

# Heisenberg models and Schur–Weyl duality

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Björnberg, J., Rosengren, H., Ryan, K. (2023). Heisenberg models and Schur–Weyl duality. Advances in Applied Mathematics, 151. http://dx.doi.org/10.1016/j.aam.2023.102572

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## Heisenberg models and Schur–Weyl duality

### J.E. Björnberg<sup>a,\*</sup>, H. Rosengren<sup>a</sup>, K. Ryan<sup>b</sup>

<sup>a</sup> Chalmers University of Technology and University of Gothenburg, Sweden
 <sup>b</sup> Technical University of Vienna, Austria

#### ARTICLE INFO

Article history: Received 2 March 2022 Received in revised form 3 May 2023 Accepted 23 June 2023 Available online xxxx

MSC: 82B10

#### ABSTRACT

We present a detailed analysis of certain quantum spin systems with inhomogeneous (non-random) mean-field interactions. Examples include, but are not limited to, the interchange- and spin singlet projection interactions on complete bipartite graphs. Using two instances of the representation theoretic framework of Schur–Weyl duality, we can explicitly compute the free energy and other thermodynamic limits in the models we consider. This allows us to describe the phase transition, the ground-state phase diagram, and the expected structure of extremal states.

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\* Corresponding author.

*E-mail addresses:* jakob.bjornberg@gu.se (J.E. Björnberg), hjalmar@chalmers.se (H. Rosengren), kieran.ryan@tuwien.ac.at (K. Ryan).

https://doi.org/10.1016/j.aam.2023.102572



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APPLIED MATHEMATICS

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#### 1. Introduction and results

This paper presents an explicit analysis of certain quantum spin systems using classical tools from representation theory. In general, quantum spin systems are used to describe magnetic properties of materials, using the following formalism. For a large number n of particles, such as electrons in a lattice, the tensor product  $(\mathbb{C}^r)^{\otimes n}$  represents a space of possible configurations, while a Hermitian linear map  $H_n : (\mathbb{C}^r)^{\otimes n} \to (\mathbb{C}^r)^{\otimes n}$  describes both the interactions between particles and the possible energy levels of the system as a whole. More precisely, the specific form of  $H_n$  encodes the interactions, while its eigenvalues (which are real) are interpreted as energy levels.  $H_n$  is called the *Hamiltonian* of the system. The parameter  $r \geq 2$  is fixed and is related to the 'spin' of the particles through S = (r-1)/2.

Arguably the most famous quantum spin system is the *Heisenberg model for ferro*magnetism. When Werner Heisenberg introduced his model, in 1928, he described it in terms of an exchange interaction between neighbouring valence electrons ("Austausch von Elektronen", [21, p. 621]). In modern notation, for the spin- $\frac{1}{2}$  system he was considering, this interaction can be written as  $T_{i,j} = 2(\mathbb{S}_i \cdot \mathbb{S}_j) + \frac{1}{2}$ , and the Hamiltonian as

$$H_n = -\sum_{1 \le i < j \le n} \alpha_{i,j} T_{i,j}, \qquad \alpha_{i,j} \ge 0, \tag{1}$$

with the  $\alpha_{i,j}$  giving the interaction strength. Here  $T_{i,j}$  acts by transposing the *i*-th and *j*-th tensor factors while  $\mathbb{S}_i = (S_i^{(1)}, S_i^{(2)}, S_i^{(3)})$  is the triple of spin- $\frac{1}{2}$ -matrices (generators for  $\mathfrak{su}(2)$ ) acting on the *i*-th tensor factor. For higher spin (r > 2), two natural generalisations suggest themselves: we can take the interaction to be the transposition  $T_{i,j}$  acting on  $(\mathbb{C}^r)^{\otimes n}$ , or to be  $\mathbb{S}_i \cdot \mathbb{S}_j$ , where the  $\mathbb{S}$  are now spin-*S*-matrices. For  $S > \frac{1}{2}$ , these choices are no longer equivalent; while both are natural generalisations, some authors reserve the name *Heisenberg model* for the model with interaction  $\mathbb{S}_i \cdot \mathbb{S}_j$ . The model with

interaction  $T_{i,j}$  has been called the *interchange model* and is one of the main topics of this paper. Note that the interaction coefficients  $\alpha_{i,j}$  allow to encode basic assumptions about the structure of the lattice where the interacting particles are located, specifically this is the graph with vertex set  $\{1, 2, ..., n\}$  and an edge between i and j when  $\alpha_{i,j} \neq 0$ .

For the antiferromagnetic spin- $\frac{1}{2}$  Heisenberg model, with Hamiltonian being the negative of (1), Aizenman and Nachtergaele [2] discovered a similar representation based on the identity  $P_{i,j} = \frac{1}{2} - 2\mathbb{S}_i \cdot \mathbb{S}_j$  where  $P_{i,j}$  is (twice) the projection onto the singlet subspace of  $\mathbb{C}^2 \otimes \mathbb{C}^2$  associated with the *i*-th and *j*-th tensor factors (meaning the eigenspace for the total spin operator with eigenvalue 0). On a bipartite graph, such as (a finite interval in) the line  $\mathbb{Z}$  considered by Aizenman and Nachtergaele, the Hamiltonian with interactions  $P_{i,j}$  is unitarily equivalent to that with interactions  $Q_{i,j}$  defined by

$$\langle e_{\alpha_1} \otimes e_{\alpha_2} | Q_{i,j} | e_{\alpha_3} \otimes e_{\alpha_4} \rangle = \delta_{\alpha_1,\alpha_2} \delta_{\alpha_3,\alpha_4}, \tag{2}$$

where the  $e_{\alpha}$  are an orthonormal basis for  $\mathbb{C}^2$  and  $\langle \cdot | \cdot \rangle$  denotes the standard scalar product. The interaction  $Q_{i,j}$  has a natural interpretation in terms of random loops, and plays a central role in the present work. The definition (2) generalises straightforwardly to higher spin.

If we take the underlying lattice to be the *complete graph*  $K_n$ , consisting of n vertices with an edge between each pair of distinct vertices, then the interchange model is a mean-field system with Hamiltonian

$$-\frac{1}{n}\sum_{1\leq i< j\leq n} T_{i,j}, \quad \text{acting on } (\mathbb{C}^r)^{\otimes n}, \quad r\geq 2.$$
(3)

This model was studied in the papers of Björnberg [8,9], where the key step of the analysis was to note that the Hamiltonian (3) is a central element of the group algebra  $\mathbb{C}[S_n]$  of the symmetric group, represented on the tensor space  $(\mathbb{C}^r)^{\otimes n}$ . This means that the eigenspace decomposition for the Hamiltonian (3) coincides with the decomposition of  $(\mathbb{C}^r)^{\otimes n}$  into irreducible  $S_n$ -modules, which is well-studied. Ryan [29] implemented a similar approach for the model with Hamiltonian

$$-\frac{1}{n}\sum_{1\leq i< j\leq n} (a\,T_{i,j} + b\,Q_{i,j}) \quad \text{acting on } (\mathbb{C}^r)^{\otimes n},\tag{4}$$

with  $a, b \in \mathbb{R}$  and  $r \geq 2$ , which can similarly be diagonalised using the irreducible representations of the *Brauer algebra* (defined below).

The unifying principle behind this approach to determining the eigenspace decomposition of the Hamiltonian is a classical algebraic theory called *Schur–Weyl duality*. This term is used for specific instances of a general result in representation theory called the *double centraliser theorem*, which states the following [14, Theorem 4.54]. Let  $\mathbb{V}$ be a finite-dimensional vector space, and  $\mathbb{A} \subseteq \text{End}(\mathbb{V})$  a semi-simple algebra of linear mappings (endomorphisms)  $\mathbb{V} \to \mathbb{V}$ . Then the centraliser  $\mathbb{B}$  of  $\mathbb{A}$ , i.e. the algebra of endomorphisms commuting with all elements of  $\mathbb{A}$ , is also semi-simple, and as a representation of  $\mathbb{A} \otimes \mathbb{B}$  we have

$$\mathbb{V} = \bigoplus_{i} U_i \otimes V_i,\tag{5}$$

where the  $U_i$  (respectively  $V_i$ ) are non-isomorphic irreducible representations of  $\mathbb{A}$  (respectively  $\mathbb{B}$ ). The most famous instances of this (and relevant in the present work) are obtained by letting  $\mathbb{V} = (\mathbb{C}^r)^{\otimes n}$ . If we let  $\mathbb{A}$  consist of all invertible endomorphisms of  $\mathbb{C}^r$ , acting diagonally on  $\mathbb{V}$ , then  $\mathbb{B}$  is generated by the permutations of the tensor factors of  $\mathbb{V}$ : this gives the Schur–Weyl duality between the general linear group  $\operatorname{GL}_r(\mathbb{C})$  and the symmetric group  $S_n$  (see (55) for details) which facilitates the analysis of the interchange model (3). If instead we take  $\mathbb{A}$  to consist of *orthogonal* matrices, then  $\mathbb{B}$  is the Brauer algebra used in the analysis of (4).

The name interchange model can be traced back to works by Harris [20], Powers [28], and Tóth [33], and is motivated by a probabilistic representation of the model. Powers [28] was first to notice that the ferromagnetic  $(\text{spin-}\frac{1}{2})$  Heisenberg model can be represented in terms of a random walk on permutations generated by transpositions. The latter random walk was constructed on infinite lattices by Harris [20]. Tóth [33] was first to use this representation to obtain an important result for the Heisenberg model: a bound on the free energy of the model on  $\mathbb{Z}^3$  that was the best known for many years [12]. The underlying random walk on permutations has come to be known as the interchange *process* in the literature on mixing times of Markov chains [3]. The present paper does not use the probabilistic representation, however; indeed our methods apply also in cases where such a representation is not available.

Let us note that the present work follows a line of papers analysing the interchange process and Heisenberg model with algebraic methods (including the aforementioned [8], [9], [29]). Alon and Kozma [4] analysed the interchange process on a general graph, and estimated the number of k-cycles at a given time; Berestycki and Kozma [7] gave an exact formula for the same on the complete graph; Alon and Kozma [5] gave an exact formula for the magnetisation of the mean-field spin- $\frac{1}{2}$  Heisenberg model.

In this work we carry the methods described above further, to inhomogeneous models on the complete graph where the coupling constants between different vertices take finitely many different values. Our setting can be thought of as a mean-field approximation of a material which is formed by combining (e.g. welding together) several materials with different properties. The models for which our analysis goes the deepest are what we call *two-block* models, where coupling constants can take at most three values (one each for the interactions within each of the two blocks, and one for interactions between the two blocks). Our results on these models come in several parts. In Theorems 1.1 and 1.2 we explicitly compute the free energy. In Propositions 1.3 to 1.6, we give results on phase transitions, and, for certain restrictions on the parameters, we compute the critical temperature. In Theorems 1.7 and 1.8 we compute a magnetisation and limits of certain correlation functions. Using the results mentioned above, in Section 1.4 we completely describe the ground-state phase diagram of the models; and in Section 1.5 we give heuristic descriptions of the extremal Gibbs states and phase diagrams at finite temperature. At the end of the paper, in Section 5, we give the free energy for what we call *multi-block* models, where coupling constants can take any finite number of values, and where we allow certain many-body interactions.

Two highlights of the new results in this paper are the following. Firstly, we give a formula for the critical temperature of the spin- $\frac{1}{2}$  quantum Heisenberg model on the complete bipartite graph; see Proposition 1.4 with a = b = 0. Secondly, a curious equality of the free energy of the model on the complete bipartite graph with interaction via transpositions  $T_{i,j}$  (3), and the model with interaction via the (scaled) spin-singlet projection  $P_{i,j}$ ; see Theorem 1.2, also with a = b = 0. We wonder whether this equality holds for arbitrary bipartite graphs.

Finally, Manai and Warzel [24] point out that for the interchange model on the complete graph (3), the results of [8] on the free energy can be deduced from the results of Fannes, Spohn and Verbeure [15], which do not rely on representation theory. However, for the two-block setting considered here, or the model (4) considered by Ryan, the results of [15] do not seem to apply easily. It would be interesting to compare the two approaches in detail.

#### 1.1. Free energy

For  $a, b, c \in \mathbb{R}$ , and  $1 \leq m \leq n$ , we define the AB-interchange-model, or AB-model for short, through its Hamiltonian

$$H_n^{\rm AB} = -\frac{1}{n} \Big( a \sum_{1 \le i < j \le m} T_{i,j} + b \sum_{m+1 \le i < j \le n} T_{i,j} + c \sum_{1 \le i \le m < j \le n} T_{i,j} \Big), \tag{6}$$

acting on  $\mathbb{V} = (\mathbb{C}^r)^{\otimes n}$ . We call this a *two-block* model since we may think of it as a spin system on a graph with vertex set  $\{1, 2, \ldots, n\}$  partitioned into the two blocks  $A = \{1, \ldots, m\}$  and  $B = \{m + 1, \ldots, n\}$ . The form of the Hamiltonian (6) means that spins at two vertices within A interact with coupling constant a, spins at two vertices within B interact with coupling constant b, and the spin at a vertex in A interacts with the spin at a vertex in B with coupling constant c. In the homogeneous case a = b = cwe obtain the interchange model on the complete graph (3), while if a = b = 0 and  $c \neq 0$ we obtain a model on the complete bipartite graph  $K_{m,n-m}$ .

Given an  $r \times r$  matrix U, we write  $U_i$  for the linear operator on  $(\mathbb{C}^r)^{\otimes n}$  which acts as U on the *i*-th tensor factor and as the identity on the other factors. In particular,  $U_i$ and  $U_i$  commute if  $i \neq j$ . For any invertible U, we have that

$$U_i U_j T_{i,j} U_j^{-1} U_i^{-1} = T_{i,j}.$$
(7)

The Hamiltonian (6) thus has the GL(r)-symmetry

$$\left(\prod_{i=1}^{n} U_{i}\right) H_{n}^{\text{AB}}\left(\prod_{i=1}^{n} U_{i}^{-1}\right) = H_{n}^{\text{AB}}, \qquad U \in \mathrm{GL}_{r}(\mathbb{C}).$$

$$(8)$$

For  $\beta > 0$ , introduce the *partition function*  $Z_n^{AB}(\beta) = \operatorname{tr}\left[e^{-\beta H_n^{AB}}\right]$ . The partition function can be written as a sum over the eigenvalues E of  $H_n^{AB}$ :

$$Z_n^{\text{AB}}(\beta) = \sum_E e^{-\beta E} m(E), \qquad (9)$$

where m(E) is the multiplicity of the eigenvalue E. Roughly speaking, as  $n \to \infty$  we expect  $Z_n^{AB}(\beta)$  to grow exponentially in n, and to be dominated by the largest few terms in (9). For large  $\beta$  we may expect the dominant terms to correspond to small values of E, while for small  $\beta$  we expect the terms with large multiplicity m(E) to dominate. This balance between 'energy' (small E) and 'entropy' (large m) will in interesting cases lead to a *phase transition*, which can be identified by analysing the maximiser of the *free* energy  $\lim_{n\to\infty} \frac{1}{n} \log Z_n^{AB}(\beta)$ . (Some authors refer to this quantity as the *pressure*, while the free energy would be given by multiplying with  $-\frac{1}{\beta}$ .)

In our case we can compute the free energy explicitly. We write

$$F(x_1, \dots, x_r; y_1, \dots, y_r) = \sum_{i=1}^r f(x_i, y_i),$$
(10)

where  $x_i, y_i \ge 0$  and

$$f(x,y) = -x\log x - y\log y + \frac{\beta}{2}(ax^2 + by^2 + 2cxy).$$
 (11)

**Theorem 1.1.** Let  $a, b, c \in \mathbb{R}$  be fixed. If  $n, m \to \infty$  such that  $m/n \to \rho \in (0, 1)$ , then the free energy of the model (6) satisfies

$$\Phi_{\beta}^{AB}(a,b,c) := \lim_{n \to \infty} \frac{1}{n} \log Z_n^{AB}(\beta) = \max F(x_1, \dots, x_r; y_1, \dots, y_r)$$
(12)

where the maximum is taken over  $x_1, \ldots, x_r, y_1, \ldots, y_r \ge 0$  subject to  $\sum_{i=1}^r x_i = 1 - \sum_{i=1}^r y_i = \rho$ .

Note that if  $(x_1, \ldots, x_r; y_1, \ldots, y_r)$  is a maximum point of F, and we order the xentries so that

$$x_1 \ge x_2 \ge \dots \ge x_r,\tag{13}$$

then for c > 0 we necessarily have  $y_1 \ge \cdots \ge y_r$ , while for c < 0 we necessarily have  $y_1 \le \cdots \le y_r$ . Indeed, the only term in F which is dependent on the relative order of the entries is the term  $\sum_{i=1}^r x_i y_i$ , which is indeed maximised when the orders are the same and minimised if they are reversed.

We next consider another two-block model but where the interaction "between" the blocks uses the operator Q defined in (2). We let

$$H_n^{\rm WB} = -\frac{1}{n} \Big( a \sum_{1 \le i < j \le m} T_{i,j} + b \sum_{m+1 \le i < j \le n} T_{i,j} + c \sum_{1 \le i \le m < j \le n} Q_{i,j} \Big).$$
(14)

The Hamiltonian  $H_n^{\text{WB}}$  satisfies a modified version of the  $\operatorname{GL}_r(\mathbb{C})$ -symmetry (8). To see this, one first checks that  $Q_{i,j}$  commutes with any matrix of the form  $U_i(U_j^{-1})^{\intercal}$ , where  $U \in \operatorname{GL}_r(\mathbb{C})$  and the superscript  $^{\intercal}$  denotes transpose. Using also (7), it follows that

$$\left(\prod_{i=1}^{m} U_{i} \prod_{j=m+1}^{n} (U_{j}^{-1})^{\mathsf{T}}\right) H_{n}^{\mathsf{WB}} \left(\prod_{i=1}^{m} U_{i}^{-1} \prod_{j=m+1}^{n} U_{j}^{\mathsf{T}}\right) = H_{n}^{\mathsf{WB}}.$$
 (15)

In particular, if  $U = (U^{-1})^{\intercal}$  we have the  $O_r(\mathbb{C})$ -symmetry

$$\left(\prod_{i=1}^{n} U_{i}\right) H_{n}^{\mathrm{WB}}\left(\prod_{i=1}^{n} U_{i}^{-1}\right) = H_{n}^{\mathrm{WB}}, \qquad U \in \mathcal{O}_{r}(\mathbb{C}).$$

$$(16)$$

Also let  $Z_n^{\text{WB}}(\beta) = \text{tr}[e^{-\beta H_n^{\text{WB}}}]$ . Let us note here that for all  $r \ge 2$ , this model is unitarily equivalent to the same model with each  $Q_{i,j}$  replaced with  $P_{i,j}$ , the latter being (r times) the projection onto the singlet state:

$$\langle e_{\alpha_1} \otimes e_{\alpha_2} | P_{i,j} | e_{\alpha_3} \otimes e_{\alpha_4} \rangle = (-1)^{\alpha_1 - \alpha_3} \delta_{\alpha_1, -\alpha_2} \delta_{\alpha_3, -\alpha_4}.$$
(17)

(Here we index the basis  $e_{\alpha}$  for  $\mathbb{C}^r$  with  $\alpha \in \{-S, -S+1, \ldots, S\}$  where S = (r-1)/2.) Indeed, for the model with a = b = 0 and c > 0 the equivalence of partition functions was proved by Aizenman and Nachtergaele in [2]; we give an algebraic proof for general  $a, b, c \in \mathbb{R}$  in Lemma B.1. We use the notation WB for this model as its analysis is based on the representation theory of the *walled Brauer algebra*, see Section 2.2. Interestingly, this model has the exact same free energy as the two-block interchange model:

**Theorem 1.2.** Let  $a, b, c \in \mathbb{R}$  be fixed. If  $n, m \to \infty$  such that  $m/n \to \rho \in (0, 1)$ , then the free energy of the model (14) satisfies

$$\Phi_{\beta}^{\rm WB}(a,b,c) := \lim_{n \to \infty} \frac{1}{n} \log Z_n^{\rm WB}(\beta) = \Phi_{\beta}^{\rm AB}(a,b,c), \tag{18}$$

where  $\Phi_{\beta}^{AB}(a, b, c)$  is given in Theorem 1.1.

In the case r = 2, Theorem 1.2 can be deduced from Theorem 1.1 in the following elementary manner. For r = 2 we have [34, Section 7.1]

$$T_{i,j} = 2(\mathbb{S}_i \cdot \mathbb{S}_j) + \frac{1}{2}, \qquad Q_{i,j} = 2(S_i^{(1)}S_j^{(1)} - S_i^{(2)}S_j^{(2)} + S_i^{(3)}S_j^{(3)}) + \frac{1}{2}.$$
(19)

Letting  $W = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$  we have that  $W_j^{-1}T_{i,j}W_j = -Q_{i,j} + 1$ , so conjugating  $H_n^{AB}(a, b, -c)$  with  $\prod_{j=m+1}^n W_j$  gives  $H_n^{\text{wB}}(a, b, c) - cm(n-m)/n$ . Thus  $\Phi_\beta^{\text{wB}}(a, b, c) = \Phi_\beta^{AB}(a, b, -c) + c\rho(1-\rho)$ . This is consistent with Theorem 1.2 since (indicating the dependence on c with a subscript)  $F_c(x_1, x_2; y_1, y_2) - F_{-c}(x_1, x_2; y_2, y_1) = c(x_1 + x_2)(y_1 + y_2) = c\rho(1-\rho)$ , meaning that by Theorem 1.1 we have  $\Phi_\beta^{AB}(a, b, -c) + c\rho(1-\rho) = \Phi_\beta^{AB}(a, b, c)$ . However, for general r the rank of  $T_{i,j}$  is r(r+1)/2 while the rank of  $Q_{i,j}$  is 1, so when r > 2, conjugating  $T_{i,j}$  cannot give a linear combination of  $Q_{i,j}$  and the identity.

#### 1.2. Phase transition and critical temperature

Next we discuss phase transitions as  $\beta$  is varied, via the maximiser of the function F. Essentially, when a transition is present, we expect the maximiser of F to be fixed (at the 'maximum entropy' point  $\omega_0$  (22)) for small  $\beta$ , and then at some critical  $\beta_c$  to begin to move. This  $\beta_c$  then corresponds to a point of phase transition in the model. For  $\beta = \beta_c$  it can happen either that  $\omega_0$  is unique or that there are other maximum points. We will see that the phase transition is also reflected in the behaviour of observables (Theorem 1.7) and the magnetisation (Theorem 1.8).

In Proposition 1.3, we characterise completely the values of a, b, c for which there exists such a phase transition. When it exists, finding explicit formulae for  $\beta_c$  seems difficult in general; we can do it in two cases, firstly in Proposition 1.4 when r = 2 (that is, spin  $\frac{1}{2}$ ), and secondly in Proposition 1.5 when  $c \ge 0$ ,  $r \ge 3$  and

$$(a-c)\rho = (b-c)(1-\rho) =: t.$$
 (20)

In the latter case, we further prove in Proposition 1.6 that for  $\beta_{\rm c} < \beta < \beta_{\rm c} + \varepsilon$  and  $\varepsilon > 0$  small, there is a unique maximiser of F that satisfies (13).

In what follows, we write  $\vec{x} = (x_1, \ldots, x_r), \ \vec{y} = (y_1, \ldots, y_r)$ , and

$$\Omega = \left\{ (\vec{x}; \vec{y}) : x_1, \dots, x_r, y_1, \dots, y_r \ge 0, \ \sum_{i=1}^r x_i = 1 - \sum_{i=1}^r y_i = \rho \right\}.$$
 (21)

Elements of  $\Omega$  will typically be denoted  $\omega = (\vec{x}; \vec{y})$ . We write

$$\omega_0 = \left(\frac{\rho}{r}, \frac{\rho}{r}, \dots, \frac{\rho}{r}; \frac{1-\rho}{r}, \frac{1-\rho}{r}, \dots, \frac{1-\rho}{r}\right) \in \partial\Omega,$$
(22)

and we write  $Q(x,y) = \frac{1}{2}(ax^2 + by^2 + 2cxy)$  for the quadratic form appearing in the function f(x,y).

**Proposition 1.3.** If Q is negative semidefinite, that is, if

$$a \le 0, \quad b \le 0, \quad and \quad ab \ge c^2,$$

$$(23)$$

then F assumes its maximum value at  $\omega_0$  for all  $\beta > 0$ , and this maximum point is unique. Otherwise, there exists a number  $\beta_c > 0$  such that F assumes it maximum value at  $\omega_0$  if and only if  $0 < \beta \leq \beta_c$ , and this maximum is unique if  $0 < \beta < \beta_c$ .

Let us write  $\beta_{\rm c}(r)$  to highlight the dependence on r. The next proposition gives  $\beta_{\rm c}(2)$  when it exists. For a simple interpretation of the value, see Lemma 3.2.

**Proposition 1.4.** Let r = 2 and assume that Q is not negative semidefinite, so that  $\beta_c(2)$  exists. Then

$$\beta_{c}(2) = \begin{cases} \frac{\rho a + (1-\rho)b - \sqrt{(\rho a - (1-\rho)b)^{2} + 4\rho(1-\rho)c^{2}}}{\rho(1-\rho)(ab-c^{2})}, & ab \neq c^{2}, \\ \frac{2}{a\rho + b(1-\rho)}, & ab = c^{2}. \end{cases}$$
(24)

Moreover, for  $\beta = \beta_c$ ,  $\omega_0$  is the unique maximum point.

In the homogeneous spin- $\frac{1}{2}$  AB-model, i.e. r = 2 and a = b = c = 1, we recover the critical point  $\beta_c = 2$  first identified by Tóth [32] and by Penrose [27]. In the bipartite case a = b = 0 we get the critical value  $\beta_c = 2/\sqrt{c^2\rho(1-\rho)}$ ; this has, to the best of our knowledge, not appeared previously in the literature.

The next proposition gives  $\beta_{\rm c}(r)$ ,  $r \ge 3$  in the special case that  $c \ge 0$  and (20) holds.

**Proposition 1.5.** Suppose that  $c \ge 0$ ,  $r \ge 3$ , that (20) holds and that Q is not negative semidefinite so that  $\beta_c$  exists. Then

$$\beta_{\rm c} = \beta_{\rm c}(r) = \frac{2(r-1)\log(r-1)}{(r-2)(c+t)}.$$
(25)

Moreover, if  $\beta = \beta_c$  there are exactly two maximum points satisfying (13), namely  $\omega_0$  of (22) and  $\omega_1 = (\vec{x}; \vec{y})$  given by

$$x_1 = \frac{(r-1)\rho}{r}, \quad x_2 = \dots = x_r = \frac{\rho}{r(r-1)},$$
 (26a)

$$y_1 = \frac{(r-1)(1-\rho)}{r}, \quad y_2 = \dots = y_r = \frac{1-\rho}{r(r-1)}.$$
 (26b)

For  $\beta > \beta_c$  and under the conditions in Proposition 1.5 we can prove that the maximum point is unique (subject to (13)) for  $\beta$  close to the critical point (see also Proposition 3.5 for another special case).

**Proposition 1.6.** Under the assumptions of Proposition 1.5, there exists  $\varepsilon > 0$  such that, if  $\beta_{\rm c} < \beta < \beta_{\rm c} + \varepsilon$ , there is a unique maximiser of F in  $\Omega$  with entries ordered as in (13). Moreover as  $\beta \searrow \beta_{\rm c}$ , this maximiser tends to  $\omega_1$  given in (26).

The fact that the maximiser jumps from  $\omega_0$  to  $\omega_1$  as one crosses the critical point suggests that this is a point of 'first order' phase transition. This will be confirmed below (see the discussion following Theorem 1.8) by showing that the magnetisation is discontinuous at this point. By contrast, in the setting of Proposition 1.4, the maximiser moves continuously away from  $\omega_0$ , indicating a second (or possibly higher) order phase transition.

#### 1.3. Correlations and magnetisation

We next move on to results about correlations which extend [9, Theorem 2.3]. To state them, introduce the function

$$R(w_1, \dots, w_r; z_1, \dots, z_r) = \det \left[ e^{w_i z_j} \right]_{i,j=1}^r \prod_{1 \le i < j \le r} \frac{j-i}{(w_i - w_j)(z_i - z_j)}.$$
 (27)

For  $\# \in \{AB, WB\}$ , we write

$$\langle \mathcal{O} \rangle_{\beta,n}^{\#} = \frac{\operatorname{tr}_{\mathbb{V}} \left[ \mathcal{O} e^{-\beta H_n^{\#}} \right]}{Z_n^{\#}(\beta)} \tag{28}$$

for the usual equilibrium state expectation of a linear operator  $\mathcal{O}$  on  $\mathbb{V}$ .

**Theorem 1.7.** Let  $a, b, c \in \mathbb{R}$  and  $\beta > 0$  be such that F has a unique maximum point  $\omega^* = (\vec{x}^*; \vec{y}^*)$  satisfying (13). Let W be an  $r \times r$  matrix with eigenvalues  $w_1, \ldots, w_r \in \mathbb{C}$ . As  $n, m \to \infty$  such that  $m/n \to \rho \in (0, 1)$ , we have that

$$\lim_{n \to \infty} \left\langle \exp\left\{\frac{1}{n} \sum_{i=1}^{n} W_i\right\} \right\rangle_{\beta,n}^{\text{AB}} = R(w_1, \dots, w_r; z_1^\star, \dots, z_r^\star),$$

$$\lim_{n \to \infty} \left\langle \exp\left\{\frac{1}{n} \left(\sum_{i=1}^{m} W_i - \sum_{i=m+1}^{n} W_i^\intercal\right)\right\} \right\rangle_{\beta,n}^{\text{WB}} = R(w_1, \dots, w_r; z_1^\dagger, \dots, z_r^\dagger),$$
(29)

where the superscript <sup>T</sup> denotes transpose, and

$$z_{j}^{\star} = x_{j}^{\star} + y_{j}^{\star}, \qquad z_{j}^{\dagger} = x_{j}^{\star} - y_{j}^{\star}.$$
 (30)

It may be instructive to give a direct explanation of the fact that (29) only depends on the spectrum of W. Consider the case of the WB-model. Let  $U \in \operatorname{GL}_r(\mathbb{C})$  and replace the matrix W by  $UWU^{-1}$ ,  $U \in \operatorname{GL}_r(\mathbb{C})$ . Then the operator

$$\mathcal{O} = \exp\left\{\frac{1}{n}\left(\sum_{i=1}^{m} W_i - \sum_{i=m+1}^{n} W_i^{\mathsf{T}}\right)\right\}$$

is replaced by  $\mathcal{UOU}^{-1}$ , where

$$\mathcal{U} = \prod_{i=1}^m U_i \prod_{i=m+1}^n (U_i^{-1})^{\mathsf{T}}.$$

As we saw in (15),  $\mathcal{U}$  commutes with  $H_n^{\text{WB}}$  and can hence be cancelled from  $\operatorname{tr}(\mathcal{UOU}^{-1}e^{-\beta H_n^{\text{WB}}})$ . This shows that  $\langle \mathcal{O} \rangle_{\beta,n}^{\text{WB}}$  only depends on the spectrum of W in the case that W is diagonalizable. The condition of diagonalizability can be removed by a continuity argument. The case of the AB-model is similar, using (8).

As a concrete example, for  $W = h \operatorname{diag}(0, 1, 2, \dots, r-1)$  we have

$$R(w_1, \dots, w_r; z_1, \dots, z_r) = \prod_{1 \le i < j \le r} \frac{e^{hz_i} - e^{hz_j}}{h(z_i - z_j)}.$$
(31)

The phase transition at  $\beta_c$  is reflected in the fact that  $R \equiv 1$  when  $\omega^* = (\vec{x}^*; \vec{y}^*) = \omega_0$ , while R is non-trivial if the entries of  $\vec{z}$  are non-constant. The latter occurs e.g. in the AB-model for  $\beta > \beta_c$ .

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For a second concrete example, let c > 0. We will prove in Proposition 3.5 that any maximiser  $(\vec{x}^*; \vec{y}^*)$  of F satisfying (13) is then of the form

$$x_1^* \ge x_2^* = \dots = x_r^*, \qquad y_1^* \ge y_2^* = \dots = y_r^*,$$
(32)

in which case  $z^*$  (30) will be of the same form. Letting W be an arbitrary rank 1 projection, with eigenvalues  $1, 0, \ldots, 0$ , and writing  $u^* = z_1^* - z_2^*$ , we have

$$\lim_{n \to \infty} \left\langle \exp\left\{\frac{1}{n} \sum_{i=1}^{n} W_i\right\} \right\rangle_{\beta,n}^{AB} = \frac{(2S)!}{(hu^*)^{2S}} e^{\frac{h}{2S+1}(1-u^*)} \sum_{j=2S}^{\infty} \frac{(hu^*)^j}{j!}.$$
 (33)

(The calculation of R is performed in [9, Section 6].)

Theorem 1.7 also shows that the AB- and WB-models are not equivalent, despite having the same free energy (for any anti-symmetric matrix W, the observables on the left in (29) are the same, while their limiting expectations are different). The result is also relevant for understanding extremal states, specifically non-triviality of R indicates phase-coexistence, see Section 1.5 for heuristics.

Finally we have the following result about the (thermodynamic) magnetisation. Let W be an  $r \times r$  matrix with real eigenvalues  $w_1 \geq \cdots \geq w_r$ , let  $h \in \mathbb{R}$ , and write

$$Z_n^{AB}(\beta, h) = \operatorname{tr}_{\mathbb{V}}[\exp\left(-\beta H_n^{AB} + h \sum_{1 \le i \le n} W_i\right)], \tag{34}$$

$$Z_n^{\text{WB}}(\beta, h) = \text{tr}_{\mathbb{V}}[\exp\left(-\beta H_n^{\text{WB}} + h\left(\sum_{1 \le i \le m} W_i - \sum_{m < i \le n} W_i^{\mathsf{T}}\right)\right)].$$
(35)

In Theorem 2.4 we will obtain explicit expressions for the limits

$$\Phi^{\#}(\beta,h) := \lim_{n \to \infty} \frac{1}{n} \log Z_n^{\#}(\beta,h), \tag{36}$$

where  $\# \in \{AB, WB\}$  (as for (29), this depends on W only through its spectrum  $\vec{w}$ ). The magnetisation is given by the left and right derivatives of this free energy with respect to h, at h = 0.

**Theorem 1.8.** Let  $\Phi$  be defined by (36), either for the AB- or WB-model. Then

$$\frac{\partial \Phi}{\partial h}\Big|_{h\downarrow 0} = \max_{(\vec{x}^\star; \vec{y}^\star)} \sum_{i=1}^r z_i w_i, \qquad \frac{\partial \Phi}{\partial h}\Big|_{h\uparrow 0} = \min_{(\vec{x}^\star; \vec{y}^\star)} \sum_{i=1}^r z_i w_{r+1-i}, \tag{37}$$

where the maxima and minima are over all maximisers  $(\vec{x}^*; \vec{y}^*) \in \Omega$  of  $F(\vec{x}; \vec{y})$  such that  $x_1^* \geq \cdots \geq x_r^*$ . The vector  $\vec{z}$  is obtained by rearranging the entries in the vector  $x^* \pm y^*$  in decreasing order, where one should take the plus sign for the AB-model and the minus sign for the WB-model.

It is natural to take W to have trace zero. Then, from Proposition 1.3, for all  $\beta < \beta_c$  the only maximiser is  $\omega_0$  (22) and we have

$$\frac{\partial \Phi}{\partial h}\Big|_{h\downarrow 0} = \frac{\partial \Phi}{\partial h}\Big|_{h\uparrow 0} = 0, \tag{38}$$

for both AB- and WB-models and for both c > 0 and c < 0. This holds also for  $\beta = \beta_c$ when r = 2.

Let us discuss the case  $r \ge 3$  in Proposition 1.5 at  $\beta = \beta_c$ . Recall that  $c \ge 0$  in this case. Calculations with the point  $\omega_1$  (26) give the following:

• In the AB-case, at  $\omega_1$  the values

$$z_1 = \frac{r-1}{r}, \quad z_2 = \dots = z_r = \frac{1}{r(r-1)}$$
 (39)

are already decreasing. Still assuming that W has trace zero, it follows that

$$\frac{\partial \Phi^{\rm AB}}{\partial h}\Big|_{h\downarrow 0} = \frac{r-2}{r-1}w_1, \qquad \frac{\partial \Phi^{\rm AB}}{\partial h}\Big|_{h\uparrow 0} = \frac{r-2}{r-1}w_r. \tag{40}$$

For W with non-zero eigenvalues we have  $w_1 > 0 > w_r$ , thus the magnetisation is discontinuous at the point of phase transition.

• In the WB-case, at  $\omega_1$  the ordering of the values  $x_i - y_i$  depends on  $\rho$ . If  $\rho > \frac{1}{2}$  we get

$$z_1 = (2\rho - 1)\frac{r-1}{r}, \quad z_2 = \dots = z_r = \frac{2\rho - 1}{r(r-1)},$$
 (41)

and from there

$$\frac{\partial \Phi^{\text{WB}}}{\partial h}\Big|_{h\downarrow 0} = (2\rho - 1)\frac{r-2}{r-1}w_1$$

$$\frac{\partial \Phi^{\text{WB}}}{\partial h}\Big|_{h\uparrow 0} = (2\rho - 1)\frac{r-2}{r-1}w_r.$$
(42)

For W with non-zero eigenvalues, this gives a discontinuous magnetisation. In the case  $\rho < \frac{1}{2}$ , the magnetisation is obtained by exchanging  $w_1$  and  $w_r$  in (42). For  $\rho = \frac{1}{2}$ , the magnetisation is continuous at the point of phase transition.

#### 1.4. Ground-state phase diagrams

Recall from (9) that when  $\beta$  is large, the free energy is dominated by the lowest energies E of the Hamiltonian. The eigenspace of the lowest eigenvalue is referred to as the ground state of the model. For finite n, as  $\beta \to \infty$  the Gibbs factor  $\frac{1}{Z_n^{\#}(\beta)}e^{-\beta H_n^{\#}}$  converges to the orthogonal projection onto the ground state. Most relevant is to characterise the ground state in the limit  $n \to \infty$ . Here we instead consider the limits in the other order, that is  $n \to \infty$  first followed by  $\beta \to \infty$ . While we do not provide full details, it is clear from our finite-n expressions (63), (65) and (87) that the limits may be swapped.

Thus, by analysing the location of the maximiser of the function F (given in (10)) in the limit as  $\beta \to \infty$ , we can identify the ground-state phase diagram. We provide

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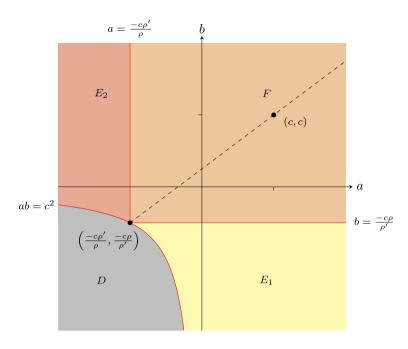


Fig. 1. The ground state phase diagram for c > 0. The dashed line indicates where we have a closed formula for the critical temperature.

two diagrams, one of the (a, b) plane for c > 0 fixed and one for c < 0 fixed. Since the diagram is invariant under the scaling  $(a, b, c) \rightarrow (\alpha a, \alpha b, \alpha c)$  with  $\alpha > 0$ , this will suffice to describe the whole diagram for  $c \neq 0$ . The case c = 0 is just two uncoupled models on complete graphs with  $T_{i,j}$  transposition interaction; this is covered by the results of [8].

The c > 0 diagram is portrayed in Fig. 1. It displays four distinct regions, separated by the curve  $ab = c^2$  (a, b < 0) and the lines  $a = -c\rho'/\rho$  and  $b = -c\rho/\rho'$ . The dashed line  $(a - c)\rho = (b - c)(1 - \rho)$  is where we have a precise formula for the critical temperature, see Proposition 1.5. The upper right region F is called *ferromagnetic*; the *c*-interaction between the two blocks is ferromagnetic and the *a*- and *b*-interactions are either ferromagnetic, or not strong enough to make a difference. In this region, we obtain from Theorem 1.8 that the magnetisation is maximal. In finite volume *n*, as *n* gets large, the ground state includes the product states  $\bigotimes_{i=1}^{n} v, v \in \mathbb{C}^r$  (think of every spin aligned in the same direction).

The lower left region D we call *disordered*; it coincides with the range of parameters for which there is no phase transition at finite temperature, by Proposition 1.3. Here the a- or b-interactions overcome the c-interactions, and the model behaves like two copies of the antiferromagnet on the complete graph, which has no phase transition [8] (spins at neighbouring sites want to be anti-aligned, but this is made impossible (frustrated) by the complete graph being non-bipartite). The magnetisation in this case is 0.

There are also two intermediate regions denoted  $E_1$  and  $E_2$ . Here, at least one of the *a*- or *b*-interactions is antiferromagnetic, and the model begins to feel this effect. In

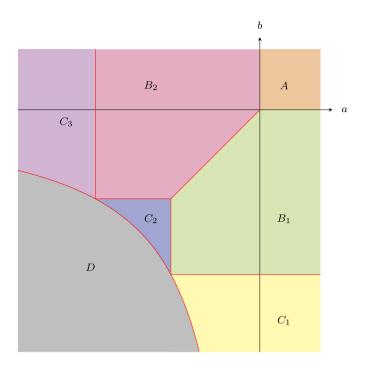


Fig. 2. The ground state phase diagram for c < 0, in the case r = 3.

these regions the magnetisation interpolates between 0 and its maximal value. As |a|+|b| becomes large, we approach the c = 0 limit of a ferromagnet on one subgraph and an antiferromagnet on the other.

When c < 0 and r = 2 the phase diagram looks identical to the case when c > 0, but we refer to the upper-right region as *antiferromagnetic*. As  $r \ge 3$ , the diagram looks more complicated, with 2r - 1 intermediate regions between the antiferromagnetic and disordered regions. This is illustrated in Fig. 2 (for r = 3) and 8 (for r = 5), and described in detail in Proposition 4.2.

We can give a tentative interpretation of the diagram when r = 3, c < 0. Here, the *c*-interaction is  $-(\mathbb{S}_i \cdot \mathbb{S}_j)^2$  in the WB model, so spins in one block want to be orthogonal to those in the other, and is  $-[(\mathbb{S}_i \cdot \mathbb{S}_j) + (\mathbb{S}_i \cdot \mathbb{S}_j)^2]$  in the AB model, so spins in one block want to be at 120° to those in the other. The *a* and *b* interactions are both  $(\mathbb{S}_i \cdot \mathbb{S}_j) + (\mathbb{S}_i \cdot \mathbb{S}_j)^2$ , so spins want to be aligned.

One might interpret the diagram as follows. The region A is truly "anti"-ferromagnetic, in the sense that spins in A are all aligned, and spins in B are all aligned, in some direction orthogonal/at 120° to those in A. We write "anti" in quotation marks since the angle between the spins is not 180°. There are two regions  $B_1, B_2$ , and three  $C_1, C_2, C_3$ . In the  $B_1$  region, the spins in A are aligned, and the spins in B are disordered, but lie on the circle which is orthogonal/at 120° to the spins in A; and vice-versa for  $B_2$ . As we decrease b into the region  $C_1$ , the spins in B become more and more disordered, until they are completely decoupled from those in A, which remain aligned. Similar for the  $C_3$  region. It is difficult to interpret the most interesting region,  $C_2$ , in this way; there is some disorder in the spins in each block, but enough *c*-interaction to prevent them from completely decoupling.

#### 1.5. Heuristics for extremal Gibbs states

By adding small perturbations to the Hamiltonian (which are sent to 0 after sending  $n \to \infty$ ), the thermal expectations (28) give rise to different so-called *Gibbs states* for the model. The set of Gibbs states is a convex set, whose extreme points represent physically 'stable' states. Typically, the set of Gibbs states is a singleton for  $\beta < \beta_c$  but non-trivial for  $\beta > \beta_c$ . In the latter case it is of interest to identify and interpret the set of extremal Gibbs states. In the setting of classical spin systems, the theory of Gibbs states is accessibly described in [16, Chapter 6]. The quantum setting parallels the classical one, for details of the general theory we recommend [22] while for the case of the complete graph details may be found in [15].

In [9], for several models including the interchange model (3), the authors give a heuristic argument which points towards the structure of the set of extremal Gibbs states at inverse temperature  $\beta$ . The description given there is expected to hold in  $\mathbb{Z}^d$  for d large enough, with  $d \geq 3$  perhaps being enough. Specifically, it is expected that for  $r \times r$  matrices W,

$$\lim_{n \to \infty} \langle e^{\frac{h}{n} \sum_{i} W_{i}} \rangle_{\beta,n} = \lim_{\Lambda \to \mathbb{Z}^{d}} \langle e^{\frac{h}{|\Lambda|} \sum_{i} W_{i}} \rangle_{\beta,\Lambda}, \tag{43}$$

where the left hand side is the limit on complete graphs of size n, while the right hand side is the limit of successively larger subsets  $\Lambda \subseteq \mathbb{Z}^d$  (covering  $\mathbb{Z}^d$  in the sense of van Hove [16, Section 3.2.1]). Apart from (43), the heuristics in [9] rest on the expected equality

$$\lim_{\Lambda \to \mathbb{Z}^d} \langle e^{\frac{h}{|\Lambda|} \sum_i W_i} \rangle_{\beta,\Lambda} = \int_{\Psi_\beta} e^{h \langle W_0 \rangle_{\psi}} d\mu(\psi), \tag{44}$$

where  $\langle \cdot \rangle_{\psi}$  is the extremal Gibbs state indexed by  $\psi \in \Psi_{\beta}$ ,  $d\mu$  is the measure on the index set  $\Psi_{\beta}$  corresponding to the symmetric Gibbs state, and  $W_0$  is the operator W at the lattice site 0. The left hand side of (43) is computed rigorously, and then, with the expected structure of  $\Psi_{\beta}$  inserted, the right hand side of (44) is also computed, and the two are shown to be the same. This working is not a proof either of the expected equalities (43), (44) or of the expected structure of  $\Psi_{\beta}$ , but it gives a consistency check for the three statements.

Using the results of the present paper, we can provide the same calculations and heuristics for the AB- and WB-models. Both models have symmetry under  $U(r) \subseteq GL(r)$ , the group of unitary  $r \times r$  matrices, see (8) and (15), and for c > 0, both models are expected to have extremal Gibbs states labelled by  $\mathbb{CP}^{r-1}$ , i.e. rank 1 projections in  $\mathbb{C}^r$ . This means that the expected identities (44) and (43) take the form

$$\lim_{n \to \infty} \left\langle e^{\frac{1}{n} \sum_{i=1}^{n} W_i} \right\rangle_{\beta, n}^{\text{AB}} = \int_{\mathbb{C}\mathbb{P}^{r-1}} e^{\rho \langle W_1 \rangle_{\psi}^{\text{AB}} + (1-\rho) \langle W_2 \rangle_{\psi}^{\text{AB}}} d\mu(\psi)$$
(45)

and

$$\lim_{n \to \infty} \left\langle e^{\frac{1}{n} \left(\sum_{i \in A} W_i - \sum_{j \in B} W_j^{\mathsf{T}}\right)} \right\rangle_{\beta, n}^{\mathsf{WB}} = \int_{\mathbb{C}\mathbb{P}^{r-1}} e^{\rho \langle W_1 \rangle_{\psi}^{\mathsf{WB}} - (1-\rho) \langle W_2^{\mathsf{T}} \rangle_{\psi}^{\mathsf{WB}}} d\mu(\psi), \tag{46}$$

where  $W_1$  and  $W_2$  represent W acting on arbitrary sites in the A- and B-parts of the graph. Using the U(r)-invariance and the Harish-Chandra–Itzykson–Zuber formula as in [9], this leads to the predictions

$$\lim_{n \to \infty} \left\langle e^{\frac{1}{n} \sum_{i=1}^{n} W_i} \right\rangle_{\beta, n}^{\text{AB}} = R(w_1, \dots, w_r; x_1 + y_1, \dots, x_r + y_r)$$
(47)

and

$$\lim_{n \to \infty} \left\langle e^{\frac{1}{n} \left( \sum_{i \in A} W_i - \sum_{j \in B} W_j^{\mathsf{T}} \right)} \right\rangle_{\beta, n}^{\mathsf{WB}} = R(w_1, \dots, w_r; x_1 - y_1, \dots, x_r - y_r),$$
(48)

where  $x_i = \langle P_1^{e_i} \rangle_{e_1}$  and  $y_i = \langle P_2^{e_i} \rangle_{e_1}$  are the expectations of the projections  $P^{e_i}$  onto the subspace spanned by the *i*-th coordinate vector  $e_i = (0, \ldots, 0, 1, 0, \ldots, 0)$  under the extremal state associated with  $\psi = e_1$ . By U(r)-invariance, we expect  $x_2 = x_3 = \cdots = x_r$ and  $y_2 = y_3 = \cdots = y_r$ , and it is further natural to assume that  $x_1 \ge x_2$  and  $y_1 \ge y_2$ . Since this fits the picture given (rigorously) by Theorem 1.7 and Proposition 3.5, we are motivated to lend some credence to the stated heuristics.

We now turn to the case of the complete bipartite graph, given by a = b = 0. By our comments below (14), the WB-model with a = b = 0, c = 1, has Hamiltonian unitarily equivalent to

$$-\frac{1}{n}\sum_{1\le i\le m< j\le n}P_{i,j},\tag{49}$$

where  $P_{i,j}$  is (r times) the projection onto the singlet state, given by (17). For spin S = 1 (r = 3) we can interpret our results and heuristics to comment on the bilinear-biquadratic model, which has Hamiltonian

$$-\frac{1}{n}\sum_{1\le i\le m< j\le n} \left( J_1(\mathbb{S}_i\cdot\mathbb{S}_j) + J_2(\mathbb{S}_i\cdot\mathbb{S}_j)^2 \right),\tag{50}$$

where  $\mathbb{S}_i \cdot \mathbb{S}_j = \sum_{k=1}^3 S_i^{(k)} S_j^{(k)}$ , and  $J_1, J_2 \in \mathbb{R}$ . Indeed, using the relations  $\mathbb{S}_i \cdot \mathbb{S}_j = T_{i,j} - P_{i,j}$  and  $(\mathbb{S}_i \cdot \mathbb{S}_j)^2 = P_{i,j} + 1$  (see Lemma 7.1 from [34]) one can rewrite (50), up to addition of a constant, as

$$-\frac{1}{n} \sum_{1 \le i \le m < j \le n} \left( J_1 T_{i,j} + (J_2 - J_1) P_{i,j} \right).$$
(51)

For our analysis to apply, we need one of the coefficients to vanish, i.e. either  $J_1 = 0$  or  $J_1 = J_2$ . Setting  $J_1 = J_2 = \pm 1$  gives the AB model with a = b = 0,  $c = \pm 1$ , while setting  $J_1 = 0$ ,  $J_2 = \pm 1$  gives the WB model with a = b = 0,  $c = \pm 1$ , in the form (49). The case  $J_1 = 0$ ,  $J_2 = 1$  (i.e. our WB-model with a = b = 0, c = 1) is the biquadratic Heisenberg model. These two special cases are exactly those described by Ueltschi ([34], Section 7B) as having SU(3) invariance; in our language this is the GL(3)-invariance that we exploit in this paper. (Note that our method unfortunately does not allow us to treat the famous AKLT-model [31, Chapter 7], which is obtained for  $J_1 = -1$ ,  $J_2 = -\frac{1}{3}$ .)

The phase diagram of the bilinear-biquadratic Heisenberg model on  $\mathbb{Z}^d$ ,  $d \geq 3$ , is given in Ueltschi [34], and we expect that the model on the complete bipartite graph has the same diagram. (See also [35], but beware that some of the predictions using Gell-Mann matrices there are inaccurate. The corresponding one-dimensional spin chain has a different phase diagram, exhibiting dimerization, see [1,10].) The biquadratic model  $(J_1 = 0, J_2 = 1)$  lies on the boundary of the nematic phase of that diagram, but actually belongs to a Néel-ordered (or antiferromagnetic) phase for bipartite graphs. Heuristically, we expect the spins in the A-part to be anti-aligned with those in the B-part. Note that for this model if we add a magnetisation term in the  $S^{(k)}$  direction at every vertex (for any k = 1, 2, 3), then, at  $\beta = \beta_c$  and for  $\rho > \frac{1}{2}$ , Theorem 1.8 tells us that the magnetisation is

$$\frac{\partial \Phi^{\rm \tiny WB}}{\partial h}\Big|_{h\downarrow 0} = \rho - \frac{1}{2},\tag{52}$$

(indeed, see Lemma B.2) which agrees with the picture of anti-aligned spins in the two blocks.

#### Acknowledgments

JEB gratefully acknowledges financial support from Vetenskapsrådet, grants 2015-05195 and 2019-04185, from *Ruth och Nils Erik Stenbäcks stiftelse*, and from Sabbatical Program at the Faculty of Science, University of Gothenburg. HR gratefully acknowledges support from Vetenskapsrådet, grant 2020-04221. KR gratefully acknowledges support from the EPSRC Studentship 1936327, and from the FWF stand-alone grant P 34713. KR would like to thank Sasha Sodin for many useful discussions. JEB and KR are grateful for hospitality at the University of Warwick and for several enlightening discussions with Daniel Ueltschi. We all thank Martin Hallnäs for stimulating discussions at the start of the project and the two anonymous referees for very helpful comments.

#### 2. Free energy and correlations

In this section we prove Theorems 1.1, 1.2, 1.7 and 1.8.

#### 2.1. Interchange model: proof of Theorem 1.1

As noted in the introduction, our method is to identify the eigenspaces of the Hamiltonian (6). This is facilitated by the classical theory of Schur–Weyl duality. We start by recalling a few basic definitions and facts. A *partition*  $\lambda \vdash n$  of n is a non-increasing sequence of non-negative integers summing to  $n: \lambda = (\lambda_1, \lambda_2, ...)$  with  $\lambda_1 \geq \lambda_2 \geq \cdots \geq 0$  and  $\sum_{k>1} \lambda_k = n$ . Its *length*  $\ell(\lambda)$  is the number of non-zero entries.

For  $\sigma \in S_n$  a permutation of 1, 2, ..., n, let  $T_{\sigma}$  be the linear operator on  $\mathbb{V} = (\mathbb{C}^r)^{\otimes n}$ which permutes the tensor factors according to  $\sigma$ :

$$T_{\sigma}(v_1 \otimes v_2 \otimes \cdots \otimes v_n) = v_{\sigma^{-1}(1)} \otimes v_{\sigma^{-1}(2)} \otimes \cdots \otimes v_{\sigma^{-1}(n)}.$$
(53)

The mapping  $\sigma \mapsto T_{\sigma}$  is a representation of  $S_n$  and hence extends to a representation of the group algebra  $\mathbb{C}[S_n]$  on  $\mathbb{V}$ . We may also regard  $\mathbb{V}$  as a module for the group  $\operatorname{GL}_r(\mathbb{C})$ of invertible  $r \times r$  matrices by the diagonal action

$$g(v_1 \otimes v_2 \otimes \cdots \otimes v_n) = g(v_1) \otimes g(v_2) \otimes \cdots \otimes g(v_n).$$
(54)

Classical Schur–Weyl duality [14, Corollary 4.59] states that these actions of  $S_n$  and of  $\operatorname{GL}_r(\mathbb{C})$  are each other's centralisers, so that  $\mathbb{V}$  may be regarded as a representation of the direct product  $\operatorname{GL}_r(\mathbb{C}) \times S_n$ , and that  $\mathbb{V}$  decomposes as a multiplicity-free direct sum of irreducible representations of  $\operatorname{GL}_r(\mathbb{C}) \times S_n$ . Specifically,

$$\mathbb{V} = \bigoplus_{\lambda \vdash n, \, \ell(\lambda) \le r} U_{\lambda} \otimes V_{\lambda}.$$
(55)

Here  $U_{\lambda}$  is the irreducible  $\operatorname{GL}_r(\mathbb{C})$ -representation indexed by (its highest weight)  $\lambda$ , and  $V_{\lambda}$  is the irreducible  $S_n$ -representation (Specht module) indexed by  $\lambda$ . We use the same notation T for the representation of  $\operatorname{GL}_r(\mathbb{C}) \times S_n$  on  $\mathbb{V}$ .

Recall our Hamiltonian  $H_n^{AB}$  given in (6). We now write this as  $H_n^{AB} = T(h_n^{AB})$  where

$$h_n^{\rm AB} = -\frac{1}{n} [(a-c)\alpha_A + (b-c)\alpha_B + c\,\alpha_{AB}],\tag{56}$$

and where  $\alpha_A, \alpha_B, \alpha_{AB}$  are the following elements of  $\mathbb{C}[S_n]$ :

$$\alpha_A = \sum_{1 \le i < j \le m} (i,j), \quad \alpha_B = \sum_{m+1 \le i < j \le n} (i,j), \quad \alpha_{AB} = \sum_{1 \le i < j \le n} (i,j). \tag{57}$$

We have that  $e^{-\beta H_n^{A^{\mathsf{B}}}} = T(e^{-\beta h_n^{A^{\mathsf{B}}}})$ . Now let W be an  $r \times r$  matrix over  $\mathbb{C}$ . Then  $e^W \in \operatorname{GL}_r(\mathbb{C})$  and we have that  $T(e^W) = \exp\left(\sum_{i=1}^n W_i\right)$ . Thus we may write

$$\exp\left(\sum_{i=1}^{n} W_i\right) e^{-\beta H_n^{\text{AB}}} = T\left(e^W e^{-\beta h_n^{\text{AB}}}\right),\tag{58}$$

where  $e^{W}e^{-\beta h_n^{AB}} \in \mathbb{C}[\operatorname{GL}_r(\mathbb{C}) \times S_n].$ 

Let us now consider how  $e^W \times e^{-\beta h_n^{AB}}$  acts on the right-hand-side of (55), starting with how  $e^{-\beta h_n^{AB}}$  acts on  $V_{\lambda}$ . The term  $\alpha_{AB}$  is the sum of all elements of a conjugacy class (the transpositions), hence it belongs to the centre of  $\mathbb{C}[S_n]$ . By Schur's Lemma, it therefore acts as a constant multiple of the identity on  $V_{\lambda}$ . The constant in question is well known [19, p. 52] to equal the *content* of the partition  $\lambda$ , defined by

$$\operatorname{ct}(\lambda) = \sum_{j \ge 1} \left( \frac{\lambda_j (\lambda_j + 1)}{2} - j \lambda_j \right).$$
(59)

(This equals the sum of the contents of all boxes in the Young diagram of  $\lambda$ , where the content of a box in position (x, y) is y - x.) We have

$$\alpha_{AB}|_{V_{\lambda}} = \operatorname{ct}(\lambda)\operatorname{Id}_{V_{\lambda}}.$$
(60)

Now, to deal with the remaining two terms  $\alpha_A$  and  $\alpha_B$ , note that as a representation of  $S_m \times S_{n-m}$ , the module  $V_{\lambda}$  splits as

$$V_{\lambda} = \bigoplus_{\mu \vdash m, \, \nu \vdash n-m} c_{\mu,\nu}^{\lambda} V_{\mu} \otimes V_{\nu}, \tag{61}$$

where  $c_{\mu,\nu}^{\lambda}$  are non-negative integers known as the *Littlewood–Richardson coefficients*. We give more details about these numbers later, for now we just note that  $c_{\mu,\nu}^{\lambda} \neq 0$  only if  $\ell(\mu), \ell(\nu) \leq \ell(\lambda)$ . On each term of the sum in (61),  $\alpha_A$  acts as  $\operatorname{ct}(\mu) \operatorname{Id}_{V_{\mu}}$  and  $\alpha_B$  acts as  $\operatorname{ct}(\nu) \operatorname{Id}_{V_{\nu}}$ , consequently  $h_n^{AB}$  acts on that term as

$$-\frac{1}{n}[(a-c)\operatorname{ct}(\mu) + (b-c)\operatorname{ct}(\nu) + c\operatorname{ct}(\lambda)]\operatorname{Id}_{V_{\mu}\otimes V_{\nu}},\tag{62}$$

and therefore  $e^{-\beta h_n^{\scriptscriptstyle AB}}$  acts as

$$\exp\left(\frac{\beta}{n}[(a-c)\operatorname{ct}(\mu)+(b-c)\operatorname{ct}(\nu)+c\operatorname{ct}(\lambda)]\right)\operatorname{Id}_{V_{\mu}\otimes V_{\nu}}.$$
(63)

As to the factor  $e^W$ , we first note that the character of the module  $U_{\lambda}$  evaluated at  $g \in \operatorname{GL}_r(\mathbb{C})$  with eigenvalues  $x_1, \ldots, x_r$  is the Schur polynomial:

$$\chi_{U_{\lambda}}[g] = s_{\lambda}(x_1, \dots, x_r) = \frac{\det[x_i^{\lambda_j + r - j}]_{i,j=1}^r}{\prod_{1 \le i < j \le r} (x_i - x_j)}.$$
(64)

If W has eigenvalues  $w_1, \ldots, w_r$ , then  $e^W$  has eigenvalues  $e^{w_1}, \ldots, e^{w_r}$ . Writing  $d_{\mu}, d_{\nu}$  for the dimensions of  $V_{\mu}, V_{\nu}$ , we may summarise these findings as follows:

**Lemma 2.1.** Suppose that W has eigenvalues  $w_1, \ldots, w_r$ . Then

$$\operatorname{tr}_{\mathbb{V}}[\exp\left(\sum_{i=1}^{n} W_{i}\right)e^{-\beta H_{n}^{AB}}] = \sum_{\lambda,\mu,\nu} s_{\lambda}(e^{w_{1}},\ldots,e^{w_{r}})c_{\mu,\nu}^{\lambda}d_{\mu}d_{\nu}$$

$$\cdot \exp\left(\frac{\beta}{n}[(a-c)\operatorname{ct}(\mu) + (b-c)\operatorname{ct}(\nu) + c\cdot\operatorname{ct}(\lambda)]\right),$$
(65)

where the sum is over  $\lambda \vdash n$  with  $\ell(\lambda) \leq r$ ,  $\mu \vdash m$ , and  $\nu \vdash n - m$ . In particular, setting W to be the zero matrix (so that  $e^W = Id$ ),

$$Z_{\beta,n}^{AB} = \sum_{\lambda,\mu,\nu} s_{\lambda}(1,\dots,1) c_{\mu,\nu}^{\lambda} d_{\mu} d_{\nu} \exp\left(\frac{\beta}{n} [(a-c)\operatorname{ct}(\mu) + (b-c)\operatorname{ct}(\nu) + c \cdot \operatorname{ct}(\lambda)]\right).$$
(66)

We will use that

$$s_{\lambda}(1,\ldots,1) = \dim(U_{\lambda}) = \prod_{1 \le i < j \le r} \frac{\lambda_i - i - \lambda_j + j}{j - i}.$$
(67)

As to  $d_{\mu}$ , a convenient formula is

$$d_{\mu} = \dim(V_{\mu}) = \frac{n!}{m_1! \cdots m_r!} \prod_{1 \le i < j \le r} (m_i - m_j)$$
(68)

where  $m_i = \mu_i + r - i$ , see [19, (4.11)].

In Lemma 2.1 we have written the partition function as a sum of terms exponentially large in n, with relatively few summands. Such a sum is dominated by its largest term. To prove Theorem 1.1 we need to understand the asymptotic behaviour of each of the factors in (66), and since only terms with  $c_{\mu,\nu}^{\lambda} \neq 0$  appear in the sum, we need a condition for  $c_{\mu,\nu}^{\lambda} \neq 0$ .

**Proof of Theorem 1.1.** First, from (67) we see that  $\dim(U_{\lambda}) = s_{\lambda}(1, \ldots, 1)$  is positive whenever  $\ell(\lambda) \leq r$ , and that  $\dim(U_{\lambda}) = \exp(o(n))$  where the o(n) is uniform in  $\lambda$ . Now consider the coefficients  $c_{\mu,\nu}^{\lambda}$ . These are known (see e.g. [17, Chapter 5, Proposition 3]) to equal the size of a certain subset of semi-standard tableaux with shape  $\lambda \setminus \mu$  filled with  $\nu_1$  1's,  $\nu_2$  2's, etc. In particular,  $c_{\mu,\nu}^{\lambda} > 0$  only if  $\mu$  is contained in  $\lambda$ , and then  $\ell(\mu) \leq \ell(\lambda) \leq r$ . Since  $c_{\mu,\nu}^{\lambda} = c_{\nu,\mu}^{\lambda}$  (see [17] again) we also need  $\ell(\nu) \leq r$  for  $c_{\mu,\nu}^{\lambda} > 0$ . The combinatorial description also gives the upper bound  $c_{\mu,\nu}^{\lambda} \leq (n+1)^{r^2} = \exp(o(n))$ where the o(n) is uniform in  $\lambda, \mu, \nu$ .

We now turn to the remaining factors in (66). First, as one can see in (68), for fixed r we have that  $d_{\mu}$  is essentially a multinomial coefficient. Thus (see e.g. [8, pp. 14–15] for details), we have

$$\frac{1}{n}\log d_{\mu} = -\sum_{j=1}^{r} \frac{\mu_{j}}{n}\log \frac{\mu_{j}}{n} + O(\frac{\log n}{n}).$$
(69)

Next, from (59) we have that

$$\operatorname{ct}(\lambda) = \frac{n^2}{2} \sum_{j=1}^r \left(\frac{\lambda_j}{n}\right)^2 + O(n).$$
(70)

Taken altogether, these facts mean that we can write (66) as

$$Z_{\beta,n}^{AB} = \sum_{\lambda,\mu,\nu} \mathbb{1}\left\{c_{\mu,\nu}^{\lambda} > 0\right\} \exp\left(n\left\{\tilde{F}(\frac{\mu}{n}, \frac{\nu}{n}, \frac{\lambda}{n}) + o(1)\right\}\right),\tag{71}$$

where  $\lambda \vdash n$ ,  $\mu \vdash m$  and  $\nu \vdash n - m$ , all having  $\leq r$  rows, and where

$$\tilde{F}(\vec{x}, \vec{y}, \vec{z}) = -\sum_{j=1}^{r} x_j \log x_j - \sum_{j=1}^{r} y_j \log y_j + \frac{\beta}{2} \left[ (a-c) \sum_{j=1}^{r} x_j^2 + (b-c) \sum_{j=1}^{r} y_j^2 + c \sum_{j=1}^{r} z_j^2 \right].$$
(72)

There is a necessary and sufficient condition for  $c_{\mu,\nu}^{\lambda} > 0$  which is very useful for our purposes, known as *Horn's conjecture*, proved by Knutson and Tao [23]. It is best stated for our purposes in terms of eigenvalues of Hermitian matrices, as follows:  $c_{\mu,\nu}^{\lambda} > 0$  if and only if there are Hermitian  $r \times r$  matrices X and Y with eigenvalues  $\mu_1, \ldots, \mu_r$ and  $\nu_1, \ldots, \nu_r$ , respectively, such that X + Y has eigenvalues  $\lambda_1, \ldots, \lambda_r$ . For information about this, see e.g. [18]. We thus have

$$c_{\mu,\nu}^{\lambda} > 0 \text{ if and only if } \left(\frac{\mu}{n}, \frac{\nu}{n}, \frac{\lambda}{n}\right) \in \Omega_{m/n}^{+}$$
 (73)

where  $\Omega_{\rho}^{+}$  is the set of triples  $(\vec{x}, \vec{y}, \vec{z})$  such that there exist positive semidefinite Hermitian matrices X, Y with  $\operatorname{tr}(X) = 1 - \operatorname{tr}(Y) = \rho$  having eigenvalues  $x_1, \ldots, x_r$  and  $y_1, \ldots, y_r$ , respectively, such that Z = X + Y has eigenvalues  $z_1, \ldots, z_r$ .

From (71) and the fact that  $\tilde{F}$  is continuous in its arguments, we conclude that

$$\frac{1}{n}\log Z^{\rm AB}_{\beta,n} \to \max_{(\vec{x},\vec{y},\vec{z})\in\Omega^+_{\rho}} \tilde{F}(\vec{x},\vec{y},\vec{z}).$$
(74)

See e.g. [8, Section 3] for a detailed argument in a similar setting. Now note that if X, Y, Z are as above, then

$$\sum_{j=1}^{r} x_j^2 = \operatorname{tr}(X^2), \qquad \sum_{j=1}^{r} y_j^2 = \operatorname{tr}(Y^2), \tag{75}$$

and also

$$\sum_{j=1}^{r} z_j^2 = \operatorname{tr}(Z^2) = \operatorname{tr}((X+Y)^2) = \operatorname{tr}(X^2) + \operatorname{tr}(Y^2) + 2\operatorname{tr}(XY).$$
(76)

Thus

$$(a-c)\sum_{j=1}^{r} x_j^2 + (b-c)\sum_{j=1}^{r} y_j^2 + c\sum_{j=1}^{r} z_j^2 = \operatorname{tr}\left[aX^2 + bY^2 + 2cXY\right].$$
(77)

So for  $(\vec{x}, \vec{y}, \vec{z}) \in \Omega_{\rho}$ , we have that

$$\tilde{F}(\vec{x}, \vec{y}, \vec{z}) = \phi(X, Y) := S(X) + S(Y) + \frac{\beta}{2} \text{tr} \big[ aX^2 + bY^2 + 2cXY \big],$$
(78)

where S is the von Neumann entropy

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$$S(X) = -\text{tr}(X \log X) = -\sum_{i=1}^{r} x_i \log x_i.$$
 (79)

It follows that

$$\frac{1}{n}\log Z_n^{\scriptscriptstyle AB}(\beta) \to \max_{X,Y} \phi(X,Y) \tag{80}$$

where the maximum is over positive definite Hermitian matrices X, Y with  $tr(X) = 1 - tr(Y) = \rho$ .

The final step is to use the fact that for positive semidefinite Hermitian matrices X, Y with fixed spectra  $x_1, \ldots, x_r$  and  $y_1, \ldots, y_r$ , respectively, ordered so that  $x_1 \ge x_2 \ge \cdots \ge x_r$  and  $y_1 \ge y_2 \ge \cdots \ge y_r$ , we have the inequality

$$\sum_{j=1}^{r} x_j y_{r+1-j} \le \operatorname{tr}[XY] \le \sum_{j=1}^{r} x_j y_j, \tag{81}$$

see e.g. [25, Prop. 9.H.1.g-h] (we discuss this result in Appendix A). In particular, both the maximum and the minimum of tr[XY] are attained when X, Y are simultaneously diagonal. Since the other terms in  $F(\vec{x}, \vec{y})$  are symmetric under permuting the  $x_i$  or the  $y_i$ , the result follows.  $\Box$ 

#### 2.2. Walled Brauer algebra: proof of Theorem 1.2

As noted above, our analysis of the model in (14) uses the walled Brauer algebra. We will now define this algebra, and collect some facts which allow us to approach a proof in a similar way to that of Theorem 1.1. An accessible introduction to the walled Brauer algebra is given in [26], and its Schur–Weyl duality is proved in [6], at least for the range  $r \ge n$ . The extension to all r, n is a straightforward extension of the work in [6].

Let us first define the (usual) Brauer algebra. Fix  $n \in \mathbb{N}, r \in \mathbb{C}$ . Arrange two rows each of n labelled vertices, one above the other. We call a *diagram* a graph on these 2nvertices, with each vertex having degree one. Let  $B_n$  be the set of such diagrams. The Brauer algebra  $\mathbb{B}_n(r)$  is the formal complex span of  $B_n$ . Multiplication of two diagrams is defined as follows. Taking two diagrams g, h, identify the upper vertices of h with the lower of g. Then form a new diagram by concatenation and removing any closed loops, as in Fig. 3. The product gh is the concatenation, multiplied by  $r^{\#\text{loops}}$ , where #loopsis the number of loops removed.

The walled Brauer algebra is a subalgebra of  $\mathbb{B}_n(r)$ . Let  $m \leq n$ . Returning to the 2n labelled vertices, draw a line (a "wall") separating the leftmost 2m vertices and the rightmost 2(n-m). Let  $B_{n,m}$  be the set of diagrams in  $B_n$  with the condition that any edge connecting two upper vertices or two lower vertices must cross the wall, and any edge connecting an upper vertex and a lower vertex must not cross the wall; see Fig. 4. The walled Brauer algebra  $\mathbb{B}_{n,m}(r)$  is the span of  $B_{n,m}$ , with multiplication as in the Brauer algebra.

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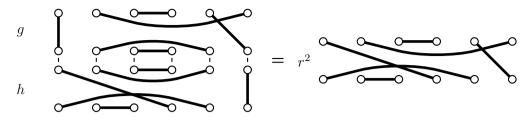


Fig. 3. Two diagrams g and h (left), and their product gh (right). The concatenation contains two loops, so we multiply the concatenation with middle vertices removed by  $r^2$ .

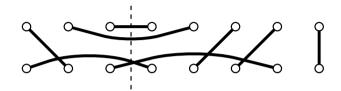
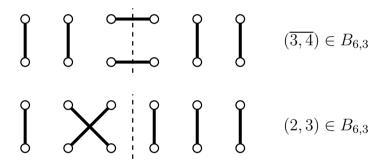


Fig. 4. A diagram in the basis  $B_{8,3}$  of the walled Brauer algebra  $\mathbb{B}_{8,3}(r)$ . Notice that all edges connecting two upper vertices (or two lower) cross the wall, and all edges connecting an upper vertex to a lower vertex do not.



**Fig. 5.** Examples of the elements  $(\overline{i, j})$  and the transpositions (i, j).

Some useful representation-theoretic facts follow. First, the group algebra  $\mathbb{C}[S_m \times S_{n-m}]$  is a subalgebra of  $\mathbb{B}_{n,m}(r)$  whose basis  $S_m \times S_{n-m}$  consists of those diagrams with no edges crossing the wall. As above, we let (i, j) denote the transposition exchanging i and j. Note that in the walled Brauer algebra, we must have  $1 \leq i, j \leq m$  or  $m+1 \leq i, j \leq n$ . For  $1 \leq i \leq m < j \leq n$ , let  $(\overline{i, j})$  denote the diagram with all edges vertical, except that the  $i^{\text{th}}$  and  $j^{\text{th}}$  upper vertices are connected, and the  $i^{\text{th}}$  and  $j^{\text{th}}$  lower vertices are connected; see Fig. 5. The elements (i, j) and  $(\overline{i, j})$  generate the walled Brauer algebra.

Next, the irreducible representations of  $\mathbb{B}_{n,m}(r)$  are indexed by

$$\{(\lambda, \mu) \mid \lambda \vdash m - t, \ \mu \vdash n - m - t, \ t = 0, \dots, \min\{m, n - m\}\},$$
(82)

where  $\lambda$  and  $\mu$  are partitions (see Proposition 2.4 of [13]). Henceforth, we will use the notation  $\hat{m} = \min\{m, n-m\}$  so that the standing condition on t is that  $t \in \{0, 1, \ldots, \hat{m}\}$ . The element



Fig. 6. The r-tuple  $\nu = (3, 2, 0, -1, -2)$  illustrated in the style of a Young diagram, where negative entries are shown by boxes to the left of the main vertical line. Here r = 5. From the figure it is straightforward to see that  $\nu = [\lambda, \mu]$ , where  $\lambda = (3, 2)$  and  $\mu = (2, 1)$ .

$$J_{n,m} = \sum_{\substack{1 \le i < j \le m \\ m < i < j < n}} (i,j) - \sum_{1 \le i \le m < j \le n} (\overline{i,j})$$
(83)

is central in  $\mathbb{B}_{n,m}(r)$ , and acts as the scalar  $\operatorname{ct}(\lambda) + \operatorname{ct}(\mu) - rt$  on the irreducible representation  $(\lambda, \mu)$ , where  $\lambda \vdash m - t$ ,  $\mu \vdash n - m - t$  and  $\operatorname{ct}(\cdot)$  denotes the content defined in (59) (a consequence of, for example, Lemma 4.1 of [13]).

The walled Brauer algebra, like the symmetric group algebra, has a Schur–Weyl duality with the general linear group. To describe this, let us first recall some facts about representations of the general linear group  $\operatorname{GL}_r(\mathbb{C})$ . The irreducible *rational* representations of  $\operatorname{GL}_r(\mathbb{C})$  are indexed by their highest weights, which are *r*-tuples  $\nu = (\nu_1 \geq \cdots \geq \nu_r) \in \mathbb{Z}^r$ . Such a tuple can be equivalently written as a pair  $\nu = [\lambda, \mu]$  of partitions  $\lambda, \mu$  with  $\ell(\lambda) + \ell(\mu) \leq r$ , by letting  $\nu_i = [\lambda, \mu]_i = \lambda_i - \mu_{r-i+1}$  for  $i = 1, \ldots, r$ . Note that at most one of the terms  $\lambda_i$  or  $\mu_{r-i+1}$  is non-zero for each *i*, due to the constraint  $\ell(\lambda) + \ell(\mu) \leq r$ , thus  $\nu$  uniquely determines  $\lambda$  and  $\mu$ . See Fig. 6 for an illustration.

We write  $U_{[\lambda,\mu]}$  for the corresponding irreducible  $\operatorname{GL}_r(\mathbb{C})$ -module. These rational representations are closely related to the polynomial representations  $U_{\lambda}$  appearing in (55); the polynomial representations are the rational representations with non-negative *r*-tuple  $\nu$ . One can also relate the rational and polynomial representations by the Pieri-rule [30]. Indeed, writing det(·) for the determinant representation of  $\operatorname{GL}_r(\mathbb{C})$ , which has highest weight  $(1, 1, \ldots, 1)$  and character  $x_1 x_2 \cdots x_r$ , we have that  $\det^{\otimes k} \otimes U_{\nu} = U_{\nu+\underline{k}}$  where  $\underline{k} = (k, k, \ldots, k)$ . For  $k = \mu_1$  we have that  $U_{[\lambda,\mu]+\underline{\mu_1}}$  is a polynomial representation. It follows from this and (64) that the character of  $U_{[\lambda,\mu]}$  is

$$\chi_{U_{[\lambda,\mu]}}[g] = \frac{s_{[\lambda,\mu]+\mu_1}(x_1,\dots,x_r)}{(x_1x_2\cdots x_r)^{\mu_1}} = \frac{\det[x_i^{[\lambda,\mu]_j+r-j}]_{i,j=1}^r}{\prod_{1\le i< j\le r}(x_i-x_j)},\tag{84}$$

where  $x_1, \ldots, x_r$  are the eigenvalues of g.

We can now state the Schur-Weyl duality for the walled Brauer algebra and the general linear group. Let  $\operatorname{GL}_r(\mathbb{C})$  act on  $\mathbb{V} = (\mathbb{C}^r)^{\otimes n} = (\mathbb{C}^r)^{\otimes m} \otimes (\mathbb{C}^r)^{\otimes (n-m)}$  as m tensor powers of its defining representation, and n-m tensor powers of the dual of its defining representation (multiplication by the inverse transpose):

$$g(v_1 \otimes \cdots \otimes v_m \otimes v_{m+1} \otimes \cdots \otimes v_n) = g(v_1) \otimes \cdots \otimes g(v_m) \otimes g^{-\intercal}(v_{m+1}) \otimes \cdots \otimes g^{-\intercal}(v_n).$$

Let  $\mathbb{B}_{n,m}(r)$  act on  $\mathbb{V}$  by sending (i,j) to the transposition operator  $T_{i,j}$ , and  $(\overline{i,j})$  to  $Q_{i,j}$  (2). Then, as a representation of  $\mathbb{C}[GL_r(\mathbb{C})] \otimes \mathbb{B}_{n,m}(r)$ ,

$$\mathbb{V} = \bigoplus_{\substack{t=0\\\mu \vdash n-m-t\\\ell(\lambda)+\ell(\mu) \le r}}^{\hat{m}} \bigoplus_{\substack{\lambda \vdash m-t\\\mu \vdash n-m-t\\\ell(\lambda)+\ell(\mu) \le r}} U_{[\lambda,\mu]} \otimes V_{(\lambda,\mu)}, \tag{85}$$

with  $V_{(\lambda,\mu)}$  irreducible  $\mathbb{B}_{n,m}(r)$ -representations as above (as noted above, this is a straightforward extension of the work in [6]).

Notice now that our Hamiltonian (14) can be rewritten as

$$H_n^{\rm WB} = -\frac{1}{n} \Big( (a+c) \sum_{1 \le i < j \le m} T_{i,j} + (b+c) \sum_{m+1 \le i < j \le n} T_{i,j} - cJ_{n,m} \Big), \tag{86}$$

where  $J_{n,m}$  is the central element given in (83). Now in an identical way to how we developed equation (66), we have

$$\operatorname{tr}_{\mathbb{V}}[e^{-\beta H_{n}^{\mathrm{WB}}}] = \sum_{\substack{\pi \vdash m \\ \tau \vdash n-m}} \sum_{\substack{t=0 \\ \mu \vdash n-m-t \\ \ell(\lambda) + \ell(\mu) \le r}}^{\hat{m}} \dim(U_{[\lambda,\mu]}) b_{(\lambda,\mu),(\pi,\tau)}^{n,m,r} d_{\pi} d_{\tau}$$

$$+ \exp\left(\frac{\beta}{n} \left[ (c+a)\operatorname{ct}(\pi) + (c+b)\operatorname{ct}(\tau) - c(\operatorname{ct}(\lambda) + \operatorname{ct}(\mu) - rt) \right] \right),$$

$$(87)$$

where  $b_{(\lambda,\mu),(\pi,\tau)}^{n,m,r}$  is the branching coefficient from  $\mathbb{C}[S_m \times S_{n-m}]$  to  $\mathbb{B}_{n,m}(r)$ , i.e. the multiplicity of the  $\mathbb{C}[S_m \times S_{n-m}]$ -module  $V_{\pi} \otimes V_{\tau}$  in  $V_{(\lambda,\mu)}$  when the latter is regarded as a  $\mathbb{C}[S_m \times S_{n-m}]$ -module. These branching coefficients play the same role as the Littlewood–Richardson coefficient did in the AB-model. Our next step is to determine when  $b_{(\lambda,\mu),(\pi,\tau)}^{n,m,r}$  is strictly positive.

**Lemma 2.2.** The branching coefficient  $b_{(\lambda,\mu),(\pi,\tau)}^{n,m,r}$  is strictly positive if and only if there exist  $r \times r$  Hermitian matrices X, Y, Z with respective spectra  $\pi, \tau, [\lambda, \mu]$ , such that X - Y = Z.

Note that the parameter t is encoded the branching coefficient, in the sense that  $b_{(\lambda,\mu),(\pi,\tau)}^{n,m,r} > 0$  implies that  $\lambda \vdash m - t = |\pi| - t$  and  $\mu \vdash n - m - t = |\tau| - t$  for some  $0 \leq t \leq \hat{m}$ . To see how t appears from the Hermitian matrices, assume for the sake of argument that X and Y commute. Then, for each i,  $[\lambda,\mu]_i = \pi_j - \tau_k$ , for some j,k. Fig. 7 then illustrates via an example how it follows that  $\lambda \vdash m - t = |\pi| - t$  and  $\mu \vdash n - m - t = |\pi| - t$  and  $\mu \vdash n - m - t = |\tau| - t$  for some  $0 \leq t \leq \hat{m}$ .

The first step to prove Lemma 2.2 is another lemma, analogous to the well known fact that the Littlewood–Richardson coefficients are both the branching coefficients from  $\mathbb{C}[S_m \times S_{n-m}]$  to  $\mathbb{C}[S_n]$ , and the coefficients of the decomposition of the tensor product of two irreducible polynomial representations of  $\mathrm{GL}_r(\mathbb{C})$ .



Fig. 7. The spectra  $\pi = (3, 0, 1, 2, 4)$  and  $\tau = (2, 1, 3, 2, 1)$ , respectively of X and Y (simultaneously diagonalised), displayed in the style of Young diagrams, either side of the main vertical line. The spectrum of Z = X - Y is (1, -1, -2, 0, 3) (and so when ordered becomes  $[\lambda, \mu] = (3, 1, 0, -1, -2)$ ). The yellow boxes are those eliminated in the subtraction. Naturally there are the same number either side of the main vertical; this is the parameter  $0 \le t \le \min |\pi|, |\tau|$ . In this example, t = 6. (For interpretation of the colours in the figure(s), the reader is referred to the web version of this article.)

**Lemma 2.3.** Let  $\pi, \tau, \lambda, \mu$  denote partitions with at most r parts, with  $\ell(\lambda) + \ell(\mu) \leq r$ , and  $U_{\pi}, U_{[\emptyset,\tau]}, U_{[\lambda,\mu]}$  denote irreducible rational representations of  $\operatorname{GL}_r(\mathbb{C})$ . Let

$$U_{\pi} \otimes U_{[\varnothing,\tau]} = \bigoplus_{\substack{\lambda,\mu\\\ell(\lambda)+\ell(\mu) \le r}} \hat{b}^{n,m,r}_{[\lambda,\mu],(\pi,\tau)} U_{[\lambda,\mu]}.$$
(88)

Then  $\hat{b}^{n,m,r}_{[\lambda,\mu],(\pi,\tau)} = b^{n,m,r}_{(\lambda,\mu),(\pi,\tau)}.$ 

**Proof.** This is proved using Schur–Weyl duality. We restrict (85) to  $\mathbb{C}[GL_r(\mathbb{C})] \otimes \mathbb{C}[S_m \times S_{n-m}]$  to see that

$$\mathbb{V} = \bigoplus_{t=0}^{m} \bigoplus_{\substack{\lambda \vdash m-t \\ \mu \vdash n-m-t \\ \ell(\lambda) + \ell(\mu) \le r}} \bigoplus_{\substack{\pi \vdash m \\ \tau \vdash n-m \\ \ell(\pi), \ell(\tau) \le r}} b^{n,m,r}_{(\lambda,\mu),(\pi,\tau)} U_{[\lambda,\mu]} \otimes (V_{\pi} \otimes V_{\tau}).$$
(89)

On the other hand, the Schur–Weyl duality between  $GL_r(\mathbb{C}) \times GL_r(\mathbb{C})$  and  $\mathbb{C}[S_m \times S_{n-m}]$  is

$$\mathbb{V} = \bigoplus_{\substack{\pi \vdash m \\ \tau \vdash n - m \\ \ell(\pi), \ell(\tau) \le r}} (U_{\pi} \otimes U_{[\varnothing, \tau]}) \otimes (V_{\pi} \otimes V_{\tau}).$$
(90)

Expanding  $U_{\pi} \otimes U_{[\emptyset,\tau]}$  as in (88) and equating coefficients from the two equations above gives the result.  $\Box$ 

**Proof of Lemma 2.2.** We take equation (88) and modify it using the Pieri rule:

$$U_{\pi} \otimes U_{[\varnothing,\tau]+\underline{\tau_1}} = \bigoplus_{\substack{\lambda,\mu\\\ell(\lambda)+\ell(\mu) \le r}} \hat{b}^{n,m,r}_{[\lambda,\mu],(\pi,\tau)} U_{[\lambda,\mu]+\underline{\tau_1}}.$$
(91)

Now the highest weights appearing on both sides have no negative parts, so by Lemma 2.3 and the Littlewood–Richardson Rule,

$$b_{(\lambda,\mu),(\pi,\tau)}^{n,m,r} = \hat{b}_{[\lambda,\mu],(\pi,\tau)}^{n,m,r} = c_{\pi,[\varnothing,\tau]+\underline{\tau_1}}^{[\lambda,\mu]+\underline{\tau_1}}.$$
(92)

We know from Horn's inequalities that  $c_{\pi,[\varnothing,\tau]+\underline{\tau_1}}^{[\lambda,\mu]+\underline{\tau_1}} > 0$  if and only if there exist  $r \times r$ Hermitian  $\bar{X}, \bar{Y}, \bar{Z}$  with respective spectra  $\pi, [\varnothing, \tau] + \underline{\tau_1}$  and  $[\lambda, \mu] + \underline{\tau_1}$  such that  $\bar{X} + \bar{Y} = \bar{Z}$ . Now it is straightforward to show that such matrices exist if and only if there exist  $r \times r$  Hermitian X, Y, Z with respective spectra  $\pi, \tau$  and  $[\lambda, \mu]$  such that X - Y = Z. Indeed, let  $X = \bar{X}, Y = -\bar{Y} + \tau_1 \mathrm{Id}$ , and  $Z = \bar{Z} - \tau_1 \mathrm{Id}$  for the first implication, and similarly for the reverse implication.  $\Box$ 

We can now return to equation (87). Using similar workings as in Section 2.1, we let  $m, n \to \infty$  such that  $m/n \to \rho \in (0, 1), \pi/n \to \vec{x}, \tau/n \to \vec{y}$  and  $[\lambda, \mu]/n \to \vec{z}$ . Note that  $\vec{z}$  can now have negative entries, and that from (59)

$$\frac{\operatorname{ct}(\lambda) + \operatorname{ct}(\mu) - rt}{n^2} = \sum_{i=1}^r \left( \left(\frac{\lambda_i}{n}\right)^2 + \left(-\frac{\mu_i}{n}\right)^2 \right) + o(1) = \sum_{i=1}^r \left(\frac{[\lambda,\mu]_i}{n}\right)^2 + o(1).$$
(93)

We find that

$$Z_n^{\text{WB}}(\beta) = \sum_{\substack{\pi \vdash m \\ \tau \vdash n - m}} \sum_{\substack{\lambda, \mu \\ (\pi/n, \tau/n, [\lambda, \mu]/n) \in \Omega_{m/n}^-}} \exp\left(n\left\{\tilde{G}(\frac{\pi}{n}, \frac{\tau}{n}, \frac{[\lambda, \mu]}{n}) + o(1)\right\}\right), \tag{94}$$

where  $\Omega_{\rho}^{-}$  is the set of triples of *r*-tuples  $\vec{x}, \vec{y}, \vec{z}$  such that  $x_1, \ldots, x_r \ge 0, y_1, \ldots, y_r \ge 0, \sum_{i=1}^r x_i = \rho = 1 - \sum_{i=1}^r y_i$ , and there exist  $r \times r$  Hermitian matrices X, Y, Z with respective spectra  $\vec{x}, \vec{y}, \vec{z}$  such that X - Y = Z, and where

$$\tilde{G}(\vec{x}, \vec{y}, \vec{z}) = \sum_{i=1}^{r} \left[ \frac{\beta}{2} ((a+c)x_i^2 + (b+c)y_i^2 - cz_i^2) - x_i \log x_i - y_i \log y_i \right].$$
(95)

Notice that the sum over t appearing in (87) is hidden in (94), as it is implicit in the definition of  $\Omega_{\rho}^{-}$ , due to our remark after the statement of Lemma 2.2. Therefore

$$\Phi_{\beta}^{\rm WB}(a,b,c) := \lim_{n \to \infty} \frac{1}{n} \log Z_n^{\rm WB}(\beta) = \max_{(\vec{x},\vec{y},\vec{z}) \in \Omega_{\rho}^-} \tilde{G}(\vec{x},\vec{y},\vec{z}).$$
(96)

As in (78) and (80), we can rewrite this in terms of the matrices X and Y:

$$\Phi_{\beta}^{\text{WB}}(a,b,c) = \max_{X,Y} \left[ S(X) + S(Y) + \frac{\beta}{2} \left( a \operatorname{tr}[X^2] + b \operatorname{tr}[Y^2] + 2c \operatorname{tr}[XY] \right) \right], \tag{97}$$

where now the maximum is only over  $r \times r$  Hermitian matrices X, Y with respective spectra  $\vec{x}, \vec{y}$  as above. This is the same as (80), and this completes the proof of Theorem 1.2.  $\Box$ 

#### 2.3. Correlation functions: proof of Theorem 1.7

Let us prove the result for the AB-model first. We use (65) and the argument leading up to (71) to get that, as  $n \to \infty$ ,

$$\left\langle \exp\left\{\frac{1}{n}\sum_{i=1}^{n}W_{i}\right\}\right\rangle_{\beta,n}^{\text{AB}} = \frac{\sum_{\lambda,\mu,\nu}\mathbbm{1}\left\{c_{\mu,\nu}^{\lambda}>0\right\}\frac{s_{\lambda}(e^{w_{1}/n},\dots,e^{w_{r}/n})}{s_{\lambda}(1,\dots,1)}\exp\left(n\left\{\tilde{F}(\frac{\mu}{n},\frac{\nu}{n},\frac{\lambda}{n})+o(1)\right\}\right)}{\sum_{\lambda,\mu,\nu}\mathbbm{1}\left\{c_{\mu,\nu}^{\lambda}>0\right\}\exp\left(n\left\{\tilde{F}(\frac{\mu}{n},\frac{\nu}{n},\frac{\lambda}{n})+o(1)\right\}\right)},$$
(98)

where  $\tilde{F}$  is as in (72). Both sums on the right-hand-side are over  $\lambda \vdash n$ ,  $\mu \vdash m$  and  $\nu \vdash n - m$ , all having at most r parts, and in the numerator we have multiplied and divided by  $\dim(U_{\lambda}) = s_{\lambda}(1, \ldots, 1)$  in order that the o(1) terms in the exponents are exactly equal. Then the arguments of [9, Section 6] apply, meaning that

$$\lim_{n \to \infty} \left\langle \exp\left\{\frac{1}{n} \sum_{i=1}^{n} W_i\right\} \right\rangle_{\beta,n}^{\text{AB}} = \lim_{\lambda/n \to \vec{z}^\star} \frac{s_\lambda(e^{w_1/n}, \dots, e^{w_r/n})}{s_\lambda(1, \dots, 1)},\tag{99}$$

where  $\vec{z}^{\star} = (z_1^{\star}, \dots, z_r^{\star})$  lists the eigenvalues of X + Y where X, Y are the Hermitian matrices which maximise the right-hand-side of (80). But we know from (81) that the maximum is attained when X, Y are simultaneously diagonal, with ordering of eigenvalues decreasing for both X and Y if c > 0, respectively decreasing for X and increasing for Y if c < 0. Then clearly the eigenvalues of Z = X + Y are the sums of the eigenvalues of X and of Y, ordered appropriately, giving  $z^{\star}$  as in (30).

Turning to the WB-model, very similarly to equation (98) we have

$$\left\langle \exp\left\{\frac{1}{n}\left(\sum_{i=1}^{m}W_{i}-\sum_{i=m+1}^{n}W_{i}^{\mathsf{T}}\right)\right\}\right\rangle_{\beta,n}^{\mathsf{WB}}\right\} = \frac{\sum_{\lambda,\mu,\pi,\tau} \mathbb{1}\left\{b_{[\lambda,\mu],(\pi,\tau)}^{n,m,r}>0\right\}\frac{\chi_{U[\lambda,\mu]}(e^{W/n})}{\dim(U_{[\lambda,\mu]})}\exp\left(n\left\{\tilde{G}(\frac{\pi}{n},\frac{\tau}{n},\frac{[\lambda,\mu]}{n})+o(1)\right\}\right)}{\sum_{\lambda,\mu,\pi,\tau} \mathbb{1}\left\{b_{[\lambda,\mu],(\pi,\tau)}^{n,m,r}>0\right\}\exp\left(n\left\{\tilde{G}(\frac{\pi}{n},\frac{\tau}{n},\frac{[\lambda,\mu]}{n})+o(1)\right\}\right),$$

$$(100)$$

where once again the o(1) terms in the exponents are exactly equal and  $\tilde{G}$  is given in (95). The arguments of [9, Section 6] apply once again, meaning that by (84) the limit equals

$$\lim_{[\lambda,\mu]/n \to z^{\dagger}} \frac{\chi_{U_{[\lambda,\mu]}}(e^{W/n})}{\dim(U_{[\lambda,\mu]})},\tag{101}$$

where this time,  $(\vec{x}^*, \vec{y}^*, \vec{z}^{\dagger})$  maximises  $\tilde{G}(\vec{x}, \vec{y}, \vec{z})$ , with the conditions that  $x_i, y_i \geq 0$ ,  $\sum_{i=1}^r x_i = \rho = 1 - \sum_{i=1}^r y_i$ , and that there exist Hermitian matrices X, Y, Z with respective spectra x, y, z with X - Y = Z. Following equation (97), we can rewrite  $\tilde{G}$  as the function of the matrices X and Y being maximised in (97). If the entries of  $\vec{x}$  are ordered decreasingly, then as before the trace-inequality (81) implies that for c > 0the entries of  $\vec{y}$  should also be ordered decreasingly, while for c < 0 they should be ordered increasingly. This gives the form of  $\vec{z}^{\dagger}$  stated in (30).

It remains only to show that

$$\lim_{[\lambda,\mu]/n \to z} \frac{\chi_{U_{[\lambda,\mu]}}(e^{W/n})}{\dim(U_{[\lambda,\mu]})} = R(w_1, \dots, w_r; z_1, \dots, z_r),$$
(102)

where R is given by (31). This is proved almost identically to Lemma 6.1 from [9]. Indeed, using (84) we get

$$\frac{\chi_{U_{[\lambda,\mu]}}(e^{W/n})}{\dim(U_{[\lambda,\mu]})} = \det[e^{w_i[\lambda,\mu]_j/n + w_i(r-j)/n}] \cdot \prod_{1 \le i < j \le r} \frac{j-i}{(e^{w_i/n} - e^{w_j/n})([\lambda,\mu]_i - [\lambda,\mu]_j + j - i)},$$
(103)

which, noting all the products (including in the determinant) are finite, tends to  $R(w_1, \ldots, w_r; z_1, \ldots, z_r)$  as  $[\lambda, \mu]/n \to z$ .  $\Box$ 

#### 2.4. Magnetisation term: proof of Theorem 1.8

We start by giving expressions for the free energy with a magnetisation term, and then afterwards we will take the appropriate derivatives. We will need the following notation:

- $\Delta^+$  will denote the set of vectors  $\vec{z} = (z_1, z_2, \dots, z_r)$  that can arise as spectra of X + Y where X and Y are positive semidefinite Hermitian matrices with  $tr[X] = 1 tr[Y] = \rho$ , ordered so that  $z_1 \ge \cdots \ge z_r$ . In fact,  $\Delta^+$  consists of all  $\vec{z}$  satisfying  $z_1 \ge \cdots \ge z_r \ge 0$  and  $\sum_{i=1}^r z_i = 1$ . Given  $\vec{z} \in \Delta^+$ , we write  $\mathcal{H}^+_{\rho}(\vec{z})$  for the set of pairs (X, Y) of such matrices with X + Y having spectrum  $\vec{z}$ .
- $\Delta_{\rho}^{-}$  will denote the set of vectors  $\vec{z} = (z_1, z_2, \dots, z_r)$  that can arise as spectra of X Y where X and Y are as above, again ordered so that  $z_1 \geq \cdots \geq z_r$ . Now  $\Delta_{\rho}^{-}$  consists of all  $\vec{z}$  satisfying  $\rho \geq z_1 \geq \cdots \geq z_r \geq -(1 \rho)$  and  $\sum_{i=1}^r z_i = 2\rho 1$ . Given  $\vec{z} \in \Delta_{\rho}^{-}$ , we write  $\mathcal{H}_{\rho}^{-}(\vec{z})$  for the set of pairs (X, Y) of such matrices with X Y having spectrum  $\vec{z}$ .

Let  $\Phi^{\#}(\beta, h) = \Phi^{\#}_{\beta, h}(a, b, c, \vec{w})$  be as in (36) and recall from (78) that

$$\phi(X,Y) = S(X) + S(Y) + \frac{\beta}{2} \operatorname{tr} \left[ aX^2 + bY^2 + 2cXY \right].$$

**Theorem 2.4.** Let  $a, b, c \in \mathbb{R}$  and  $w_1 \geq \cdots \geq w_r$  be fixed. If  $n, m \to \infty$  such that  $m/n \to \rho \in (0, 1)$ , then the free energy of the models (34) and (35) satisfy:

$$\Phi^{AB}(\beta,h) = \max_{\vec{z}\in\Delta^{+}} \left( \max_{(X,Y)\in\mathcal{H}_{\rho}^{+}(\vec{z})} \phi(X,Y) + \begin{cases} h\sum_{i=1}^{r} z_{i}w_{i}, & \text{if } h > 0, \\ h\sum_{i=1}^{r} z_{i}w_{r+1-i}, & \text{if } h < 0, \end{cases} \right) \\
\Phi^{WB}(\beta,h) = \max_{\vec{z}\in\Delta_{\rho}^{-}} \left( \max_{(X,Y)\in\mathcal{H}_{\rho}^{-}(\vec{z})} \phi(X,Y) + \begin{cases} h\sum_{i=1}^{r} z_{i}w_{i}, & \text{if } h > 0, \\ h\sum_{i=1}^{r} z_{i}w_{r+1-i}, & \text{if } h < 0, \end{cases} \right).$$
(104)

**Proof.** Let us start with the AB case. Using the expression (65) and arguing similarly to (71) we have

$$Z_{n,h}^{AB} = \sum_{\mu,\nu,\lambda} s_{\lambda}(e^{hw_{1}},\dots,e^{hw_{r}})$$

$$\cdot c_{\mu,\nu}^{\lambda}d_{\mu}d_{\nu}\exp\left(\frac{\beta}{n}[(a-c)\operatorname{ct}(\mu)+(b-c)\operatorname{ct}(\nu)+c\cdot\operatorname{ct}(\lambda)]\right)$$

$$= \sum_{(\mu/n,\nu/n,\lambda/n)\in\Omega_{m/n}^{+}} s_{\lambda}(e^{hw_{1}},\dots,e^{hw_{r}})\exp\left(n\left\{\tilde{F}(\frac{\mu}{n},\frac{\nu}{n},\frac{\lambda}{n})+o(1)\right\}\right),$$
(105)

where  $\tilde{F}$  is given in (72) and  $\Omega_{\rho}^{+}$  in (73). Recall that [17, Section 2.2]

$$s_{\lambda}(e^{hw_1}, \dots, e^{hw_r}) = \sum_{\mathbb{T}} \prod_{i=1}^r e^{hm_i w_i} = \sum_{\mathbb{T}} e^{\sum_{i=1}^r hm_i w_i},$$
 (106)

where the sum is over all semistandard Young tableaux  $\mathbb{T}$  with shape  $\lambda$  and entries in  $\{1, \ldots, r\}$ , and where for each i,  $m_i$  is the number of times the number i appears in  $\mathbb{T}$ . The tableau with each box in the  $i^{\text{th}}$  row labelled i appears in the sum, and in fact, for h > 0, it maximises the sum in the exponent:

$$e^{\sum_{i=1}^{r} hm_i w_i} \le e^{\sum_{i=1}^{r} h\lambda_i w_i},\tag{107}$$

for each valid  $\mathbb{T}$ . Indeed, note that in a semistandard tableau, the entries of row *i* must be at least *i*. Then, taking any semistandard  $\mathbb{T}$ , shape  $\lambda$ , changing an entry  $j \geq i$  in row *i* to *i* changes the sum in the exponent by  $h(w_i - w_j)$ , which is non-negative by our ordering of  $\vec{w}$  as  $w_1 \geq \cdots \geq w_r$ . Hence for h > 0,

$$e^{\sum_{i=1}^{r}h\lambda_{i}w_{i}} \leq s_{\lambda}(e^{hw_{1}},\dots,e^{hw_{r}}) \leq \dim(U_{\lambda})e^{\sum_{i=1}^{r}h\lambda_{i}w_{i}}.$$
(108)

Recalling that  $\frac{1}{n} \log \dim(U_{\lambda}) \to 0$  we get, for h > 0,

$$Z_{n,h}^{\text{AB}} = \sum_{(\mu/n,\nu/n,\lambda/n)\in\Omega_{m/n}^+} \exp\left(n\left\{\tilde{F}(\frac{\mu}{n},\frac{\nu}{n},\frac{\lambda}{n}) + h\sum_{i=1}^r \frac{\lambda_i}{n}w_i + o(1)\right\}\right).$$
(109)

In the case h < 0, the sum in the exponent in (106) is maximised when  $m_i = \lambda_{r+1-i}$  for each *i*; indeed, let h' = -h, and  $w'_i = -w_{r+1-i}$ , and apply the same reasoning as above. So, for h < 0, we have

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$$e^{\sum_{i=1}^{r}h\lambda_{r+1-i}w_i} \le s_{\lambda}(e^{hw_1},\dots,e^{hw_r}) \le \dim(U_{\lambda})e^{\sum_{i=1}^{r}h\lambda_{r+1-i}w_i}, \tag{110}$$

and consequently

$$Z_{n,h}^{\text{AB}} = \sum_{(\mu/n,\nu/n,\lambda/n)\in\Omega_{m/n}^+} \exp\left(n\left\{\tilde{F}(\frac{\mu}{n},\frac{\nu}{n},\frac{\lambda}{n}) + h\sum_{i=1}^r \frac{\lambda_i}{n} w_{r+1-i} + o(1)\right\}\right).$$
(111)

The result for the AB-case then follows by arguing as in (74) and [8, Lemma 3.4].

For the WB-case, a very similar argument as for (105) gives

$$Z_n^{\rm WB}(\beta,h) = \sum_{(\pi/n,\tau/n,[\lambda,\mu]/n)\in\Omega_{m/n}^-} \chi_{U_{[\lambda,\mu]}}(e^{hw_1},\dots,e^{hw_r}) \exp\left(n\left\{\tilde{G}(\frac{\mu}{n},\frac{\nu}{n},\frac{\lambda}{n})+o(1)\right\}\right),\tag{112}$$

where  $\tilde{G}$  is given in (95),  $\Omega_{\rho}^{-}$  is defined just above (95), and  $\chi_{U_{[\lambda,\mu]}}$  is given in (84). In particular, from (84), we see that upper and lower bounds from (108) and (110) extend to this case. The result for the WB-case then follows by arguing as in (97) and [8, Lemma 3.4] again.  $\Box$ 

**Proof of Theorem 1.8.** The proof closely follows that of Theorem 4.1 from [8]. We start from the expressions (104) where, for ease of notation, we drop the superscript. We give details only in the AB-case with h > 0 as the other cases are very similar.

Let  $F_{\max} = \Phi(\beta, 0) = \max_{\vec{z} \in \Delta^+} \left( \max_{(X,Y) \in \mathcal{H}_a^+(\vec{z})} \phi(X, Y) \right)$  and let

$$K = \left\{ \vec{z} \in \Delta^+ : \max_{(X,Y) \in \mathcal{H}_{\rho}^+(\vec{z})} \phi(X,Y) = F_{\max} \right\}$$
(113)

denote the set of maximisers. Note that K is compact. Clearly,

$$\frac{\Phi(\beta,h) - \Phi(\beta,0)}{h} = \max_{\vec{z} \in \Delta^+} \left[ \sum_{i=1}^r z_i w_i + \frac{\max_{(X,Y) \in \mathcal{H}_{\rho}^+(\vec{z})} \phi(X,Y) - F_{\max}}{h} \right]$$

$$\geq \max_{\vec{z} \in K} \sum_{i=1}^r z_i w_i.$$
(114)

We want to prove that the left-hand side of (114) tends to the right-hand side as  $h \to 0$ . For a contradiction, assume that there is a sequence  $h_n \to 0$  such that the corresponding limit exists and is strictly larger than the right-hand side. For each  $h_n$ , pick an element  $\vec{z}(h_n) \in \Delta^+$  that achieves the first maximum in (114). Since  $\Delta^+$  is compact, we can assume after passing to a subsequence if necessary that  $\vec{z}(h_n) \to \vec{z}^*$  as  $h_n \to 0$ . We claim that  $\vec{z}^* \in K$ . Otherwise,  $\max_{(X,Y)\in \mathcal{H}_{\mu}^+(\vec{z}^*)} \phi(X,Y) < F_{\max}$ , which would mean that the left-hand side of (114) tends to  $-\infty$  as  $h = h_n \to 0$ , contradicting the lower bound on the right. It follows that

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$$\frac{\Phi(\beta, h_n) - \Phi(\beta, 0)}{h_n} = \sum_{i=1}^r z_i(h_n)w_i + \frac{\max_{(X,Y)\in\mathcal{H}_{\rho}^+(\vec{z}(h_n))}\phi(X,Y) - F_{\max}}{h_n}$$

$$\leq \sum_{i=1}^r z_i(h_n)w_i \to \sum_{i=1}^r z_i^*w_i \leq \max_{\vec{z}\in K} \sum_{i=1}^r z_i^*w_i,$$
(115)

as required.

In the WB-case, we follow the same reasoning but with  $\Delta^+$  replaced by  $\Delta_{\rho}^-$ , with  $\mathcal{H}_{\rho}^+$  replaced by  $\mathcal{H}_{\rho}^-$ , and the maxima in (114) replaced by minima (as well as  $w_i \leftrightarrow w_{r+1-i}$ ).

It remains to show that the  $z_i$  may be expressed as in the statement of the Theorem. Indeed, we know from (81) that  $\phi(X, Y)$  is maximised when X and Y are simultaneously diagonal, with entries  $x_1, \ldots, x_r$  and  $y_1, \ldots, y_r$ , respectively, ordered as follows:

• if 
$$c > 0$$
, if  $x_1 \ge \cdots \ge x_r \ge 0$  then  $y_1 \ge \cdots \ge y_r \ge 0$ ;

• if c < 0, if  $x_1 \ge \cdots \ge x_r \ge 0$  then  $0 \le y_1 \le \cdots \le y_r$ .

This gives the result.  $\Box$ 

#### 3. The phase transition

In this section we prove Propositions 1.3, 1.4, 1.5 and 1.6. Let us start by recalling the basic quantities of interest: we wish to maximise the function

$$F(\omega) = F(\vec{x}; \vec{y}) = \sum_{i=1}^{r} f(x_i, y_i),$$
(116)

over the domain

$$\Omega = \left\{ \omega = (\vec{x}; \vec{y}) : x_1, \dots, x_r, y_1, \dots, y_r \ge 0, \ \sum_{i=1}^r x_i = 1 - \sum_{i=1}^r y_i = \rho \right\}.$$
 (117)

Here

$$f(x,y) = -x\log x - y\log y + \frac{\beta}{2}(ax^2 + by^2 + 2cxy),$$
(118)

and we write  $Q(x, y) = \frac{1}{2} (ax^2 + by^2 + 2cxy)$  for the quadratic form appearing in f(x, y). We will write  $\rho' = 1 - \rho$  to lighten the notation.

We are particularly interested in whether the maximum of F is attained at the point

$$\omega_0 = \left(\frac{\rho}{r}, \frac{\rho}{r}, \dots, \frac{\rho}{r}; \frac{\rho'}{r}, \frac{\rho'}{r}, \dots, \frac{\rho'}{r}\right),\tag{119}$$

or at some other point in  $\Omega$ .

#### 3.1. Existence of a phase transition: proof of Proposition 1.3

We are now ready to prove our result on the existence of a critical point. Recall that we want to prove that  $\beta_c$  exists (is positive and finite) if and only if Q is not negative

semidefinite, where  $\beta_c$  is the maximum of the  $\beta$  for which  $\omega_0$  is a maximiser of F. We will need the following elementary identity.

#### **Lemma 3.1.** If Q is a quadratic form of two variables, then

$$r\sum_{j=1}^{r} Q(x_j, y_j) = Q(x_1 + \dots + x_r, y_1 + \dots + y_r) + \sum_{1 \le i < j \le r} Q(x_i - x_j, y_i - y_j).$$
(120)

**Proof.** When Q(x, y) = xy we need to prove that

$$r\sum_{j=1}^{r} x_j y_j = (x_1 + \dots + x_r)(y_1 + \dots + y_r) + \sum_{1 \le i < j \le r} (x_i - x_j)(y_i - y_j).$$
(121)

This is easy to see by comparing the coefficient of each monomial on the two sides. Specializing  $x_j = y_j$  proves the result for  $Q(x, y) = x^2$  and  $Q(x, y) = y^2$ , and the general case then follows by linearity.  $\Box$ 

#### **Proof of Proposition 1.3.** We will write

$$F(\omega) - F(\omega_0) = \beta \mathcal{E}(\omega) + \mathcal{H}(\omega), \qquad (122)$$

where

$$\mathcal{E}(\vec{x};\vec{y}) = \sum_{j=1}^{r} Q(x_j, y_j) - rQ\left(\frac{\rho}{r}, \frac{\rho'}{r}\right),\tag{123}$$

and

$$\mathcal{H}(\vec{x}; \vec{y}) = \sum_{j=1}^{r} (-x_j \log x_j - y_j \log y_j) + \rho \log \frac{\rho}{r} + \rho' \log \frac{\rho'}{r}.$$
 (124)

The term  $\mathcal{E}$  is in some sense an energy term, and  $\mathcal{H}$  an entropy term. Note that F is maximised at  $\omega_0$  if and only if  $\beta \mathcal{E}(\omega) + \mathcal{H}(\omega) \leq 0$  on  $\Omega$ .

On  $\Omega$ , we can write

$$\frac{1}{r}\mathcal{H}(\vec{x};\vec{y}) = -h\left(\frac{x_1 + \dots + x_r}{r}\right) + \frac{h(x_1) + \dots + h(x_r)}{r} - h\left(\frac{y_1 + \dots + y_r}{r}\right) + \frac{h(y_1) + \dots + h(y_r)}{r},$$

where  $h(x) = -x \log x$ . Since h is strictly concave,  $\mathcal{H}(\omega) \leq 0$  with equality only at the point  $\omega_0$ . Moreover, by Lemma 3.1,

$$\mathcal{E}(\vec{x}; \vec{y}) = \frac{1}{r} \sum_{1 \le i < j \le r} Q(x_i - x_j, y_i - y_j).$$
(125)

Thus, if Q is negative semidefinite, we have  $\mathcal{E}(\omega) \leq 0$  and consequently  $\omega_0$  is the unique maximum point of F.

Assume now that Q is not negative semidefinite. We claim that  $\mathcal{E}$  assumes strictly positive values in  $\Omega$ . To see this, it suffices to consider the case when  $x_2 = \cdots = x_r$ ,  $y_2 = \cdots = y_r$ . Then

$$\mathcal{E}(\vec{x};\vec{y}) = \frac{r-1}{r} Q(\xi,\eta), \qquad (126)$$

where  $\xi = x_1 - x_2$  and  $\eta = y_1 - y_2$ . Here  $(\xi, \eta)$  can take any value in  $\left[-\frac{\rho}{r-1}, \rho\right] \times \left[-\frac{\rho'}{r-1}, \rho'\right]$ . By assumption, Q takes on positive values in parts of this rectangle. Then it is clear that  $\mathcal{E}$  takes positive values, hence that  $\mathcal{H}(\omega) + \beta \mathcal{E}(\omega)$  assumes positive values for  $\beta$  large enough, and that the set of  $\beta > 0$  for which this is true is an interval  $\beta > \beta_c$ . To see that  $\omega_0$  is the unique maximiser for  $\beta < \beta_c$ , take  $\omega \in \Omega \setminus \{\omega_0\}$ . Then either  $\mathcal{E}(\omega) > 0$ , in which case  $\mathcal{H}(\omega) + \beta \mathcal{E}(\omega) < \mathcal{H}(\omega) + \beta_c \mathcal{E}(\omega) \leq 0 = \mathcal{H}(\omega_0) + \beta \mathcal{E}(\omega_0)$ , or  $\mathcal{E}(\omega) \leq 0$ , in which case  $\mathcal{H}(\omega) + \beta \mathcal{E}(\omega) \leq \mathcal{H}(\omega) < 0 = \mathcal{H}(\omega_0) + \beta \mathcal{E}(\omega_0)$ .

It remains to show that  $\beta_c \neq 0$ , that is, that F assumes its maximum value at  $\omega_0$  for  $\beta$  close to zero. We will show that this is in fact true if we maximise F over the larger set

$$U = \{ (\vec{x}; \vec{y}) : 0 \le x_j \le \rho, 0 \le y_j \le \rho', j = 1, \dots, r \}.$$
 (127)

To do this we will show that the Hessian H(F) is negative definite in U for  $\beta$  close to 0, meaning that F is concave in U for such  $\beta$  and that  $\omega_0$  is a global maximum in U. The Hessian H(F) is a direct sum of the Hessians

$$H(f) = \begin{pmatrix} f_{xx} & f_{xy} \\ f_{xy} & f_{yy} \end{pmatrix} = \begin{pmatrix} \beta a - \frac{1}{x} & \beta c \\ \beta c & \beta b - \frac{1}{y} \end{pmatrix},$$
(128)

which is negative definite if and only if

$$\left(\beta a - \frac{1}{x}\right)\left(\beta b - \frac{1}{y}\right) > \beta^2 c^2, \qquad \frac{1}{x} > \beta a, \qquad \frac{1}{y} > \beta b.$$
 (129)

By monotonicity, when  $x \leq \rho$  and  $y \leq \rho'$  the inequalities (129) are implied by

$$\left(\beta a - \frac{1}{\rho}\right)\left(\beta b - \frac{1}{\rho'}\right) > \beta^2 c^2, \qquad \frac{1}{\rho} > \beta a, \qquad \frac{1}{\rho'} > \beta b.$$
 (130)

But (130) holds for  $\beta = 0$ , hence by continuity also for small positive  $\beta$ , as required.  $\Box$ 

From the proof above we note that  $\beta \leq \beta_c$  if and only if  $\mathcal{H}(\omega) + \beta \mathcal{E}(\omega) \leq 0$  for all  $\omega \in \Omega$ , and also that we have the expression

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$$\beta_{\rm c} = \inf_{\omega \in \Omega^+} \left( -\frac{\mathcal{H}(\omega)}{\mathcal{E}(\omega)} \right), \quad \text{where } \Omega^+ = \left\{ \omega \in \Omega : \, \mathcal{E}(\omega) > 0 \right\}. \tag{131}$$

#### 3.2. Formulas for $\beta_c$ : proofs of Propositions 1.4 and 1.5

We now turn to the proofs of our formulas for  $\beta_c$ , Proposition 1.4 for the case r = 2and Proposition 1.5 for the case  $r \ge 3$ ,  $c \ge 0$  and  $(a - c)\rho = (b - c)\rho' =: t$ .

Our strategy is to obtain general lower and upper bounds on  $\beta_c(r)$ , given in Propositions 3.3 and 3.4 respectively, which are tight in the two cases that we consider. Both bounds are given in terms of the critical temperature  $\beta_c^h(r)$  of the homogeneous case a = b = c = 1 (the superscript h is for "homogeneous"). In [8, Theorem 4.2], it was found that

$$\beta_{\rm c}^{\rm h}(r) = \begin{cases} 2, & r = 2, \\ \frac{2(r-1)\log(r-1)}{r-2}, & r \ge 3. \end{cases}$$
(132)

Note that this agrees with our Proposition 1.5; the corresponding form  $Q(x, y) = \frac{1}{2}(x + y)^2$  is not negative semidefinite and (20) holds with t = 0.

To get a better understanding of Proposition 1.5, we note that (20) implies the explicit diagonalization

$$Q(x,y) = \frac{t\rho\rho'}{2} \left(\frac{x}{\rho} - \frac{y}{\rho'}\right)^2 + \frac{c+t}{2}(x+y)^2.$$
 (133)

That Q is not negative semidefinite means that at least one of t and c + t are positive. Since we assume that  $c \ge 0$  this means that c + t > 0. In particular, the expression for  $\beta_{\rm c}(r)$  in Proposition 1.5 is always positive.

Let us now obtain a lower bound for  $\beta_c$ . We deduce from (131) and [8, Theorem 4.2] with  $\rho = 1$  that  $-\mathcal{H}(\vec{x}; \vec{0}) \geq \beta_c^{h}(r)\mathcal{E}(\vec{x}; \vec{0})$ . This inequality takes the form

$$\sum_{j=1}^{r} x_j \log x_j - \log \frac{1}{r} \ge \frac{\beta_{\rm c}^{\rm h}(r)}{2r} \sum_{1 \le i < j \le r} (x_j - x_i)^2, \quad \text{where } \sum_{j=1}^{r} x_j = 1.$$
(134)

Replacing each  $x_j$  by  $x_j/\rho$  gives

$$\sum_{j=1}^{r} x_j \log x_j - \rho \log \frac{\rho}{r} \ge \frac{\beta_c^{\rm h}(r)}{2\rho r} \sum_{1 \le i < j \le r} (x_j - x_i)^2, \quad \text{where } \sum_{j=1}^{r} x_j = \rho.$$
(135)

As was observed in [8], equality in (135) holds both at the point  $x_1 = \cdots = x_r = \rho/r$ and at (26a). (They are the same point if r = 2.)

We will temporarily write  $\gamma$  for the explicit expression (24) (we aim to show that  $\beta_{\rm c}(2) = \gamma$ ). We will need the following description of  $\gamma$ .

**Lemma 3.2.** Assume that  $Q(x,y) = \frac{1}{2}(ax^2 + by^2 + 2cxy)$  is not negative semidefinite and that  $\beta$ ,  $\rho$ ,  $\rho' > 0$ . Then, the form

$$\beta Q(x,y) - \frac{x^2}{\rho} - \frac{y^2}{\rho'}$$
(136)

is negative semidefinite if and only if  $\beta \leq \gamma$ , and negative definite if and only if  $\beta < \gamma$ .

**Proof.** By assumption, the first term in (136) can assume positive values, and the second term is always non-positive. It follows that the range of  $\beta$  for which (136) is negative semidefinite is of the form  $\beta \leq \beta_0$  and that it is negative definite if and only if  $\beta < \beta_0$ . The precise conditions for (136) to be negative semidefinite are

$$\left(\beta a - \frac{1}{2\rho}\right) \left(\beta b - \frac{1}{2\rho'}\right) \ge \beta^2 c^2, \qquad \beta a \le \frac{1}{2\rho}, \qquad \beta b \le \frac{1}{2\rho'}.$$
(137)

By continuity,

$$\left(\beta_0 a - \frac{1}{2\rho}\right) \left(\beta_0 b - \frac{1}{2\rho'}\right) = \beta_0^2 c^2.$$

If  $ab = c^2$ , this is a linear equation with the solution  $\beta_0 = 2/(a\rho + b\rho') = \gamma$ . Otherwise, it has two solutions

$$\beta_{\pm} = \frac{\rho a + (1-\rho)b \pm \sqrt{(\rho a - (1-\rho)b)^2 + 4\rho(1-\rho)c^2}}{\rho(1-\rho)(ab-c^2)},$$
(138)

which satisfy  $(ab - c^2)\beta_+\beta_- = 1/4\rho\rho' > 0$ . If  $ab > c^2$ , both solutions are positive and  $\beta_0$  equals the smallest solution  $\beta_- = \gamma$ . If  $ab < c^2$  the solutions have opposite sign. In this case  $\beta_0$  is the largest solution, which is again  $\beta_- = \gamma$ .  $\Box$ 

**Proposition 3.3.** Assume that Q is not negative semidefinite, so that  $\beta_c$  exists. Then,

$$\beta_{\rm c} \ge \frac{1}{2} \beta_{\rm c}^h(r) \gamma. \tag{139}$$

**Proof.** Using the estimate (135) in (124) gives

$$-\mathcal{H}(\omega) \ge \frac{\beta_{\rm c}^{\rm h}(r)}{2r} \sum_{1 \le i < j \le r} \left( \frac{(x_i - x_j)^2}{\rho} + \frac{(y_i - y_j)^2}{\rho'} \right). \tag{140}$$

It follows that

$$\mathcal{H}(\omega) + \beta \mathcal{E}(\omega) \le \frac{1}{r} \sum_{1 \le i < j \le r} \tilde{Q}(x_j - x_i, y_j - y_i),$$
(141)

where

$$\tilde{Q}(x,y) = \beta Q(x,y) - \frac{\beta_{\rm c}^{\rm h}(r)}{2} \left(\frac{x^2}{\rho} + \frac{y^2}{\rho'}\right).$$
(142)

By Lemma 3.2,  $\tilde{Q}$  is negative semidefinite if and only if  $\beta \leq \frac{1}{2}\beta_{c}^{h}(r)\gamma$ . For  $\beta$  in this range it follows that  $\mathcal{H}(\omega) + \beta \mathcal{E}(\omega) \leq 0$  on  $\Omega$ . This gives the desired bound on  $\beta_{c}$ .  $\Box$ 

Let us now move to upper bounds for  $\beta_c$ . We need to find a value of  $\beta$  such that  $F(\omega) > F(\omega_0)$  for some points  $\omega \in \Omega$ . We want to find upper bounds that in some cases equal the lower bound in Proposition 3.3. We can only expect this to work if we used the inequality (135) in cases when it holds with equality. By the results of [8] mentioned above, it is natural to take  $\omega$  either close to  $\omega_0$ , or to  $\omega_1$  as in (26). This leads to the following two upper bounds.

**Proposition 3.4.** Assume that Q is not negative semidefinite, so that  $\beta_c$  exists. Then,

$$\beta_{\rm c} \le \frac{1}{2} r \gamma. \tag{143}$$

If, in addition,  $Q(\rho, \rho') > 0$  and  $r \ge 3$ , then

$$\beta_{\rm c} \le \frac{\beta_{\rm c}^h(r)}{2Q(\rho, \rho')}.\tag{144}$$

In fact, (144) holds also when r = 2, but in that case it is weaker than (143).

**Proof.** We first consider the behaviour of F near  $\omega_0$ . More precisely, consider the points

$$\omega_{t,u} = \omega_0 + (t, -t, 0, \dots, 0; u, -u, 0, \dots, 0), \tag{145}$$

which belong to  $\Omega$  for t, u close to 0. We have the Taylor expansion

$$F(\omega_{t,u}) - F(\omega_0) = f\left(\frac{\rho}{r} + t, \frac{\rho'}{r} + u\right) + f\left(\frac{\rho}{r} - t, \frac{\rho'}{r} - u\right) - 2f\left(\frac{\rho}{r}, \frac{\rho'}{r}\right) \\ = \left(t^2 f_{xx} + u^2 f_{yy} + 2tu f_{xy}\right) \left(\frac{\rho}{r}, \frac{\rho'}{r}\right) + \mathcal{O}((t^2 + u^2)^{3/2}).$$

By (128), the quadratic term is

$$2\beta Q(t,u) - r\left(\frac{t^2}{\rho} + \frac{u^2}{\rho'}\right).$$
 (146)

By Lemma 3.2, if  $\beta > r\gamma/2$ , this form is not negative semidefinite. It follows that  $\omega_0$  is not a local maximum of F. This gives the first result.

Next, we consider the point  $\omega_1$  from (26) and assume  $r \geq 3$ . By a straightforward computation,

$$\mathcal{H}(\omega_1) = -\frac{r-2}{r}\log(r-1) \tag{147}$$

and, by (126),

$$\mathcal{E}(\omega_1) = \frac{r-1}{r} Q\left(\frac{\rho(r-2)}{r-1}, \frac{\rho'(r-2)}{r-1}\right) = \frac{(r-2)^2}{r(r-1)} Q(\rho, \rho').$$
(148)

The second upper bound now follows from (131).  $\Box$ 

We can now put our upper and lower bounds together to prove Propositions 1.4 and 1.5.

**Proof of Proposition 1.4.** When r = 2, (139) and (143) reduce to  $\gamma \leq \beta_c \leq \gamma$ , that is,  $\beta_c(2) = \gamma$ . For the statement about uniqueness of the maximiser, note that if  $\beta = \beta_c(2)$ and  $\omega = (\vec{x}; \vec{y})$  is a maximiser, then the left-hand-side of (141) equals zero. Then also the right-hand-side of (141) equals zero, since  $\tilde{Q} \leq 0$  for  $\beta \leq \frac{1}{2}\beta_c^{h}(2)\gamma = \beta_c(2)$  by the proof of Proposition 3.3. Hence (140) holds with equality and therefore (135) holds with equality, as does the corresponding statement for  $\vec{y}$ . But it follows from the proof of Theorem 4.2 in [8] that (for r = 2) equality in (135) holds only at the point  $\omega_0$ .  $\Box$ 

**Proof of Proposition 1.5.** Note that the lower bound in (139) and the upper bound in (144) are equal if  $\gamma = Q(\rho, \rho')^{-1}$ . Assuming (20), we can parametrise

$$a = c + \frac{t}{\rho}, \qquad b = c + \frac{t}{\rho'}.$$
(149)

It is then straight-forward to check that

$$(\rho a - \rho' b)^2 + 4\rho \rho' c^2 = c^2$$
, and  $ab - c^2 = \frac{t(c+t)}{\rho \rho'}$ , (150)

which gives

$$\gamma = \frac{2t + c - \sqrt{c^2}}{t(c+t)} = \frac{2}{c+t}, \qquad c \ge 0.$$
(151)

By (133),

$$Q(\rho, \rho') = \frac{c+t}{2}.$$
 (152)

This shows that, under the conditions of Proposition 1.5, the upper and lower bound for  $\beta_c$  agree and hence  $\beta_c = \beta_c^h(r)/(c+t)$ .

To see that the point  $\omega_1$  in (26) gives another maximiser at  $\beta = \beta_c$ , take  $\beta = \beta_c(r) = \beta_c^{\rm h}(r)/2Q(\rho,\rho')$  to see from (147) and (148) that  $\mathcal{H}(\omega_1) + \beta \mathcal{E}(\omega_1) = 0$  which is also the maximum value of  $\mathcal{H}(\omega) + \beta \mathcal{E}(\omega)$ . To see that  $\omega_1$  is the only other maximiser we argue as at the end of the proof of Proposition 1.4. Namely, for  $\beta = \beta_c(r) = \frac{1}{2}\beta_c^{\rm h}(r)\gamma$ , we have that (135) holds with equality, as does the corresponding statement for  $\vec{y}$ . From [8], equality in (135) holds only at the points  $\omega_0$  and  $\omega_1$  (assuming (13)).  $\Box$ 

We can now complete the final proof of this section, that of Proposition 1.6, that the maximiser is unique for  $\beta > \beta_c$  close to  $\beta_c$  under the conditions in Proposition 1.5.

**Proof of Proposition 1.6.** We first show that F is strictly concave in neighbourhoods of  $\omega_0$  and  $\omega_1$  in  $\Omega$ . More generally, consider  $F(\vec{x} + \vec{t}; \vec{y} + \vec{u})$ , where  $(\vec{x}; \vec{y}) \in \Omega$  is a point with  $x_2 = \cdots = x_r$  and  $y_2 = \cdots = y_r$  and  $(\vec{t}; \vec{u})$  a small perturbation with

$$\sum_{j=1}^{r} t_j = \sum_{j=1}^{r} u_j = 0.$$
(153)

By (128), the quadratic term in the Taylor expansion of F is

$$Q_1(t_1, u_1) + \sum_{j=2}^r Q_2(t_j, u_j), \qquad (154)$$

where

$$Q_k(t, u) = \beta Q(t, u) - \frac{t^2}{2x_k} - \frac{u^2}{2y_k}$$

At the point  $\omega_0$ , we have

$$Q_1(t,u) = Q_2(t,u) = \beta Q(t,u) - \left(\frac{rt^2}{2\rho} + \frac{ru^2}{2\rho'}\right).$$

It follows from Lemma 3.2 that this is negative definite if  $\beta < \beta_0 = r\gamma/2$ . By continuity, it follows that F is strictly concave near  $\omega_0$ . Since  $\omega_0$  is a stationary point it must then be a local maximum, that is,  $F(\vec{x}; \vec{y}) \leq F(\omega_0)$  for  $(\vec{x}; \vec{y})$  near  $\omega_0$  and  $\beta < \beta_0$ . Using that

$$\beta_{\rm c} = \frac{(r-1)\log(r-1)}{r-2} \gamma_{\rm c}$$

it is easy to check that  $\beta_{\rm c} < \beta_0 = r\gamma/2$ , so this applies in particular to  $\beta$  near  $\beta_{\rm c}$ .

The point  $\omega_1$  cannot be handled as easily since  $Q_1$  is then not negative definite. Instead, we use Lemma 3.1 and (153) to write

$$(r-1)\sum_{j=2}^{r} Q_2(t_j, u_j) = Q_2(t_1, u_1) + \sum_{2 \le i < j \le r} Q_2(t_i - t_j, u_i - u_j).$$

It follows that (154) equals

$$Q_1(t_1, u_1) + \frac{1}{r-1} Q_2(t_1, u_1) + \frac{1}{r-1} \sum_{2 \le i < j \le r} Q_2(t_i - t_j, u_i - u_j).$$

We compute

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$$Q_1(t,u) + \frac{1}{r-1} Q_2(t,u) = \frac{r}{r-1} \left( \beta Q(t,u) - \left(\frac{rt^2}{2\rho} + \frac{ru^2}{2\rho'}\right) \right).$$

As before, this is negative definite for  $\beta < \beta_0$ . Moreover,

$$Q_2(t,u) = \beta Q(t,u) - \frac{r(r-1)t^2}{2\rho} - \frac{r(r-1)u^2}{2\rho'}$$

is negative definite for  $\beta < (r-1)\beta_0$ , which is a weaker condition. We conclude that F is strictly concave for  $\beta < \beta_0$  and  $(\vec{x}; \vec{y})$  near  $\omega_1$ . We note that from (122),

$$F(\omega_1) - F(\omega_0) = \mathcal{H}(\omega_1) + \beta_{\rm c} \mathcal{E}(\omega_1) + (\beta - \beta_{\rm c}) \mathcal{E}(\omega_1),$$

where the sum of the first two terms on the right hand side vanishes and the last term is computed by (148) and (152). This gives

$$F(\omega_1) - F(\omega_0) = (\beta - \beta_c) \frac{(r-2)^2 (c+t)}{2r(r-1)},$$

which is clearly positive for  $\beta > \beta_c$ .

For each  $\beta > \beta_c$ , let  $\omega(\beta)$  be a maximiser of F in  $\Omega$ . Permute the coordinates so that (13) holds. We claim that then  $\omega(\beta) \to \omega_1$  as  $\beta \searrow \beta_c$ . Otherwise, there exists a sequence  $\omega(\beta_n)$ ,  $\beta_n \searrow \beta_c$ , that avoids a neighbourhood of  $\omega_1$ . Since  $\Omega$  is compact we may assume that this sequence converges. It must then converge to a maximiser of F for  $\beta = \beta_c$  that satisfies (13). There are only two such points,  $\omega_0$  and  $\omega_1$ , by Proposition 1.5. However, we have seen that for  $\beta_c < \beta < \beta_0$  we have  $F(\vec{x}; \vec{y}) \leq F(\omega_0)$  for  $(\vec{x}; \vec{y})$  near  $\omega_0$ whereas  $F(\omega_1) > F(\omega_0)$ . Thus, a sequence of global maximisers cannot converge to  $\omega_0$ . This is a contradiction, and we conclude that  $\omega(\beta) \to \omega_1$ . These points must then enter a region where F is strictly concave and hence maximisers are unique. This completes the proof.  $\Box$ 

### 3.3. Form of the maximiser of F for c > 0

In this section we will prove that, for c > 0, any maximiser of F(10) is of the form (155). This is useful for the heuristic discussion of Gibbs states in Section 1.5 and for the results on ground state phase diagrams in Section 4.

We assume throughout this section that  $\vec{x}$  is ordered as in (13), that is  $x_1 \ge x_2 \ge \cdots \ge x_r$ . Recall from the discussion after (13) that, for c > 0, F is maximised when the orders of  $\vec{x}$  and  $\vec{y}$  match, that is when also  $y_1 \ge \cdots \ge y_r$ . We will adapt the arguments in [8] and in the appendix of [9] to show the following.

**Proposition 3.5.** For c > 0, any maximiser  $(\vec{x}^*; \vec{y}^*)$  of F in the set  $\Omega$  (21) is of the form

$$x_1^{\star} \ge x_2^{\star} = \dots = x_r^{\star}, 
 y_1^{\star} \ge y_2^{\star} = \dots = y_r^{\star}.$$
 (155)

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Moreover for the special case a = b = 0, c > 0,  $\rho = 1/2$ , and  $\beta \neq \beta_c$  we have that the maximiser is unique, and  $x_i^* = y_i^*$  for all i = 1, ..., r.

The proof of this proposition is divided into several steps. We first prove that a maximum point  $(\vec{x}; \vec{y})$  only has positive coordinates, and that  $x_j = x_k$  if and only if  $y_j = y_k$  (this holds also for c < 0). Then we prove that, when c > 0, the entries  $x_i$  (and therefore  $y_i$ ) can take at most two distinct values. This reduces the number of variables we need to consider, leading to (155) and the uniqueness statement via direct calculations.

**Lemma 3.6.** For any  $a, b, c \in \mathbb{R}$  with  $c \neq 0$ , if  $(\vec{x}; \vec{y})$  is a maximum point of F in  $\Omega$ , then

(1) all x<sub>j</sub> and y<sub>j</sub> are strictly positive,
(2) x<sub>j</sub> = x<sub>k</sub> if and only if y<sub>j</sub> = y<sub>k</sub>.

**Proof.** In this proof we write  $e_j$  for the unit vector with a 1 in the  $x_j$ -coordinate and remaining entries equal to 0. For the first part, suppose that  $\omega = (\vec{x}; \vec{y}) \in \Omega$  is a maximum point such that  $x_j = 0$  for some j, and that j is the smallest index with this property. Then,  $\omega(t) = \omega + t(e_j - e_{j-1}) \in \Omega$  for small enough t > 0 (recall that  $x_{j-1} \ge x_j$  by (13)). By a direct computation,  $F(\omega(t)) - F(\omega) = -t \log t + O(t)$  as  $t \to 0$ . It follows that  $F(\omega(t)) > F(\omega)$  for small t, which contradicts  $\omega$  being a maximum point. The same argument works for the variables  $y_j$ .

For the second part, suppose that  $x_j = x_k$  and  $y_j \neq y_k$ . If necessary, redefine jand k so that  $\{l : x_l = x_k\} = \{j, j + 1, ..., k\}$ . We still have  $y_j \neq y_k$ . Then  $\omega(t) :=$  $(\vec{x}; \vec{y}) + t(e_j - e_k) \in \Omega$  for small enough t > 0. (Here we use the first part of the lemma in the case k = r.) We have that  $\frac{\partial}{\partial t} F(\omega(t))|_{t=0} = c(y_j - y_k) > 0$ . This contradicts  $\omega$  being a maximum point. The same argument proves the reverse implication.  $\Box$ 

Lemma 3.6 shows that at a maximum point there is a composition  $r = k_1 + \cdots + k_m$ so that

$$(x_1^{\star}, \dots, x_r^{\star}) = (\underbrace{\xi_1, \dots, \xi_1}_{k_1}, \dots, \underbrace{\xi_m, \dots, \xi_m}_{k_m}), \tag{156a}$$

$$(y_1^{\star}, \dots, y_r^{\star}) = (\underbrace{\eta_1, \dots, \eta_1}_{k_1}, \dots, \underbrace{\eta_m, \dots, \eta_m}_{k_m}),$$
(156b)

where  $\xi_j \neq \xi_k$  and  $\eta_j \neq \eta_k$  for  $j \neq k$ . This leads to the problem of maximizing

$$\overline{F}(\xi;\eta) = k_1 f(\xi_1,\eta_1) + \dots + k_m f(\xi_m,\eta_m)$$
 (157)

over the set  $\Omega^{(m)}$  defined by

$$\xi_1 > \xi_2 > \dots > \xi_m > 0, \qquad k_1 \xi_1 + \dots + k_m \xi_m = \rho,$$
 (158a)

$$\eta_1 > \eta_2 > \dots > \eta_m > 0, \qquad k_1 \eta_1 + \dots + k_m \eta_m = 1 - \rho.$$
 (158b)

For  $m \ge 2$ , the set  $\Omega^{(m)}$  is open, so we may find local extreme points by using Lagrange multipliers. At any such point we have

$$\nabla F(\xi;\eta) = \lambda \nabla (k_1 \xi_1 + \dots + k_m \xi_m) + \mu \nabla (k_1 \eta_1 + \dots + k_m \eta_m), \tag{159}$$

for some  $\lambda, \mu \in \mathbb{R}$ . Equivalently

$$\frac{\partial f}{\partial \xi}(\xi_i, \eta_i) = \lambda, \quad \frac{\partial f}{\partial \eta}(\xi_i, \eta_i) = \mu, \qquad 1 \le i \le m.$$
 (160)

The system (160) can in turn be rewritten in the form

$$\eta_i = \phi_\lambda(\xi_i), \qquad \xi_i = \psi_\mu(\eta_i), \qquad 1 \le i \le m, \tag{161}$$

where

$$\phi_{\lambda}(x) = \frac{\lambda + 1 + \log(x) - ax}{c}, \qquad \psi_{\mu}(y) = \frac{\mu + 1 + \log(y) - by}{c}.$$
 (162)

If we let  $P_{\lambda,\mu}$  denote the intersection of the graphs  $y = \phi_{\lambda}(x)$  and  $x = \psi_{\mu}(y)$ , we can summarise these findings as follows: the maximum of F in  $\Omega$  is attained either at the point  $\omega_0$  (22), or at a point of the form (156), where  $2 \leq m \leq r$ ,  $(\xi, \eta) \in \Omega^{(m)}$  and  $(\xi_i, \eta_i) \in P_{\lambda,\mu}$  for  $1 \leq i \leq m$ . Note that  $\phi''_{\lambda}(x) = -1/cx^2$ ,  $\psi''_{\mu}(y) = -1/cy^2$ , so for c > 0the graphs are concave. We can now prove that for c > 0, a maximiser of F can have at most two distinct entries  $x_i$  (and therefore the same for  $y_i$ ). Henceforth we suppress the indices  $\lambda, \mu$  from  $\phi, \psi$ .

# **Proposition 3.7.** If c > 0 then the m of (156) satisfies $m \leq 2$ .

**Proof.** Suppose first that b < 0. Then,  $\psi$  is increasing and concave, so  $\psi^{-1}$  is increasing and convex. The graph of  $\psi^{-1}$  can intersect the graph of the concave function  $\phi$  in at most two points. If a < 0 the same argument works with  $\phi$  and  $\psi$  interchanged.

This leaves the case when a > 0 and b > 0. In the region

$$\mathcal{R} = \{ (x, y) : 0 < x < 1/a, \ 0 < y < 1/b \},$$
(163)

 $\phi$  is increasing and concave whereas the local inverse  $\psi^{-1}$  is increasing and convex. Thus, there are at most two crossing points in  $\mathcal{R}$ . If there are zero or two crossing points in  $\mathcal{R}$ , then an elementary convexity argument shows that there are no crossing points outside  $\mathcal{R}$ .

In all the cases considered so far there are at most two crossing points, which implies  $m \leq 2$ . In the remaining case, when there is exactly one crossing point in  $\mathcal{R}$ , there can be several crossing points outside  $\mathcal{R}$ . They can be ordered as a sequence  $(x_j, y_j)$  with  $x_j$ 

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decreasing and  $y_j$  increasing. We are only interested in subsequences of crossing points with  $x_j$  and  $y_j$  decreasing. The maximum length of such a subsequence is 2, where we may pick the unique crossing point in  $\mathcal{R}$  and an arbitrary crossing point outside  $\mathcal{R}$ . This proves that  $m \leq 2$  also in this case.  $\Box$ 

We are now ready to prove Proposition 3.5.

**Proof of Proposition 3.5.** We absorb  $\beta$  in a, b, c, effectively setting  $\beta = 1$ . It will be convenient to use  $\xi = x_1 - x_r$  and  $\eta = y_1 - y_r$  as parameters. By Proposition 3.7 (using k in place of m) we can write  $\vec{x}$  and  $\vec{y}$  as

$$x_{1} = \dots = x_{k} = \frac{\rho + (r - k)\xi}{r}, \qquad x_{k+1} = \dots = x_{r} = \frac{\rho - k\xi}{r},$$
  

$$y_{1} = \dots = y_{k} = \frac{\rho' + (r - k)\eta}{r}, \qquad y_{k+1} = \dots = y_{r} = \frac{\rho' - k\eta}{r},$$
(164)

where  $\rho' = 1 - \rho$ . The function (10) can then be written

$$F(\xi,\eta,k) = kf\left(\frac{\rho + (r-k)\xi}{r}, \frac{\rho' + (r-k)\eta}{r}\right) + (r-k)f\left(\frac{\rho - k\xi}{r}, \frac{\rho' - k\eta}{r}\right).$$

We need to show that the maximum of F over  $\xi \in [\rho, k]$ ,  $\eta \in [\rho', k]$  and  $k \in \{0, 1, \ldots, r\}$  is achieved at k = 1. Note that k = 0, which corresponds to the point  $\omega_0$  (22), is included in that case as k = 1,  $\xi = \eta = 0$ . The idea is now to consider k as continuous. We will show the stronger statement that the maximum of F on the domain

$$0 \le \xi \le \frac{\rho}{k}, \qquad 0 \le \eta \le \frac{\rho'}{k}, \qquad 1 \le k \le r \tag{165}$$

is achieved at k = 1.

We first show that F does not have any stationary points in the interior. By a straightforward computation,

$$\begin{split} \frac{\partial F}{\partial \xi} &= \frac{k(r-k)}{r} \left( a\xi + c\eta - \log \frac{\rho + (r-k)\xi}{\rho - k\xi} \right), \\ \frac{\partial F}{\partial \eta} &= \frac{k(r-k)}{r} \left( c\xi + b\eta - \log \frac{\rho' + (r-k)\eta}{\rho' - k\eta} \right), \\ \frac{\partial F}{\partial k} &= \xi + \eta + \frac{r-2k}{r} Q(\xi, \eta) \\ &- \frac{\rho + (r-2k)\xi}{r} \log \frac{\rho + (r-k)\xi}{\rho - k\xi} - \frac{\rho' + (r-2k)\eta}{r} \log \frac{\rho' + (r-k)\eta}{\rho' - k\eta}. \end{split}$$

By the first two equations, at any stationary point we have

$$\log \frac{\rho + (r-k)\xi}{\rho - k\xi} = a\xi + c\eta, \qquad \log \frac{\rho' + (r-k)\eta}{\rho' - k\eta} = c\xi + b\eta.$$
(166)

Inserting this in the third equation and using

$$Q(\xi,\eta) = \frac{1}{2} \left( \xi(a\xi + c\eta) + \eta(c\xi + b\eta) \right)$$

gives

$$\frac{\partial F}{\partial k} = \xi + \eta - \frac{2\rho + (r-2k)\xi}{2r}(a\xi + c\eta) - \frac{2\rho' + (r-2k)\eta}{2r}(c\xi + b\eta).$$

We now observe that (166) implies

$$\operatorname{coth} \frac{a\xi + c\eta}{2} = \frac{2\rho + (r - 2k)\xi}{\xi r}, \qquad \operatorname{coth} \frac{c\xi + b\eta}{2} = \frac{2\rho' + (r - 2k)\eta}{\eta r},$$

which in turn gives

$$\frac{\partial F}{\partial k} = \xi \left( 1 - \frac{a\xi + c\eta}{2} \coth \frac{a\xi + c\eta}{2} \right) + \eta \left( 1 - \frac{c\xi + b\eta}{2} \coth \frac{c\xi + b\eta}{2} \right). \tag{167}$$

Note that  $1 - (x/2) \coth(x/2) \le 0$  for all x, with equality only if x = 0. So a stationary point must satisfy  $\xi(a\xi + c\eta) = \eta(c\xi + b\eta) = 0$ . However, if  $a\xi + c\eta = 0$  then (166) gives  $\xi = 0$  and similarly if  $c\xi + b\eta = 0$  then  $\eta = 0$ . Thus, F has no stationary points in the interior of (165).

It remains to study F on the boundary of (165). At the boundary component  $\xi = 0$ , all x-variables are equal. By Lemma 3.6, at any such maximum point also the y-variables are equal, so it must be the point  $\omega_0$ . Similarly, any maximum point with  $\eta = 0$  is  $\omega_0$ . If  $\xi = \rho/k$  then  $x_r = 0$ , but we know from Lemma 3.6 that F is not maximised at such a point. Similarly, we exclude the case  $\eta = \rho'/k$ . The case k = r again corresponds to  $\omega_0$ . The only remaining boundary component is k = 1. This shows that any maximiser of Fhas the form (155).

To finish the proof of Proposition 3.5, it remains to show that in the case a = b = 0, c > 0,  $\rho = \frac{1}{2}$ , and  $\beta \neq \beta_c$ , the maximiser is unique and satisfies  $x_i = y_i$  for all  $i = 1, \ldots, r$ . Without loss of generality we can let c = 1. Using the fact that the maximiser must be of the form (155), and setting  $x_1 = x$ ,  $y_1 = y$ , we can write

$$F(\vec{x}; \vec{y}) = F_0(x, y) := \beta \left( xy + \frac{(\frac{1}{2} - x)(\frac{1}{2} - y)}{r - 1} \right) - x \log x - y \log y - \left(\frac{1}{2} - x\right) \log \frac{\frac{1}{2} - x}{r - 1} - \left(\frac{1}{2} - y\right) \log \frac{\frac{1}{2} - y}{r - 1}.$$
(168)

We are maximising  $F_0$  in the box  $[\frac{1}{2r}, \frac{1}{2}]^2$ . Calculations yield that when x > y,  $\frac{\partial F_0}{\partial x} < \frac{\partial F_0}{\partial y}$ , and vice-versa, so that the maximum points of  $F_0$  must satisfy x = y or lie on the boundary. Lemma 3.6 shows that they cannot lie on the boundary unless  $(\vec{x}; \vec{y}) = \omega_0$ . So, substituting x = y, and reparametrising with z = 2x, we have

$$F_0\left(\frac{z}{2}, \frac{z}{2}\right) = \frac{\beta}{4} \left(z^2 + \frac{(1-z)^2}{r-1}\right) - z \log z - (1-z) \log \frac{1-z}{r-1} + \log 2.$$
(169)

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Now, apart from the constant log 2, this is precisely the function maximised in [8, Theorem 1.1], with  $\beta$  in that paper replaced with  $\beta/2$  here, and  $\vec{x}$  in that paper of the form  $x_1 \ge x_2 = \cdots = x_r$ . By the working in that paper and the Appendix of [9], the maximiser is unique for all  $\beta \ne \beta_c = \frac{4(r-1)\log(r-1)}{r-2}$  from (25). This concludes the proof of Proposition 3.5.  $\Box$ 

It would be interesting to determine the structure of the maximisers also for c < 0, but that seems more difficult than the case c > 0 considered above. It is still true that any maximiser has the form (156), where the points  $(\xi_i, \eta_i)$  solve a system of the form (161). However, it is no longer true that all maximisers satisfy m = 2 or  $k_1 = 1$ . In fact, in Proposition 4.2 we will see that more complicated maximisers exist even in the zero-temperature limit  $\beta \to \infty$ .

# 4. The ground-state phase diagram

In this section we justify the ground-state phase diagrams given in Figs. 1 and 2 of the introduction. In the zero temperature limit  $\beta \to \infty$ , the logarithmic terms in the function  $F(\vec{x}; \vec{y})$  of (10) become negligible, and the maximisation problem in Theorem 1.1 and 1.2 reduces to maximising the function

$$G(\vec{x};\vec{y}) = \sum_{i=1}^{r} Q(x_i, y_i) = \sum_{i=1}^{r} \frac{1}{2} \left( ax_i^2 + by_i^2 + 2cx_i y_i \right)$$
(170)

on the domain  $\Omega$  defined in (21). We will determine all maximisers of G for  $c \neq 0$ , starting with the easier case c > 0. As has been mentioned, the case c = 0 can be reduced to results of [8].

## 4.1. Diagram for c > 0

We first introduce some notation. For fixed c, we split the ab-plane into five disjoint regions, defined by

$$D = \left\{ a, b < 0, ab > c^2 \right\}, \qquad \qquad \partial D = \left\{ a, b < 0, ab = c^2 \right\},$$
$$E_1 = \left\{ b \le \frac{-c\rho}{\rho'}, ab < c^2 \right\}, \qquad \qquad E_2 = \left\{ a \le \frac{-c\rho'}{\rho}, ab < c^2 \right\},$$
$$F = \left\{ a > \frac{-c\rho'}{\rho}, b > \frac{-c\rho}{\rho'} \right\}.$$

We refer to D as the disordered and F as the ferromagnetic region. The regions  $E_1$  and  $E_2$  are intermediate between D and F. This is illustrated in Fig. 1.

We also introduce the following points in  $\mathbb{R}^r \times \mathbb{R}^r$ :

$$\begin{split} \omega_D &= \left(\frac{\rho}{r}, \dots, \frac{\rho}{r}; \frac{\rho'}{r}, \dots, \frac{\rho'}{r}\right),\\ \omega_{E_1} &= \left(\rho, 0, \dots, 0; \frac{b\rho' - (r-1)c\rho}{br}, \frac{b\rho' + c\rho}{br}, \dots, \frac{b\rho' + c\rho}{br}\right),\\ \omega_{E_2} &= \left(\frac{a\rho - (r-1)c\rho'}{ar}, \frac{a\rho + c\rho'}{ar}, \dots, \frac{a\rho + c\rho'}{ar}; \rho', 0, \dots, 0\right),\\ \omega_F &= (\rho, 0, \dots, 0; \rho', 0, \dots, 0). \end{split}$$

(Above, we used the notation  $\omega_D = \omega_0$ .)

The following result completely describes the maximisers of  $G|_{\Omega}$ . As before, we may restrict attention to maximisers  $(\vec{x}^*; \vec{y}^*)$  such that  $x_i^*$  and  $y_i^*$  are decreasing.

**Proposition 4.1.** Assume that c > 0 and let  $\omega^* = (\vec{x}^*; \vec{y}^*)$  be a maximiser of  $G|_{\Omega}$  with  $x_i^*$  and  $y_i^*$  decreasing. If  $(a, b) \in X$ , where X is one of D,  $E_1$ ,  $E_2$  and F, then  $\omega^*$  is unique and equals  $\omega_X$ . In the remaining case  $(a, b) \in \partial D$  there are infinitely many maximisers. Explicitly, they are given by all points  $(x^*; y^*) \in \Omega$  such that

$$\sqrt{-a}\left(x_i^{\star} - \frac{\rho}{r}\right) = \sqrt{-b}\left(y_i^{\star} - \frac{\rho'}{r}\right), \qquad 1 \le i \le r.$$
(171)

**Proof.** We first consider the case when Q is negative semidefinite, that is,  $(a, b) \in \overline{D}$ . Recall the identity (125), which can be written

$$G(\vec{x}; \vec{y}) = G(\omega_D) + \frac{1}{r} \sum_{1 \le i < j \le r} Q(x_i - x_j, y_i - y_j).$$
(172)

As we already saw in the proof of Proposition 1.3, this immediately implies that  $\omega_D$  is the unique maximiser in case D. If  $(a, b) \in \partial D$ , then

$$Q(x,y) = -\frac{1}{2}(\sqrt{-a}x - \sqrt{-b}y)^2.$$
(173)

Then, (172) implies that G is maximised at all points such that  $\sqrt{-a} x_i - \sqrt{-b} y_i$  is independent of *i*. Summing over *i* gives  $r(\sqrt{-a} x_i - \sqrt{-b} y_i) = \sqrt{-a} \rho - \sqrt{-b} \rho'$ , which leads to (171). Note that if  $(x_1^*, \ldots, x_r^*)$  is any decreasing sequence of non-negative numbers summing to  $\rho$  and we solve (171) for  $y_i^*$ , then  $(x^*; y^*) \in \Omega$  provided that

$$x_r^* \ge \frac{\rho}{r} - \sqrt{\frac{b}{a}} \frac{\rho'}{r}.$$
(174)

Since the right-hand-side is  $< \rho/r$ , this shows that the number of maximisers is indeed infinite in this case.

From now on we assume that Q is not negative semidefinite. Let k and l denote the number of non-zero entries in  $x^*$  and  $y^*$ , respectively. Suppose first that  $k \leq l$ . Then,  $\omega^*$  is a maximiser of

$$H(\vec{x}; \vec{y}) = \sum_{j=1}^{k} Q(x_j, y_j) + \sum_{j=k+1}^{l} Q(0, y_j)$$

on the set

$$U = \left\{ (\vec{x}; \vec{y}); x_1, \dots, x_k, y_1, \dots, y_l > 0, \sum_{j=1}^k x_j = \rho, \sum_{j=1}^l y_j = \rho' \right\}.$$

There must then exist Lagrange multipliers  $\lambda$  and  $\mu$  such that

$$\frac{\partial H}{\partial x_j}(\omega^\star) = ax_j^\star + cy_j^\star = \lambda, \qquad 1 \le j \le k, \qquad (175a)$$

$$\frac{\partial H}{\partial y_j}(\omega^\star) = cx_j^\star + by_j^\star = \mu, \qquad 1 \le j \le k, \qquad (175b)$$

$$\frac{\partial H}{\partial y_j}(\omega^\star) = by_j^\star = \mu, \qquad k+1 \le j \le l.$$
(175c)

If  $ab \neq c^2$ , the system (175a)–(175b) has a unique solution, so  $x_1^* = \cdots = x_k^*$  and  $y_1^* = \cdots = y_k^*$ . This also holds if  $ab = c^2$ , where a, b > 0. In that case, (175a) gives  $a(x_1^* - x_j^*) + c(y_1^* - y_j^*) = 0$  for  $j \leq k$ . Since a > 0 and c > 0, we can still conclude that  $x_1^* = x_j^*$  and  $y_1^* = y_j^*$ .

If  $b \neq 0$ , (175c) gives  $y_{k+1}^{\star} = \cdots = y_l^{\star}$ . Again, this also holds for b = 0. Indeed, in that case, if k < l, then (175b) gives  $cx_k^{\star} = \mu$  and (175c) gives  $0 = \mu$ . This is impossible since c and  $x_k^{\star}$  are both assumed positive. Thus, k = l and the equalities  $y_{k+1}^{\star} = \cdots = y_l^{\star}$  are trivially valid.

The above arguments show that, under the assumption  $k \leq l$ ,

$$\omega^{\star} = (\underbrace{x_1^{\star}, \dots, x_1^{\star}}_{k}, \underbrace{0, \dots, 0}_{r-k}; \underbrace{y_1^{\star}, \dots, y_1^{\star}}_{k}, \underbrace{y_l^{\star}, \dots, y_l^{\star}}_{l-k}, \underbrace{0, \dots, 0}_{r-l}).$$

Next, we prove that either l = k or l = r. To see this, assume that k < l < r. On the one hand, (175b) and (175c) give  $\mu = cx_1^* + by_1^* = by_l^*$ . This implies  $b(y_l^* - y_1^*) = cx_1^* > 0$  and hence b < 0. On the other hand, if t is a small positive number, then  $(\vec{x}^*; \vec{y}^* + t(e_{l+1} - e_l)) \in U$  and hence  $G(\vec{x}^*; \vec{y}^*) \ge G(\vec{x}^*; \vec{y}^* + t(e_{l+1} - e_l))$ , where  $e_j$  are unit vectors. It follows that

$$0 \geq \frac{\partial H}{\partial y_{l+1}}(\omega^{\star}) - \frac{\partial H}{\partial y_{l}}(\omega^{\star}) = c(x_{l+1}^{\star} - x_{l}^{\star}) + b(y_{l+1}^{\star} - y_{l}^{\star}) = -by_{l}^{\star},$$

which contradicts b < 0. After a change of variables, we conclude that

$$\omega^{\star} = (\underbrace{x_1^{\star}, \dots, x_1^{\star}}_{k}, \underbrace{0, \dots, 0}_{r-k}; \underbrace{y_1^{\star}, \dots, y_1^{\star}}_{k}, \underbrace{y_2^{\star}, \dots, y_2^{\star}}_{r-k}),$$
(176)

where the previous cases l = k and l = r correspond to  $y_2^{\star} = 0$  and  $y_2^{\star} \neq 0$ , respectively.

If k > 1 in (176) then

$$G(\vec{x}^{\star} + t(e_1 - e_k); \vec{y}^{\star} + u(e_1 - e_k)) - G(\omega^{\star})$$
  
=  $Q(x_1 + t, y_1 + u) + Q(x_1 - t, y_1 - u) - 2Q(x_1, y_1) = 2Q(t, u).$  (177)

Since we assume that Q is not negative semidefinite, it assumes positive values in any neighbourhood of (0,0). This contradicts that  $\omega^*$  is a maximiser. It follows that k = 1, that is,

$$\omega^{\star} = (\rho, 0, \dots, 0; y_1^{\star}, y_2^{\star}, \dots, y_2^{\star}).$$
(178)

If (178) holds with  $y_2^* = 0$  then  $y_1^* = \rho'$ , that is,  $\omega^* = \omega_F$ . If  $y_2^* \neq 0$ , then the variables  $y_i^*$  can be determined from

$$y_1^{\star} + (r-1)y_2^{\star} = \rho', \qquad c\rho + by_1^{\star} = by_2^{\star},$$

where the second equation follows from (175b) and (175c). Solving these equations, we find that  $\omega^* = \omega_{E_1}$ .

So far we have assumed that  $k \leq l$ . The complementary case follows by interchanging the roles of the x- and y-variables. It leads to the additional possibility  $\omega^* = \omega_{E_2}$ . That is, if  $(a, b) \in E_1 \cup E_2 \cup F$ , then the maximum is achieved at one of the points  $\omega_{E_1}$ ,  $\omega_{E_2}$ and  $\omega_F$ .

It is easy to check that, at the point  $\omega_{E_1}$ , the conditions  $y_1^* \ge y_2^* \ge 0$  are equivalent to  $b \le -c\rho/\rho'$ . Likewise,  $\omega_{E_2}$  is only an admissible point if  $a \le -c\rho'/\rho$ . In region F, neither of these conditions hold and the only possibility is  $\omega^* = \omega_F$ . In region  $E_1$ , we have ruled out  $\omega_{E_2}$ , so we only need to compare the values at  $\omega_{E_1}$  and  $\omega_F$ . By an elementary computation,

$$G(\omega_F) - G(\omega_{E_1}) = \frac{(r-1)(c\rho + b\rho')^2}{2br} \le 0$$

since b < 0 in this case. Equality holds only at the boundary with region F, where  $\omega_{E_1} = \omega_F$ . This proves the result in case  $E_1$  and case  $E_2$  follows by symmetry.  $\Box$ 

To give an example of how the model behaves in the different regions, we compute the magnetisation (see Theorem 1.8)

$$\mathcal{M} = \frac{\partial \Phi^{\rm AB}}{\partial h}\Big|_{h\downarrow 0} = \sum_{i=1}^r (x_i^\star + y_i^\star) w_i.$$

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We will assume that  $(a, b) \notin \partial D$  and that  $w_1 + \cdots + w_r = 0$ . Since  $x_2^* = \cdots = x_r^*$  and  $y_2^* = \cdots = y_r^*$  we obtain

$$\mathcal{M} = (x_1^{\star} + y_1^{\star} - x_2^{\star} - y_2^{\star})w_1.$$

Inserting the explicit expressions from Proposition 4.1 gives

$$\mathcal{M} = \begin{cases} 0, & (a,b) \in D, \\ \left(1 - \frac{c}{b}\right) \rho w_1, & (a,b) \in E_1, \\ \left(1 - \frac{c}{a}\right) \rho' w_1, & (a,b) \in E_2, \\ w_1, & (a,b) \in F. \end{cases}$$

We see that  $\mathcal{M}$  has a discontinuity across the curve  $\partial D$ . At the half-lines separating region F from  $E_1$  and  $E_2$ , it is continuous but not differentiable.

## 4.2. Diagram for c < 0

We now turn to the case c < 0. As before, we view c as fixed and describe the phase diagram in the *ab*-plane; see Fig. 8. There is then an anti-ferromagnetic phase

$$A = \{a, b > 0\},\tag{179}$$

and a disordered phase

$$D = \{a, b < 0, ab > c^2\},\tag{180}$$

which agrees with the case c > 0. There are also a number of intermediate phases. To describe them geometrically, we introduce the points

$$P_k = \left(\frac{k\rho'c}{(r-k)\rho}, \frac{(r-k-1)\rho c}{(k+1)\rho'}\right), \qquad k = 1, 2, \dots, r-2,$$
(181)

which are all in the region  $\{a, b < 0, ab < c^2\}$ , and

$$Q_k = \left(\frac{k\rho'c}{(r-k)\rho}, \frac{(r-k)\rho c}{k\rho'}\right), \qquad k = 1, 2, \dots, r-1$$
(182)

which are on  $\partial D = \{a, b < 0, ab = c^2\}$ . We draw r - 2 line segments connecting the origin a = b = 0 to the points  $P_j$ . We also draw a zig-zag line, consisting of the horizontal half-line to the right of  $Q_1$ , a vertical line segment from  $Q_1$  to  $P_1$ , a horizontal segment from  $P_1$  to  $Q_2$ , a vertical segment from  $Q_2$  to  $P_2$ , continuing in this way and ending with the vertical half-line above  $Q_{r-1}$ . Together with the boundaries of A and D, these line segments divide the plane into 2r - 1 additional open regions. We will write  $B_1, \ldots, B_{r-1}$  for the regions above and  $C_1, \ldots, C_r$  for those below the zig-zag line, in both cases numbered from southeast to northwest. More explicitly,

$$B_{1} = \left\{ a > \frac{\rho'c}{(r-1)\rho}, \frac{(r-1)\rho c}{\rho'} < b < 0, \ \rho^{2}(r-1)(r-2)a > 2(\rho')^{2}b \right\},$$

$$B_{k} = \left\{ a > \frac{k\rho'c}{(r-k)\rho}, \ b > \frac{(r-k)\rho c}{k\rho'}, \\ (r-k)(r-k-1)\rho^{2}a > k(k+1)(\rho')^{2}b, \\ (r-k+1)(r-k)\rho^{2}a < (k-1)k(\rho')^{2}b \right\}, \qquad 2 \le k \le r-2,$$

$$B_{r-1} = \left\{ \frac{(r-1)\rho'c}{\rho} < a < 0, \ b > \frac{\rho c}{(r-1)\rho'}, \ 2\rho^{2}a < (\rho')^{2}(r-1)(r-2)b \right\},$$
(183)

and

$$C_{1} = \left\{ b < \frac{(r-1)\rho c}{\rho'}, ab < c^{2} \right\},$$

$$C_{k} = \left\{ a < \frac{(k-1)\rho' c}{(r-k+1)\rho}, b < \frac{(r-k)\rho c}{k\rho'}, ab < c^{2} \right\}, \qquad 2 \le k \le r-1, \qquad (184)$$

$$C_{r} = \left\{ a < \frac{(r-1)\rho' c}{\rho}, ab < c^{2} \right\}.$$

As before, we write

$$\omega_D = \left(\frac{\rho}{r}, \dots, \frac{\rho}{r}; \frac{\rho'}{r}, \dots, \frac{\rho'}{r}\right).$$

The maximiser in the anti-ferromagnetic phase is

$$\omega_A = (\rho, 0, \dots, 0; 0, \dots, 0, \rho').$$

We will see that the intermediate regions correspond to the maximisers

$$\omega_{B_k} = \left(\underbrace{\frac{\rho}{k}, \dots, \frac{\rho}{k}}_{k}, \underbrace{0, \dots, 0}_{r-k}; \underbrace{0, \dots, 0}_{k}, \underbrace{\frac{\rho'}{r-k}, \dots, \frac{\rho'}{r-k}}_{r-k}\right)$$
(185)

and

$$\omega_{C_k} = \left(\underbrace{x_1, \dots, x_1}_{k-1}, x_2, \underbrace{0, \dots, 0}_{r-k}; \underbrace{0, \dots, 0}_{k-1}, y_1, \underbrace{y_2, \dots, y_2}_{r-k}\right),$$

where

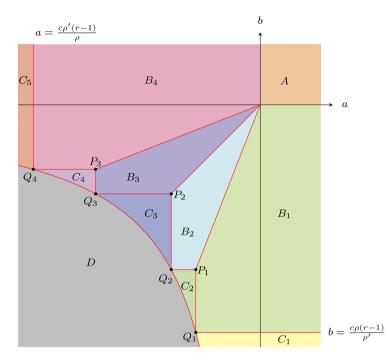


Fig. 8. The ground state phase diagram for c < 0, in the case r = 5, with the points  $P_k$  (181) and  $Q_k$  (182) as well as the regions A (179),  $B_k$  (183),  $C_k$  (184) and D (180) indicated.

$$x_1 = \frac{(r+1-k)\rho ab + \rho' bc - (r-k)\rho c^2}{k(r+1-k)ab - (k-1)(r-k)c^2},$$
(186a)

$$x_2 = \frac{(r+1-k)\rho ab - (k-1)\rho' bc}{k(r+1-k)ab - (k-1)(r-k)c^2},$$
(186b)

$$y_1 = \frac{k\rho'ab - (r-k)\rho ac}{k(r+1-k)ab - (k-1)(r-k)c^2},$$
(186c)

$$y_2 = \frac{k\rho'ab + \rho ac - (k-1)\rho'c^2}{k(r+1-k)ab - (k-1)(r-k)c^2}.$$
(186d)

The complete description of the ground state phase diagram for c < 0 is then as follows.

**Proposition 4.2.** Assume that c < 0,  $r \ge 3$  and let  $\omega^* = (\vec{x}^*; \vec{y}^*)$  be a maximiser of  $G|_{\Omega}$  with  $x_i^*$  decreasing and  $y_i^*$  increasing. If  $(a, b) \in X$ , where X is one of A,  $B_k$ ,  $C_k$  or D, then  $\omega^*$  is unique and equal to  $\omega_X$ . If (a, b) is in the interior of the line segment separating  $B_k$  from  $C_k$ , then  $\omega^*$  is also unique and given by  $\omega^* = \omega_{B_k} = \omega_{C_k}$ . Likewise, if (a, b) is in the interior of the line segment separating  $B_k$  from  $C_{k+1}$  then  $\omega^* = \omega_{B_k} = \omega_{C_{k+1}}$ . If (a, b) is in the interior of the line segment separating  $B_k$  from  $B_{k+1}$ , then there are exactly two maximisers, namely,  $\omega_{B_k}$  and  $\omega_{B_{k+1}}$ . If  $(a, b) = P_k$  (the corner between  $B_k$ ,  $B_{k+1}$  and  $C_{k+1}$ ) then there are infinitely many maximisers, which form the line segment

 $t\omega_{B_k} + (1-t)\omega_{B_{k+1}}$  for  $0 \le t \le 1$ . In the remaining cases,  $(a,b) \in \partial A$  or  $(a,b) \in \partial D$ there are also infinitely many maximisers. In the case  $\partial D$  they are determined by the conditions

$$\sqrt{-a}\left(x_i^{\star} - \frac{\rho}{r}\right) + \sqrt{-b}\left(y_i^{\star} - \frac{\rho'}{r}\right) = 0, \qquad 1 \le i \le r, \tag{187}$$

in the case a > 0, b = 0 by the conditions

$$x_1^{\star} = \rho, \qquad x_2^{\star} = \dots = x_r^{\star} = y_1^{\star} = 0,$$
 (188a)

in the case a = 0, b > 0 by the conditions

$$x_r^{\star} = y_1^{\star} = \dots = y_{r-1}^{\star} = 0, \qquad y_r^{\star} = \rho'$$
 (188b)

and, finally, for a = b = 0 by

$$x_1^* y_1^* = \dots = x_r^* y_r^* = 0. \tag{188c}$$

For convenience, we formulated Proposition 4.2 only for  $r \ge 3$ . In the case r = 2 the same statement is correct, except for the fact that the equations (188) have the unique solution  $\omega = \omega_A$ . In this case  $\omega_{B_1} = \omega_A$ , so  $\partial A$  and  $B_1$  should be considered as parts of the anti-ferromagnetic phase. Note also that there are no points  $P_k$ , and only one region  $B_k$ . This leads to exactly the same diagram as for c > 0. We already know this from the discussion after Theorem 1.2.

The proof of Proposition 4.2 follows the same strategy as that of Proposition 4.1. Since the details are more involved, we divide it into a series of lemmas.

**Lemma 4.3.** Proposition 4.2 holds if  $(a, b) \in \overline{A}$  or  $(a, b) \in \overline{D}$ .

**Proof.** The case  $(a,b) \in D$  follows immediately from (172). If  $(a,b) \in \partial D$ , (173) is replaced by

$$Q(x,y) = -\frac{1}{2}(\sqrt{-a}x + \sqrt{-b}y)^2.$$

This leads to the sign change in (187) compared to (171). Moreover the condition (174) is replaced by

$$x_1^\star \le \frac{\rho}{r} + \sqrt{\frac{b}{a}} \frac{\rho'}{r},$$

which shows that the number of maximisers is indeed infinite.

If  $(a, b) \in \overline{A}$ , that is,  $a, b \ge 0$ , we can estimate

$$Q(\vec{x}; \vec{y}) = \sum_{j=1}^{r} \left( \frac{a}{2} x_j^2 + c x_j y_j + \frac{b}{2} y_j^2 \right)$$
  
$$\leq \frac{a}{2} (x_1 + \dots + x_r)^2 + \frac{b}{2} (y_1 + \dots + y_r)^2 = \frac{a \rho^2 + b(\rho')^2}{2},$$

where we deleted the non-positive terms  $cx_jy_j$  and added the non-negative terms  $ax_ix_j$ and  $by_iy_j$  for i < j. Equality holds if and only if all those terms vanish. If a > 0 and b > 0 this can only happen if  $\omega = \omega_A$ . It is also clear that if  $(a, b) \in \partial A$  it happens under the conditions (188).  $\Box$ 

**Lemma 4.4.** Assume that  $(a,b) \notin \overline{A} \cup \overline{D}$ . Then the maximiser  $\omega^*$  in Proposition 4.2 is equal to one of the points  $\omega_{B_k}$ ,  $\omega_{C_k}$  or  $t\omega_{B_k} + (1-t)\omega_{B_{k+1}}$  for  $0 \le t \le 1$ . The last case can only happen if  $(a,b) = P_k$ .

**Proof.** Let k and l be the number of non-zero entries in  $x^*$  and  $y^*$ , respectively. Then,  $\omega^*$  is a maximiser of

$$\sum_{j=1}^{\min(k,r-l)} Q(x_j,0) + \sum_{j=r-l+1}^k Q(x_j,y_j) + \sum_{j=\max(k+1,r-l+1)}^r Q(0,y_j),$$

where the middle sum is empty if  $k+l \leq r$ . This gives the Lagrange multiplier equations

$$ax_j^{\star} = \lambda, \qquad 1 \le j \le \min(k, r - l), \qquad (189a)$$

$$ax_j^{\star} + cy_j^{\star} = \lambda, \qquad r - l + 1 \le j \le k, \qquad (189b)$$

$$cx_j^{\star} + by_j^{\star} = \mu, \qquad \qquad r - l + 1 \le j \le k, \qquad (189c)$$

$$by_j^{\star} = \mu, \qquad \max(k+1, r-l+1) \le j \le r.$$
 (189d)

We will first show that the variables  $x_j^*$  and  $y_j^*$  involved in each group of equations (189a), (189b)–(189c) and (189d) are independent of j. This is obvious if, respectively,  $a \neq 0$ ,  $ab \neq c^2$  (which holds by assumption) and  $b \neq 0$ . By symmetry, it remains to consider the case a = 0, when we must show that  $x_1^* = \cdots = x_{\min(k,r-l)}^*$ . If l = r there is nothing to prove. If l < r and k + l > r then (189a) and (189b) give  $\lambda = ax_1^* = 0$  and  $\lambda = ax_k^* + cy_k^* = cy_k^*$ , which is impossible. Finally, suppose  $k + l \leq r$ . Note that b < 0 since  $(a, b) \notin \partial A$ . It then follows from (189d) that  $y_j^* = \rho'/l$  for  $j \geq r - l + 1$ . This gives

$$G(\omega^{\star}) = \sum_{j=1}^{k} Q(x_j^{\star}, 0) + lQ(0, \frac{\rho'}{l}) = 0 + \frac{b(\rho')^2}{l},$$

which is maximised when l = r - 1 and hence k = 1, so the condition we want to prove holds automatically. So far we have proved that, if  $k + l \leq r$ ,

$$\omega^{\star} = \left(\underbrace{\frac{\rho}{k}, \dots, \frac{\rho}{k}}_{k}, \underbrace{0, \dots, 0}_{r-k}; \underbrace{0, \dots, 0}_{r-l}, \underbrace{\frac{\rho'}{l}, \dots, \frac{\rho'}{l}}_{l}\right),$$
(190)

and if k + l > r (after a change of variables)

$$\omega^{\star} = \left(\underbrace{x_1, \dots, x_1}_{r-l}, \underbrace{x_2, \dots, x_2}_{k+l-r}, \underbrace{0, \dots, 0}_{r-k}; \underbrace{0, \dots, 0}_{r-l}, \underbrace{y_1, \dots, y_1}_{k+l-r}, \underbrace{y_2, \dots, y_2}_{r-k}\right).$$
(191)

In the case (190) we have

$$G(\omega^{\star}) = kQ(\rho/k, 0) + lQ(0, \rho'/l) = \frac{a\rho^2}{2k} + \frac{b(\rho')^2}{2l}.$$

Since we assume that at least one of a and b is negative, this can only be a global maximum if k + l = r, that is,  $\omega^* = \omega_{B_k}$  (see (185)).

In the case (191), we claim that k + l = r + 1. Indeed, if  $k + l \ge r + 2$  we find as in (177) that

$$G(\vec{x}^{\star} + t(e_{r-l+1} - e_{r-l+2}); \vec{y}^{\star} + u(e_{r-l+1} - e_{r-l+2})) = G(\omega^{\star}) + 2Q(t, u),$$

which shows that  $\omega^{\star}$  is not a local maximum. We now know that

$$\omega^{\star} = \left(\underbrace{x_1, \dots, x_1}_{k-1}, x_2, \underbrace{0, \dots, 0}_{r-k}; \underbrace{0, \dots, 0}_{k-1}, y_1, \underbrace{y_2, \dots, y_2}_{r-k}\right),$$

where  $1 \le k \le r$ . Suppose first that  $2 \le k \le r - 1$ . Then, the Lagrange equations (189) give

$$ax_1 = ax_2 + cy_1, \qquad cx_2 + by_1 = by_2.$$

Inserting  $x_2 = \rho - (k-1)x_1$  and  $y_1 = \rho' - (r-k)y_2$  gives

$$kax_1 + (r-k)cy_2 = a\rho + c\rho',$$
 (192a)

$$(k-1)cx_1 + (r-k+1)by_2 = c\rho + b\rho'.$$
(192b)

If the determinant  $k(r+1-k)ab - (k-1)(r-k)c^2 \neq 0$ , we can solve this system and find that  $\omega^* = \omega_{C_k}$ . If k = 1, there is no  $x_1$  and we must have  $x_2 = \rho$ . We can still determine  $y_2$  from (192b) and obtain  $\omega^* = \omega_{C_1}$ . Similarly, the case k = r gives  $\omega^* = \omega_{C_r}$ .

It remains to consider solutions of (192) when

$$k(r+1-k)ab = (k-1)(r-k)c^{2}$$
(193)

with  $2 \le k \le r-2$ . For solutions to exist we must have (from (192))

$$(k-1)c(a\rho+c\rho') = ka(c\rho+b\rho'),$$
  
$$(r-k+1)b(a\rho+c\rho') = (r-k)c(c\rho+b\rho')$$

It is easy to solve this for (a, b), and obtain that either  $(a, b) = (-c\rho'/\rho, -c\rho/\rho')$  or  $(a, b) = P_{k-1}$ . The first solution does not satisfy (193) and can be discarded. At the point  $P_{k-1}$ , (192) reduces to

$$k(k-1)\rho'x_1 + (r-k)(r-k+1)\rho y_2 = r\rho\rho'.$$
(194)

The conditions  $x_1 \ge x_2 \ge 0$  and  $0 \le y_1 \le y_2$  mean that  $(x_1, y_2)$  is in the rectangle  $[\rho/k, \rho/(k-1)] \times [\rho'/(r-k+1), \rho'/(r-k)]$ . The line (194) passes through the corners  $(\rho/k, \rho'/(r-k)), (\rho/(k-1), \rho'/(r-k+1))$  which correspond to the points  $\omega_{B_k}$  and  $\omega_{B_{k-1}}$ . Thus, there are potential maximisers at the line segment between these points.  $\Box$ 

It remains to pair up the maximisers with the correct region.

**Lemma 4.5.** In the context of Lemma 4.4, if  $\omega^* = \omega_{C_k}$ , then either  $(a, b) \in \overline{C}_k$  or (a, b) is on the extensions of the line segments separating  $C_k$  from  $B_k$  and  $B_{k-1}$ . In the latter case,  $\omega_{C_k} = \omega_{B_k}$  and  $\omega_{C_k} = \omega_{B_{k-1}}$ , respectively.

**Proof.** Since  $(a, b) \notin A$ , at least one of a and b is negative. Suppose that a < 0. We compute

$$G(\omega_{C_k}) - G(\omega_{B_k}) = -\frac{a(k\rho'b - (r-k)\rho c)^2}{2k(r-k)\Delta_k},$$
(195)

where  $\Delta_k = k(r+1-k)ab - (k-1)(r-k)c^2$ . If  $\omega_{C_k}$  is a global maximiser, it follows that either  $\Delta_k > 0$  or  $k\rho'b = (r-k)\rho c$ . The second case is the extensions of the line segment separating  $C_k$  from  $B_k$ . It is easy to verify that in that case  $\omega_{C_k} = \omega_{B_k}$ . If  $\Delta_k > 0$  then both a and b are negative. It is then clear from (186) that the conditions  $x_2, y_1 \ge 0$  give  $(a,b) \in \overline{C}_k$ .

The case when b < 0 follows in the same way, using instead

$$G(\omega_{C_k}) - G(\omega_{B_{k-1}}) = -\frac{b((r+1-k)\rho a - (k-1)\rho' c)^2}{2(k-1)(r+1-k)\Delta_k}.$$
 (196)

**Lemma 4.6.** In the context of Lemma 4.4, if  $\omega^* = \omega_{B_k}$ , then  $(a, b) \in \overline{B}_k$ .

**Proof.** For  $2 \le k \le r-1$ , we compute

$$G(\omega_{B_k}) - G(\omega_{B_{k-1}}) = \frac{k(k-1)(\rho')^2 a - (r-k)(r+1-k)\rho^2 b}{2k(r-k)(k-1)(r+1-k)}$$

It follows that, if  $\omega_{B_k}$  is a global maximiser, then (a, b) is above or on the line separating  $B_k$  from  $B_{k-1}$ . Replacing k by k + 1 we see that, if  $1 \le k \le r-2$  then (a, b) is below or on the line separating  $B_k$  from  $B_{k+1}$ . This means that either  $(a, b) \in \overline{B}_k$ ,  $(a, b) \in C_k$  or  $(a, b) \in C_{k+1}$ . However, if  $(a, b) \in C_k$  then the expression (195) is strictly positive, so  $\omega_{B_k}$  is not a maximiser. Similarly, the case  $(a, b) \in C_{k+1}$  is excluded by (196).  $\Box$ 

We can now complete the proof of Proposition 4.2. The case  $(a, b) \in \overline{A} \cup \overline{D}$  is handled by Lemma 4.3. In all other cases except at the points  $P_k$  it follows from Lemma 4.4 that  $\omega^* = \omega_{B_j}$  or  $\omega^* = \omega_{C_j}$  for some j. We can then use Lemma 4.5 and Lemma 4.6 to exclude all possibilities for  $\omega^*$  except those mentioned in Proposition 4.2. In most cases this leaves a unique possibility. At the boundary between  $B_k$  and  $B_{k+1}$  there are two possibilities, but it is easy to verify (and clear from continuity arguments) that  $G(\omega_{B_k}) = G(\omega_{B_{k+1}})$ in this case. At the points  $P_k$  there are infinitely many possibilities, but it is again easy to verify (and clear from the Lagrange equations) that they are all maximisers.

#### 5. Multi-block models

In this section we generalise the free energy calculation of Theorem 1.1 to a class of models with  $p \ge 1$  blocks rather than just the two blocks A and B, and with certain many-body interactions.

We first need some notation. Let  $\gamma$  be a partition with all parts > 1, that is  $\gamma = (\gamma_1, \ldots, \gamma_\ell)$  is a sequence of integers  $\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_\ell \geq 2$ . We say that a permutation  $\sigma \in S_n$  has cycle-type  $\gamma$  if its non-trivial cycles, ordered from longest to shortest, have lengths  $\gamma_1, \ldots, \gamma_\ell$ . Then  $|\gamma| := \gamma_1 + \cdots + \gamma_\ell \leq n$ . Let  $C_n^{\gamma}$  be the set of permutations in  $S_n$  with cycle-type  $\gamma$ ; this is a conjugacy-class of  $S_n$ . For example, if  $\gamma = (2)$  then  $C_n^{\gamma} = C_n^{(2)}$  is the set of transpositions in  $S_n$ , and if  $\gamma = (3)$  then  $C_n^{\gamma} = C_n^{(3)}$  is the set of three-cycles in  $S_n$ . Similarly, for  $A \subseteq \{1, 2, \ldots, n\}$ , let  $C_A^{\gamma}$  denote the set of permutations of the elements of A with cycle-type  $\gamma$ .

Let  $A_1, \ldots, A_p$  form a partition of  $\{1, \ldots, n\}$  with  $|A_k| = m_k$ . Fix a finite set  $\Gamma$  of partitions  $\gamma$  with all parts > 1. We assume that n and all  $m_k$  are large enough that  $C_n^{\gamma} \neq \emptyset$  and  $C_{A_k}^{\gamma} \neq \emptyset$  for all  $\gamma \in \Gamma$ . For  $a_1^{\gamma}, \ldots, a_p^{\gamma}, c^{\gamma} \in \mathbb{R}$ , consider the Hamiltonian

$$H_n^{\rm MB} = -n \sum_{\gamma \in \Gamma} \Big( \sum_{k=1}^p \frac{a_k^{\gamma}}{|C_{A_k}^{\gamma}|} \sum_{\sigma \in C_{A_k}^{\gamma}} T_{\sigma} + \frac{c^{\gamma}}{|C_n^{\gamma}|} \sum_{\sigma \in C_n^{\gamma}} T_{\sigma} \Big), \tag{197}$$

and the partition function  $Z_n^{\text{MB}}(\beta) = \text{tr}_{\mathbb{V}}[e^{-\beta H_n^{\text{MB}}}]$ . Note that we have the scaling factor n in front of (197) rather than  $\frac{1}{n}$  as in (6). This is because the sizes of the conjugacy classes  $C_A^{\gamma}$  depend on n, for example for transpositions we have  $|C_n^{(2)}| = \binom{n}{2}$ .

The form of the Hamiltonian (197) means that spins at vertices in each block  $A_k$ interact with each other through the many-body interaction  $T_{\sigma}$  (as opposed to the pairinteraction  $T_{i,j} = T_{(i,j)}$  before), with strength constants  $a_k^{\gamma}$  dependent on the cycle type  $\gamma$  of  $\sigma$ ; as well as this, spins in all blocks together interact with each other similarly, this time with strength constants  $c^{\gamma}$ .

The operators  $T_{\sigma}$  appearing in (197) may all be written in terms of spin-matrices. Indeed, for transpositions  $\sigma = (i, j)$  this was discussed above, and for general  $\sigma$  we may write  $T_{\sigma}$  as a product of  $T_{i,j}$ 's. However, we do not pursue an explicit formula for  $T_{\sigma}$  in terms of spin-matrices.

Our result about the free energy of this model is most compactly expressed in terms of positive semidefinite Hermitian  $r \times r$  matrices X. For such a matrix, having eigenvalues  $x_1, \ldots, x_r \ge 0$ , we use the von Neuman entropy (79). We have the following:

**Theorem 5.1.** Let  $p \ge 1$  be fixed, and suppose that for all k = 1, ..., p we have that  $m_k/n \to \rho_k \in (0, 1)$  as  $n \to \infty$ . For the Hamiltonian (197), we have that the free energy is given by

$$\lim_{n \to \infty} \frac{1}{n} \log Z_n^{\rm MB}(\beta) = \max \phi_\beta(X_1, \dots, X_p), \tag{198}$$

where the maximum is taken over all positive semidefinite Hermitian  $r \times r$  matrices  $X_1, \ldots, X_p$  with  $tr[X_k] = \rho_k$ , and where

$$\phi_{\beta}(X_1, \dots, X_p) = \sum_{k=1}^p S(X_k)$$

$$+ \beta \sum_{\gamma \in \Gamma} \Big( \sum_{k=1}^p a_k^{\gamma} \prod_{j \ge 1} \operatorname{tr}[X_k^{\gamma_j}] + c^{\gamma} \prod_{j \ge 1} \operatorname{tr}[(X_1 + \dots + X_p)^{\gamma_j}] \Big).$$
(199)

Before proving Theorem 5.1 we discuss a few special cases. If we set p = 2,  $\Gamma = \{(2)\}$  and  $a_1^{(2)} = (a-c)/2$ ,  $a_2^{(2)} = (b-c)/2$  and  $c^{(2)} = c/2$ , then

$$\phi_{\beta}(X_1, X_2) = S(X_1) + S(X_2) + \frac{\beta}{2} \operatorname{tr} \left[ aX_1^2 + bX_2^2 + 2cX_1X_2 \right].$$
(200)

In fact, in this case we recover Theorem 1.1, i.e. we have max  $\phi_{\beta}(X_1, X_2) = \Phi_{\beta}^{AB}(a, b, c)$ . For details, see the discussion around (81).

If instead we set p = 1 and all  $a_k^{\gamma} = 0$  then (197) becomes

$$H_n^{\rm MB} = -n \sum_{\gamma \in \Gamma} \frac{c^{\gamma}}{|C_n^{\gamma}|} \sum_{\sigma \in C_n^{\gamma}} T_{\sigma}.$$
 (201)

We thus obtain a homogeneous model of many-body interaction on the complete graph  $K_n$ . (In fact, (201) is the image of a general central element of  $\mathbb{C}[S_n]$  under the representation T.) In this case we get that

$$\frac{1}{n}\log Z_{\beta,n}^{\rm MB} \to \max\Big(-\sum_{i=1}^r x_i\log x_i + \beta\sum_{\gamma\in\Gamma}c^{\gamma}p_{\gamma}(x_1,\ldots,x_r)\Big),\tag{202}$$

where the maximum is over all  $x_1, \ldots, x_r$  satisfying  $x_i \ge 0$  and  $\sum_{i=1}^r x_i = 1$ , and where  $p_{\gamma}(x_1, \ldots, x_r)$  denotes the power-sum symmetric polynomial

$$p_{\gamma}(x_1, \dots, x_r) = \prod_{j=1}^{\ell} (x_1^{\gamma_j} + \dots + x_r^{\gamma_j}).$$
(203)

It seems likely that Theorems 1.7 and 1.8 can be extended to multi-block cases, though we do not pursue such extensions here.

We now turn to the proof of Theorem 5.1, which follows a similar pattern to that of Theorem 1.1. We start by writing

$$H_n^{\rm MB} = -nT\Big(\sum_{\gamma\in\Gamma}\Big[\sum_{k=1}^p a_k^{\gamma}\alpha_{A_k}^{\gamma} + c^{\gamma}\alpha_n^{\gamma}\Big]\Big) = -n\sum_{\gamma\in\Gamma}\Big[\sum_{k=1}^p a_k^{\gamma}T(\alpha_{A_k}^{\gamma}) + c^{\gamma}T(\alpha_n^{\gamma})\Big]\Big), \quad (204)$$

where T is the representation of  $\mathbb{C}[S_n]$  on  $\mathbb{V}$  given in (53), and

$$\alpha_{A_k}^{\gamma} = \frac{1}{|C_{A_k}^{\gamma}|} \sum_{\sigma \in C_{A_k}^{\gamma}} \sigma \in \mathbb{C}[S_{A_k}], \qquad \alpha_n^{\gamma} = \frac{1}{|C_n^{\gamma}|} \sum_{\sigma \in C_n^{\gamma}} \sigma \in \mathbb{C}[S_n].$$
(205)

As in (55) we have a decomposition

$$\mathbb{V} \cong \bigoplus_{\lambda \vdash n, \ell(\lambda) \le r} \dim(U_{\lambda}) V_{\lambda}.$$
 (206)

Here we consider  $\mathbb{V}$  as an  $\mathbb{C}[S_n]$ -module only (we do not need the  $\operatorname{GL}_r(\mathbb{C})$ -part since we consider only the free energy and not correlations). As a  $\mathbb{C}[S_{m_1} \times \cdots \times S_{m_p}]$ -module, we have the decomposition

$$V_{\lambda} \cong \bigoplus_{\mu(1),\dots,\mu(p)} c^{\lambda}_{\mu(1),\dots,\mu(p)} V_{\mu(1)} \otimes \dots \otimes V_{\mu(p)},$$
(207)

which generalises (61). Here  $\mu(k) \vdash m_k$  for each k and the multiplicities  $c^{\lambda}_{\mu(1),\dots,\mu(p)}$  are analogs of the Littlewood–Richardson coefficients  $c^{\lambda}_{\mu,\nu}$  and have many similar properties. In particular, a full analog of Horn's inequalities holds:  $c^{\lambda}_{\mu(1),\dots,\mu(p)} > 0$  if and only if there are Hermitian matrices  $M(1),\dots,M(p)$  with spectra  $\mu(1),\dots,\mu(p)$  such that  $M(1) + \dots + M(p)$  has spectrum  $\lambda$  (see Theorem 17 of [18]).

Let us next see how  $T(\alpha_{A_k}^{\gamma})$  and  $T(\alpha_n^{\gamma})$  act on these subspaces  $V_{\mu(k)}$ . For  $m \leq n$  and  $C = C_m^{\gamma}$  the conjugacy class of  $\gamma$  in  $S_m$ , consider  $\alpha = \frac{1}{|C|} \sum_{\sigma \in C} \sigma \in \mathbb{C}[S_m]$ . For  $\mu \vdash m$ , since  $\alpha$  is central in  $\mathbb{C}[S_m]$ , it acts on the irreducible  $V_{\mu}$  as a scalar, and in fact we have

$$\alpha|_{V_{\mu}} = \frac{\chi_{\mu}(\alpha)}{d_{\mu}} \operatorname{Id}_{V_{\mu}} = \frac{\chi_{\mu}(\gamma)}{d_{\mu}} \operatorname{Id}_{V_{\mu}}, \qquad (208)$$

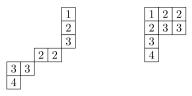


Fig. 9. Left: A skew tableau with shape  $\nu$  formed from the three partitions  $\mu(1) = (2, 1), \mu(2) = (2)$  and  $\mu(3) = (1, 1, 1)$ . Right: its rectification.

where  $\chi_{\mu}(\gamma)$  is the character of  $V_{\mu}$  evaluated at any permutation of cycle-type  $\gamma$ . This leads to the following expression analogous to (66):

$$Z_n^{\text{MB}} = \sum_{\lambda \vdash n, \ell(\lambda) \le r} \dim(U_\lambda) \sum_{\mu(1), \dots, \mu(p)} c_{\mu(1), \dots, \mu(p)}^{\lambda} d_{\mu(1)} \cdots d_{\mu(p)} \cdot \exp\left(n\beta \sum_{\gamma \in \Gamma} \left[\sum_{k=1}^p a_k^{\gamma} \frac{\chi_{\mu(k)}(\gamma)}{d_{\mu(k)}} + c^{\gamma} \frac{\chi_{\lambda}(\gamma)}{d_{\lambda}}\right]\right).$$
(209)

As before, the relevant scaling for the limit  $\lim_{n\to\infty} \frac{1}{n} \log Z_n^{\text{MB}}$  is given by letting  $\lambda/n \to \vec{z}$  and  $\mu(k)/n \to \vec{x}(k)$  for all k. Also as before,  $\dim(U_\lambda)$  is negligible on the relevant scale, and the  $d_{\mu(k)}$  obey the asymptotics of (69). Below, we prove that  $c_{\mu(1),\dots,\mu(p)}^{\lambda} \leq (n+1)^{pr^2}$  which is also too small to contribute to the limit.

What remains is to identify the limits of the expressions of the form  $\frac{\chi_{\mu}(\gamma)}{d_{\mu}}$ . The latter limits are well-known in the asymptotic representation theory of the symmetric group: Thoma's Theorem and the Vershik–Kerov Theorem (see e.g. [11, Corollary 4.2 and Theorem 6.16]) imply that if  $\mu/n \to \vec{x} = (x_1, \ldots, x_r)$ , then

$$\frac{\chi_{\mu}(\gamma)}{d_{\mu}} \to p_{\gamma}(x_1, \dots, x_r), \tag{210}$$

where  $p_{\gamma}$  is the power-sum symmetric polynomial given in (203). Writing  $\vec{x}(k) = \lim_{n \to \infty} \mu(k)/n$  and  $\vec{z} = \lim_{n \to \infty} \lambda/n$ , we conclude that the contributing  $\vec{x}(k)$  and  $\vec{z}$  are spectra of Hermitian matrices  $X_1, \ldots, X_p$  and  $Z = X_1 + \cdots + X_p$ , respectively, where  $\operatorname{tr}[X_k] = \rho_k$ . Re-writing the free energy in terms of these matrices, as in (80) and (97), we obtain the claim (199).

It remains to verify the bound  $c_{\mu(1),\dots,\mu(p)}^{\lambda} \leq (n+1)^{pr^2}$ . We use the following combinatorial description of  $c_{\mu_1,\dots,\mu_p}^{\lambda}$  which is mentioned just after Proposition 13 of [18]. Form a skew shape  $\nu$  by stacking  $\mu(1),\dots,\mu(p)$  from bottom left to top right, such that the lower left corner of  $\mu(k)$  just touches the upper right corner of  $\mu(k-1)$  as in Fig. 9. Fix any semistandard tableau  $\tau_{\lambda}$  of shape  $\lambda$ , to be concrete let us say that the first row of  $\tau_{\lambda}$  consists of  $\lambda_1$  1's, the second row of  $\lambda_2$  2's etc. Then  $c_{\mu(1),\dots,\mu(p)}^{\lambda}$  is the number of semistandard tableaux  $\sigma_{\nu}$  of skew shape  $\nu$  whose *rectification* equals  $\tau_{\lambda}$ . For a full description of the rectification, see [17, Section 1.2], but in brief terms the rectification is obtained by 'sliding' the numbered boxes of  $\sigma_{\nu}$  until a non-skew shape is obtained. To see the claimed bound, note that in order to obtain the tableau  $\tau_{\lambda}$ , the number of boxes labelled 1 in  $\nu$  must equal the number of boxes labelled 1 in  $\lambda$ , and similarly for labels 2, 3, etc. Thus, for each row of  $\nu$  we have at most

$$(\lambda_1+1)(\lambda_2+1)\cdots(\lambda_r+1) \le (n+1)^r$$

choices of entries (from 0 to  $\lambda_1$  1's, from 0 to  $\lambda_2$  2's etc). Since  $\nu$  has at most pr rows, the total number of choices is  $\leq [(n+1)^r]^{pr}$ , as claimed.  $\Box$ 

## Appendix A. The trace-inequality (81)

The inequality (81) appears e.g. in [25, Prop. 9.H.1.g-h], but we give here an almost self-contained proof based on Birkhoff's theorem, adapted from the discussion in [36]. The problem is to maximise (respectively, minimise) tr[XY] subject to the condition that X, Y are nonnegative definite Hermitian matrices with fixed spectra  $x_1 \ge x_2 \ge$  $\cdots \ge x_r \ge 0$  and  $y_1 \ge y_2 \ge \cdots \ge y_r \ge 0$ . Equivalently, since there are unitary matrices U and V such that  $U^*XU = D_x = \text{diag}(x_1, \ldots, x_r)$  and  $V^*YV = D_y = \text{diag}(y_1, \ldots, y_r)$ , the goal is to extremise

$$\operatorname{tr}[UD_x U^* V D_y V^*] = \operatorname{tr}[D_x U^* V D_y V^* U]$$
(211)

over unitaries U, V. Writing  $W = U^*V$  we may equivalently extremise over the unitary W,

$$\operatorname{tr}[D_x W D_y W^*] = \sum_{i,j=1}^r x_i w_{i,j} y_j w_{j,i}^* = \sum_{i,j=1}^r x_i y_j |w_{i,j}|^2.$$
(212)

Define the matrix  $P = (p_{i,j})_{i,j=1}^r$  where  $p_{i,j} = |w_{i,j}|^2$ . Since W is unitary, P is doubly stochastic (rows and columns sum to 1). We have by the above

$$\max_{W} \operatorname{tr}[D_x W D_y W^*] \le \max_{P} \sum_{i,j=1}^r x_i y_j p_{i,j},$$
(213)

where the second max is over doubly-stochastic matrices P (and similarly for the min). The function to be maximised on the right-hand-side is linear in P and the set of doublystochastic matrices is convex and compact. Thus the maximum (as well as the minimum) is attained at an extreme point of the set of doubly-stochastic matrices. By Birkhoff's theorem [25, Theorem 2.A.2], the extreme points are the permutation matrices  $\Pi$ . Since permutation matrices are real orthogonal (hence unitary) it follows that

$$\max_{W} \operatorname{tr}[D_x W D_y W^*] = \max_{\Pi} \operatorname{tr}[D_x \Pi D_y \Pi^*]$$
(214)

and similarly for the minimum. Thus, we must only find the permutation  $\pi$  which maximises or minimises the function

$$\sum_{j=1}^{r} x_j y_{\pi(j)}.$$
(215)

The maximum is obtained for the identity permutation and the minimum for the reversal of  $12 \dots r$ .  $\Box$ 

#### Appendix B. Equivalence of $Q_{i,j}$ and $P_{i,j}$ in the wb-model

In this second appendix we study two representations of the walled Brauer algebra  $\mathbb{B}_{n,m}(r)$ . We will prove in Lemma B.1 that they are isomorphic for all  $r \geq 2$ . This will in particular give the equivalence of our WB-model with the same model, but with each  $Q_{i,j}$  replaced with  $P_{i,j}$ . More generally Lemma B.1 gives the same statement on general graphs. To be precise, if  $G = A \cup B$  is any graph (with  $A \cap B = \emptyset$ ), with  $E_A$  the set of edges between two vertices in  $A, E_B$  similar, and  $E_{AB}$  those between a vertex of A and a vertex of B, then for all  $a, b, c \in \mathbb{R}$ , the following two Hamiltonians are unitarily equivalent:

$$H = -\sum_{\{i,j\}\in E_A} aT_{i,j} - \sum_{\{i,j\}\in E_B} bT_{i,j} - \sum_{\{i,j\}\in E_{AB}} cP_{i,j}$$

$$H' = -\sum_{\{i,j\}\in E_A} aT_{i,j} - \sum_{\{i,j\}\in E_B} bT_{i,j} - \sum_{\{i,j\}\in E_{AB}} cQ_{i,j}.$$
(216)

This in particular shows that the models with interactions  $P_{i,j}$  and  $Q_{i,j}$  are equivalent on any bipartite graph; the equivalence of partition functions was proved by Aizenman and Nachtergaele in [2]. The same statement (and in fact slightly stronger) holds on non-bipartite graphs, but only for r odd. Indeed, (216) is very similar to a statement on the model (4): for any graph G with edge set E, for any  $L_1, L_2 \in \mathbb{R}$ , the following two Hamiltonians are unitarily equivalent for r odd:

$$H = -\sum_{\{i,j\}\in E} L_1 T_{i,j} + L_2 P_{i,j}$$
  
$$H' = -\sum_{\{i,j\}\in E} L_1 T_{i,j} + L_2 Q_{i,j}.$$
 (217)

This is proved with Lemma B.1 of [29], which is the equivalent of our Lemma B.1 below, but for the full Brauer algebra.

The representations we consider are defined as follows. First, we let  $|a\rangle$  denote the standard basis for  $\mathbb{C}^r$ , indexed using  $a \in \{-S, -S+1, \ldots, S\}$  where S = (r-1)/2, and recall that  $\mathbb{V} = (\mathbb{C}^r)^{\otimes n}$ . Let  $T : \mathbb{B}_{n,m}(r) \to \operatorname{End}(\mathbb{V})$  satisfy

$$T(\overline{i,j}) = Q_{i,j}, \qquad T(i,j) = T_{i,j}, \qquad (218)$$

where we recall that  $T_{i,j}$  is the transposition operator, and  $\langle a_i, a_j | Q_{i,j} | b_i, b_j \rangle = \delta_{a_i,a_j} \delta_{b_i,b_j}$ . Similarly, define  $\tilde{T} : \mathbb{B}_{n,m}(r) \to \operatorname{End}(\mathbb{V})$  by

$$\tilde{T}(\overline{i,j}) = P_{i,j}, \qquad \tilde{T}(i,j) = T_{i,j}, \qquad (219)$$

where we recall that  $\langle a_i, a_j | P_{i,j} | b_i, b_j \rangle = (-1)^{a_i - b_i} \delta_{a_i, -a_j} \delta_{b_i, -b_j}$ .

**Lemma B.1.** For all  $r \geq 2$ , and all n, the representations T and  $\tilde{T}$  of  $\mathbb{B}_{n,m}(r)$  are isomorphic via a unitary transformation.

**Proof.** The proof follows closely that of Lemma B.1 of [29]. For r odd, the lemma actually follows from that result by restricting the two representations there to the walled Brauer algebra. So let r be even. The elements (i, j) and  $(\overline{i, j})$  generate the algebra  $\mathbb{B}_{n,m}(r)$ , so we aim to find an invertible linear function  $A : \mathbb{V} \to \mathbb{V}$  such that

$$A^{-1}T_{i,j}A = T_{i,j}, (220)$$

for all  $1 \leq i < j \leq m$  and  $m < i < j \leq n$ , and

$$A^{-1}Q_{i,j}A = P_{i,j}, (221)$$

for all  $1 \leq i \leq m < j \leq n$ . By the Schur–Weyl duality for the general linear and symmetric groups (55), the first condition holds if and only if  $A = \alpha^{\otimes m} \otimes \gamma^{\otimes n-m}$  for some  $\alpha, \gamma \in \operatorname{GL}_r(\mathbb{C})$ . Then the second condition also holds if and only if  $(\alpha \otimes \gamma)^{-1}Q_{i,j}(\alpha \otimes \gamma) = P_{i,j}$  for all  $1 \leq i \leq m < j \leq n$ , which holds if and only if:

$$(-1)^{a_{i}-b_{i}}\delta_{a_{i},-a_{j}}\delta_{b_{i},-b_{j}} = \sum_{c_{i},c_{j},d_{i},d_{j}} (\alpha^{-1})_{a_{i},c_{i}} (\gamma^{-1})_{a_{j},c_{j}} \delta_{c_{i},c_{j}} \delta_{d_{i},d_{j}} \alpha_{d_{i},b_{i}} \gamma_{d_{j},b_{j}}$$

$$= \sum_{c,d} (\alpha^{-1})_{a_{i},c} (\gamma^{-1})_{a_{j},c} \alpha_{d,b_{i}} \gamma_{d,b_{j}}$$

$$= (\alpha^{-1}\gamma^{-\intercal})_{a_{i},a_{j}} (\alpha^{\intercal}\gamma)_{b_{i},b_{j}}.$$
(222)

Now recall that we assumed r to be even, meaning that S and all the indices  $a_i, a_j, b_i, b_j$  are odd multiples of  $\frac{1}{2}$ . Thus  $(-1)^{a_i} = -(-1)^{-a_i}$  and (222) holds if

$$\alpha^{\mathsf{T}}\gamma = -(\gamma^{\mathsf{T}}\alpha)^{-1} = \begin{bmatrix} & & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & & \\$$

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The matrix on the right in (223) is an involution whose transpose is its negative, so it suffices to check this for  $\alpha^{\intercal}\gamma$ . Further, the matrix consists of the block matrices  $(-1)^{r/2} \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}$  aligned along the antidiagonal, where  $i = \sqrt{-1}$ .

Such a pair  $\alpha$ ,  $\gamma$  exists: for example let

$$g_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} i & i \\ -1 & 1 \end{bmatrix}, \qquad g_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 & 1 \\ -i & -i \end{bmatrix},$$

take  $\alpha$  to be block-antidiagonal with blocks  $g_1$ , and take  $\gamma$  to be block-diagonal with blocks  $(-1)^{r/2}g_2$ . Since  $g_1^{\mathsf{T}}g_2 = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}$ ,  $\alpha^{\mathsf{T}}\gamma$  is as required. Further, since both  $\alpha$  and  $\gamma$  are unitary, so is A.  $\Box$ 

We can further prove the following statement, that in the S = 1 (r = 3) case, under a certain choice of the isomorphism of representations, the spin matrices are antisymmetric. This verifies that we can use Theorems 1.8 and 1.7 on the S = 1 (r = 3)nematic model with magnetisation term given by a spin matrix  $S^{(k)}$ , k = 1, 2, 3, at each vertex, as noted at the end of Section 1.5.

**Lemma B.2.** For all k = 1, 2, 3, there exists a (unitary) isomorphism  $\psi_n = \psi^{\otimes n}$  of the representations T and  $\tilde{T}$  of  $\mathbb{B}_{n,m}(3)$  (with  $\psi_n^{-1}\tilde{T}(b)\psi_n = T(b)$  for all  $b \in \mathbb{B}_{n,m}(3)$ ), such that  $\psi_n^{-1}S^{(k)}\psi_n$  is anti-symmetric (its transpose is its negative).

**Proof.** In Lemma B.1, we showed that representations T and  $\tilde{T}$  of  $\mathbb{B}_{n,m}(3)$  are isomorphic. In particular, since r = 3 odd, we used the Lemma B.1 of [29]. In that Lemma, one found that a valid isomorphism  $\psi_n$  was given by  $\psi_n = \psi^{\otimes n}$ , where  $\psi$  is a  $3 \times 3$  (unitary) matrix

$$\psi = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{-1}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} \end{bmatrix},$$
(224)

where  $i = \sqrt{-1}$ . One then can verify the required identities directly, using the explicit spin matrices

$$S^{(1)} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0 \end{bmatrix}, \ S^{(2)} = \frac{1}{i\sqrt{2}} \begin{bmatrix} 0 & 1 & 0\\ -1 & 0 & 1\\ 0 & -1 & 0 \end{bmatrix}, \ S^{(3)} = \begin{bmatrix} 1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1 \end{bmatrix}. \quad \Box$$
(225)

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