{N \rightarrow \infty} N^{-1} \ln \text{Det}(I - \zeta^{-1} |J|) = \beta^{-1} (2\pi)^{-d} \int_0^{2\pi} \int d\mathbf{\theta} \ln(1 - \zeta^{-1} |\lambda(\mathbf{\theta})|). \tag{3.25}$$

Here  $\lambda(\mathbf{\theta})$  is given by (3.5) with either  $J(0) = 0$  or  $J(0) = \gamma^d \varrho(0)$  as appropriate.

In each of the two limits  $d \rightarrow \infty, \gamma \rightarrow 0+$  the remainder term (3.25) vanishes. For the  $d \rightarrow \infty$  limit, this was proved in [12]. For the long-range  $\gamma \rightarrow 0+$  limit it has been proved in [13]. Evaluating the trace in (3.24) (Appendix A) and taking the limits  $n \rightarrow \infty, \zeta \rightarrow J+$  [see (3.23)] after all other limits, we conclude that

$$\lim_{d \rightarrow \infty} \psi_d(\beta) \geq \psi_{\text{MF}}(\beta, J), \tag{3.26}$$

and

$$\lim_{\gamma \rightarrow 0+} \psi_\gamma(\beta) \geq \psi_{\text{MF}}(\beta, J), \tag{3.27}$$

where  $\psi_{\text{MF}}(\beta, J)$  is the mean-field free energy given by (1.13). These inequalities, along with the reverse inequality (2.1), prove the theorem stated in Sect. 1.

### Appendix A

In this appendix we prove the following:

**Lemma.** For arbitrary  $x$  and  $\eta$ ,

$$\begin{aligned}
 \text{Tr} \exp(x \mathbf{1} \cdot \mathbf{\Omega} + \eta \mathbf{1} \cdot \mathbf{M}) &= \exp[\frac{1}{2} (q-2)(x + \eta)] \\
 &\quad \cdot \{ 2 \cosh[\frac{1}{2} (q^2 x^2 - 2q(q-2)x\eta + q^2 \eta^2)^{1/2}] \\
 &\quad + (q-2) \exp[-\frac{1}{2} q(x + \eta)] \}.
 \end{aligned} \tag{A.1}$$

*Proof.* We wish to find the eigenvalues of the  $q \times q$  matrix

$$x \mathbf{1} \cdot \mathbf{\Omega} + \eta \mathbf{1} \cdot \mathbf{M} = \begin{bmatrix} (q-1)x & \eta & \dots & \eta & \eta \\ \eta & -x & \dots & \eta & \eta \\ \vdots & & \ddots & \vdots & \vdots \\ \eta & \eta & \dots & -x & \eta \\ \eta & \eta & \dots & \eta & -x \end{bmatrix}. \tag{A.2}$$

Such a matrix has been studied in [8]: it has two eigenvectors of the form  $(a, 1, 1, \dots, 1)$  with eigenvalues

$$\lambda_{1,2} = \frac{1}{2} (q-2)(x + \eta) \pm \frac{1}{2} [q^2 x^2 - 2q(q-2)x\eta + q^2 \eta^2]^{1/2}, \tag{A.3}$$

and  $(q-2)$  eigenvectors of the form  $(0, 1, w, w^2, \dots, w^{q-2})$ , where  $w \neq 1$  is a  $(q-1)^{\text{th}}$  root of unity, with degenerate eigenvalues

$$\lambda_3 = \lambda_4 = \dots = \lambda_q = -(x + \eta). \tag{A.4}$$

Hence

$$\text{Tr} \exp(x\mathbf{1} \cdot \mathbf{\Omega} + \eta\mathbf{1} \cdot \mathbf{M}) = e^{\lambda_1} + e^{\lambda_2} + (q-2)e^{\lambda_3} \tag{A.5}$$

from which (A.1) follows.

### Appendix B

Our aim here is to prove the inequality (3.14). To do this we first prove the following:

**Lemma.** *If  $A$  and  $B$  are  $q \times q$  matrices and  $n$  a positive integer, then*

$$|\text{Tr}[\exp(n^{-1}A)\exp(n^{-1}B)]^n| \leq \{1 + 2n^{-1} \exp[3(\|A\| + \|B\|)]\} |\text{Tr} \exp(A+B)|, \tag{B.1}$$

where the norm  $\|A\|$  is given by

$$\|A\| = \sup_{\|\mathbf{v}\|=1} \|A\mathbf{v}\| \tag{B.2}$$

with  $\|\mathbf{v}\|^2 = \mathbf{v} \cdot \mathbf{v}$  for  $\mathbf{v} \in \mathbb{C}^q$ .

*Proof.* Let us set

$$T = \exp(n^{-1}A)\exp(n^{-1}B), \tag{B.3}$$

$$S = \exp[n^{-1}(A+B)]; \tag{B.4}$$

then

$$\left| \frac{\text{Tr}(T^n)}{\text{Tr}(S^n)} \right| = \left| \frac{\text{Tr}(T^n S^{-n} S^n)}{\text{Tr}(S^n)} \right| \leq \varrho(T^n S^{-n}) \leq \|T^n S^{-n}\|, \tag{B.5}$$

where  $\varrho(A)$  denotes the spectral radius of  $A$ . Using the elementary properties of the norm (B.2), i.e.

$$\|A+B\| \leq \|A\| + \|B\|, \quad \|AB\| \leq \|A\| \|B\|, \quad \|I\| = 1, \tag{B.6}$$

we further estimate that

$$\|T^n S^{-n}\| = \|I + (T^n - S^n)S^{-n}\| \leq 1 + \|T^n - S^n\| \|S^{-n}\|. \tag{B.7}$$

The required result (B.1) thus follows from the estimates (see, for example, Reed and Simon [22, p. 295]):

$$\|S^{-n}\| \leq \exp(\|A\| + \|B\|), \tag{B.8}$$

$$\|S^n - T^n\| \leq 2n^{-1} \exp[2(\|A\| + \|B\|)]. \tag{B.9}$$

To obtain the inequality (3.14), we can now use the Hölder inequality [24]

$$\left| \text{Tr} \prod_{t=1}^n T_t \right| \leq \prod_{t=1}^n [\text{Tr}(T_t^\dagger T_t)^{n/2}]^{1/n}, \tag{B.10}$$

with

$$T_t = \exp(n^{-1}A_t)\exp(n^{-1}B_t), \tag{B.11}$$

$$A_t = q^{-1}\mathbf{z}_t \cdot \boldsymbol{\Omega}, \quad B_t = q^{-1}\eta \mathbf{1} \cdot \mathbf{M}. \tag{B.12}$$

Since  $A_t$  and  $B_t$  are Hermitian we find

$$\begin{aligned} \text{Tr}(T_t^\dagger T_t)^{n/2} &= \text{Tr}[\exp(n^{-1}B_t)\exp(2n^{-1}A_t)\exp(n^{-1}B_t)]^{n/2} \\ &= \text{Tr}[\exp(2n^{-1}A_t)\exp(2n^{-1}B_t)]^{n/2}. \end{aligned} \tag{B.13}$$

In this last step we have assumed that  $n$  is *even* and used the cyclic property of the trace. Applying the preceding lemma to (B.10) now gives

$$\begin{aligned} &\left| \text{Tr} \prod_{t=1}^n \exp(n^{-1}A_t)\exp(n^{-1}B_t) \right| \\ &\leq \prod_{t=1}^n \{ [1 + 4n^{-1} \exp(3(\|A_t\| + \|B_t\|))] \text{Tr} \exp(A_t + B_t) \}^{1/n}. \end{aligned} \tag{B.14}$$

Recalling the definitions (B.12) of  $A_t$  and  $B_t$ , we see that (B.14) gives the desired inequality (3.14), once  $\|A_t\|$  and  $\|B_t\|$  have been replaced by the simple estimates:

$$\|A_t\| \leq q^{-1} \sum_{\alpha=1}^{q-1} |z_{t\alpha}| \|\boldsymbol{\Omega}\|^\alpha = q^{-1} \sum_{\alpha=1}^{q-1} |z_{t\alpha}| \leq \|\mathbf{z}_t\|, \tag{B.15}$$

$$\|B_t\| \leq q^{-1}\eta \sum_{\alpha=1}^{q-1} \|M\|^\alpha = q^{-1}(q-1)\eta \leq \eta. \tag{B.16}$$

### Appendix C

In this appendix we prove the inequality (3.15). This inequality follows immediately from the following stronger result:

**Lemma.** *Let  $A, B, C$  be the  $q \times q$  Hermitian matrices given by*

$$A = \mathbf{z} \cdot \boldsymbol{\Omega} + (q-1)^{-1/2} \|\mathbf{z}\| I, \tag{C.1}$$

$$B = (q-1)^{-1/2} \|\mathbf{z}\| (\mathbf{1} \cdot \boldsymbol{\Omega} + I), \tag{C.2}$$

$$C = \eta(\mathbf{1} \cdot \mathbf{M} + I). \tag{C.3}$$

Then, for any positive integer  $n$ ,

$$\text{Tr}(A + C)^n \leq \text{Tr}(B + C)^n. \tag{C.4}$$

*Proof.* We first show that

$$\text{Tr} A^n \leq \text{Tr} B^n. \tag{C.5}$$

For  $n=1$ , equality holds, i.e.  $\text{Tr} A = \text{Tr} B$ , because

$$\text{Tr} \boldsymbol{\Omega} = \mathbf{0}. \tag{C.6}$$

For  $n=2$ , a straightforward calculation gives

$$\begin{aligned} \text{Tr } A^2 &= (q/4) \sum_{\alpha=1}^{q-1} |z_\alpha + \bar{z}_{q-\alpha}|^2 + q(q-1)^{-1} \|\mathbf{z}\|^2 \\ &\leq q^2(q-1)^{-1} \|\mathbf{z}\|^2 = \text{Tr } B^2, \end{aligned} \tag{C.7}$$

where the last equality is easily obtained by noting that

$$\mathbf{1} \cdot \boldsymbol{\Omega} + I = \text{diag}(q, 0, 0, \dots, 0). \tag{C.8}$$

For  $n \geq 3$ , we have

$$\text{Tr } A^n \leq (\text{Tr } A^2)^{n/2} \leq [q(q-1)^{-1/2} \|\mathbf{z}\|]^n = \text{Tr } B^n. \tag{C.9}$$

Here the first inequality is a generalization of a standard inequality for  $l^p$  norms and the second inequality follows from (C.7).

To prove (C.4) we now observe that the entries of the matrix  $C$  are all equal to  $\eta$ . Because it is of this special form, the matrix  $C$  can be eliminated from the trace of any product, formed with a diagonal  $q \times q$  matrix  $D$ , by using the cyclic property of the trace and the following identities:

$$C^2 = q\eta C, \quad CDC = \eta(\text{Tr } D)C, \quad \text{Tr } CD = \eta \text{Tr } D. \tag{C.10}$$

Using (C.7) it follows, for example, that

$$\text{Tr } ACA^2C^2 = q\eta^3 \text{Tr } A \cdot \text{Tr } A^2 \leq q\eta^3 \text{Tr } B \cdot \text{Tr } B^2 = \text{Tr } BCB^2C^2. \tag{C.11}$$

Since this argument holds for any such product, (C.4) can be obtained by using the binomial expansion for non-commuting operators and comparing the traces term-by-term. Likewise, by expanding the exponentials, we can prove

$$\text{Tr } e^{A+C} \leq \text{Tr } e^{B+C}. \tag{C.12}$$

This inequality is equivalent to (3.15).

### Appendix D

In this appendix we prove the following:

**Lemma.** *Suppose  $x \geq 0$  and  $\eta \geq 0$ . Then*

$$\frac{\partial}{\partial x} \text{Tr } \exp(x\mathbf{1} \cdot \boldsymbol{\Omega} + \eta\mathbf{1} \cdot \mathbf{M}) = \text{Tr}(\mathbf{1} \cdot \boldsymbol{\Omega}) \exp(x\mathbf{1} \cdot \boldsymbol{\Omega} + \eta\mathbf{1} \cdot \mathbf{M}) \geq 0, \tag{D.1}$$

*Proof.* Let  $C$  and  $D$  be the  $q \times q$  Hermitian matrices given by

$$C = \eta(\mathbf{1} \cdot \mathbf{M} + I), \tag{D.2}$$

$$D = \mathbf{1} \cdot \boldsymbol{\Omega} = \text{diag}(q-1, -1, -1, \dots, -1). \tag{D.3}$$

Then to prove (D.1), i.e.

$$\text{Tr } D \exp(C + xD) \geq 0, \tag{D.4}$$

we expand the exponential, take the trace term-by-term using (C.10), and use the inequalities

$$\text{Tr} D^n = (q-1)^n \pm (q-1) \geq 0. \quad (\text{D.5})$$

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**Note added in proof.** One of the authors (P.A.P.) has now shown that the mean-field theory for the quantum Potts model becomes exact in the  $q \rightarrow \infty$  limit. The details will appear elsewhere.

