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Three-spin models in two dimensions: generalisations of the Baxter–Wu model

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Abstract. We show that a large class of two-dimensional pure three-spin statistical mechanical models can be analysed using a vector Coulomb gas. This can be done with the same methods previously applied to the 2D XY model and results of similar rigour obtained. The models considered here are generalisations of the Baxter–Wu model, with the Hamiltonian being given by a sum of three-spin interactions over a triangular lattice.

1. Introduction

A large class of 2D models, the so-called Z_n or vector Potts models, are defined by the Hamiltonian

$$H = J \sum_{\langle ij \rangle} V(\theta_i - \theta_j). \tag{1}$$

Here V is a periodic function of θ and $\langle ij \rangle$ label nearest-neighbour sites on a lattice. If θ_i is defined continuously, we have the familiar XY model (Kosterlitz and Thouless 1973), and if $\theta_i = 2\pi n/p$ takes on discrete values, given by n integer, the resultant model is called a p-state clock model or Z_p model since the Hamiltonian is invariant under the symmetry operations corresponding to the cyclic group of order p. Using the duality structure of this class of models, it is possible to show that for $p > p_c$ (and for the Z_p model $p_c = 4$) there is a 'massless' phase where correlations in the order parameter decay algebraically as a function of distance (José *et al* 1977, Elitzur *et al* 1979).

These models are by now thoroughly understood. The analysis relies heavily on renormalisation group ideas applied to a 2D Coulomb gas. The reader is referred to a seminal paper (José *et al* 1977) for the background to this problem. By contrast, this paper considers an *a priori* very different type of model on a triangular lattice with a three-spin interaction instead of a two-spin interaction as in (1).

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2. Model

The simplest type of three-spin model is the Baxter–Wu model (Baxter and Wu 1973) on a triangular lattice. The Hamiltonian for this model is written in the form

$$-\beta H = J \sum_{\langle \boldsymbol{R}, \boldsymbol{R}', \boldsymbol{R}'' \rangle} S(\boldsymbol{R}) S(\boldsymbol{R}') S(\boldsymbol{R}'') \tag{2}$$

where $\langle \boldsymbol{R}, \boldsymbol{R}', \boldsymbol{R}'' \rangle$ denotes all triplets ('plaquettes') on a triangular lattice, the spin $S(\boldsymbol{R}) = \pm 1$ and β is the reduced temperature. This model is easily seen to be one of a class of models defined by

$$-\beta H = J \sum_{\langle t \rangle} \cos(\theta_t). \tag{3}$$

We here define $\langle t \rangle$ to be all triplets $\langle \boldsymbol{R}, \boldsymbol{R}', \boldsymbol{R}'' \rangle$ and $\theta_t = \theta(\boldsymbol{R}) + \theta(\boldsymbol{R}') + \theta(\boldsymbol{R}'')$. The angles θ are given by $\theta = 2\pi n/p$. For the Baxter–Wu model, $p = 2$ so that $\theta = 0$ or π. Clearly, any value of p defines a model and in the limit of $p = \infty$, we have a three-spin generalisation of the XY model with a continuous symmetry. These models will be called the $Z_p \times Z_p$ or $U(1) \times U(1)$ models depending on whether or not p is finite or infinite. The reason for this notation will become clear shortly.

It has been shown (Alcaraz and Jacobs 1982a, b) that these models have a self-dual structure similar to that of the XY and clock models on the square lattice. Numerical Monte Carlo simulations suggest (Alcaraz and Jacobs 1982a, b) the existence of a massless phase for $p \geqslant p_c$ where $p_c = 5$. In this paper, we will show that these models can be analysed using an analysis similar to that which has previously been applied to the XY model and clock models. In particular, we derive a Coulomb gas reformulation of the three-spin models using a duality transformation and analyse this using a renormalisation group approach analogous to that employed for the XY model (Kosterlitz and Thouless 1973). With the Villain form (Villain 1975) for the interaction potential replacing the cosine in equation (3), these models are self-dual and correlation inequalities are proved in the appendix which show that for sufficiently large p, there must exist three phases as the temperature is raised from zero. The phase that exists for intermediate values of temperature is massless, i.e. there is no long-range order in the system, and correlations decay algebraically with distance.

In order to gain some familiarity with the model defined by equation (3), we shall first explore some symmetries of this model. We first take θ to be defined continuously on the interval 0 to 2π (i.e. $p = \infty$). The ground state has a $U(1) \times U(1)$ symmetry, determined by two angles arbitrarily labelled ψ_a and ψ_b. The ground state is shown in figure 1. The value of the angle $\Phi(\boldsymbol{R})$ at each site is either ψ_a, ψ_b or $-(\psi_a + \psi_b) = \psi_c$ depending on which of the three sublattices a, b or c the site '$\boldsymbol{R}$' occupies. Thus there are two independent U(1) generators for the ground state configurations.

We define the order parameter $\Psi(\boldsymbol{R})$ by

$$\Psi(\boldsymbol{R}) = \exp[\mathrm{i}\theta(\boldsymbol{R})] \tag{4}$$

and the order parameter correlation function $C_2(\boldsymbol{R} - \boldsymbol{R}')$ by

$$C_2(\boldsymbol{R} - \boldsymbol{R}') = \langle \Psi(\boldsymbol{R}) \Psi^*(\boldsymbol{R}') \rangle. \tag{5}$$

Since the Hamiltonian is invariant under the replacement $\theta(\boldsymbol{R}) \to \theta(\boldsymbol{R}) + \Phi(\boldsymbol{R})$ where $\Phi(\boldsymbol{R}) = \Phi_a$, Φ_b or $(-\Phi_a - \Phi_b)$ depending on whether site '$\boldsymbol{R}$' is on sublattice a, b or c, the Mermin–Wagner theorem (Mermin and Wagner 1966) implies that fluctuations

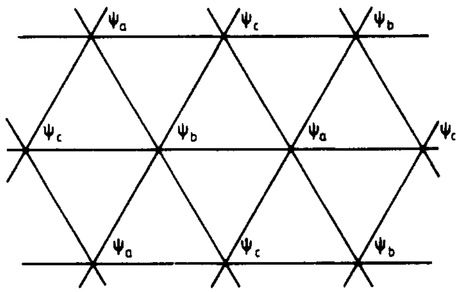

Figure 1. The degenerate ground states of the three-spin model are shown. The spins on each of the sublattices a, b or c are defined by the angles ψ_a, ψ_b or $\psi_c = -(\psi_a + \psi_b)$. Since there is freedom to choose ψ_a and ψ_b, the ground state has a U(1) × U(1) symmetry.

are large enough to cause $C_2(\boldsymbol{R} - \boldsymbol{R}')$ to vanish for any finite separation at finite temperature if $\boldsymbol{R}$ and $\boldsymbol{R}'$ are on different sublattices. In the case where $\theta(\boldsymbol{R})$ takes on p discrete values, we find a p^2 degenerate ground state. For the $p = 2$ Baxter–Wu model, this corresponds to the four-fold degenerate ground state shown in figures 2(a) and (b). (The two other ground states equivalent to that shown in 2(a) but translated by an elementary lattice vector are not shown.)

The case $p = 3$ of our model corresponds to being on the ferromagnetic–antiferromagnetic coexistence line of the model considered by Schick and Griffiths (1977). It has been established that the transition on this line is a first-order transition (Enting and Wu 1982, Saito 1982, Wu 1982), and this is consistent with the results that we shall present.

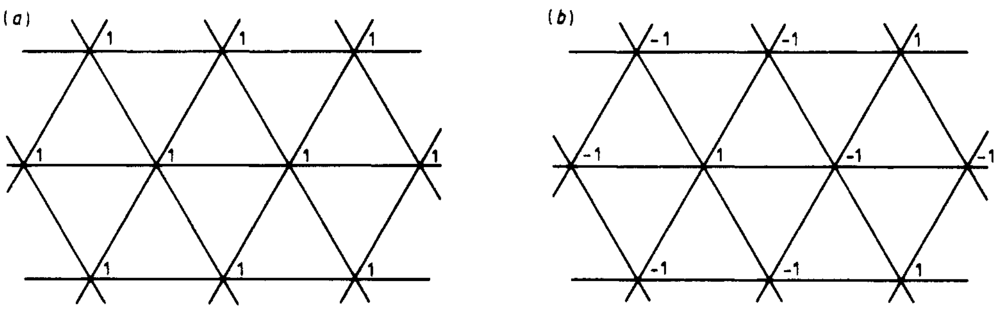

Figure 2. (a) The singlet ground state of the $p = 2$ Baxter–Wu model is shown. (b) One of the three equivalent states in the triplet ground state of the Baxter–Wu model is shown. The other two are related to this by a translation by an elementary lattice vector.

3. Gaussian approximation

In order to obtain a more precise understanding of the model in equation (3) in the case $p = \infty$, let us consider the Gaussian model defined by

$$-\beta H = \tfrac{1}{2} J \sum_{\langle t \rangle} (\theta_t)^2 \tag{6}$$

where the sum $\langle t \rangle$ again is over all triplets of a triangular lattice. This approximates equation (3) at low temperature for the cosine potential. We can write the angle $\theta(\boldsymbol{R})$ using a Fourier transform as

$$\theta(\boldsymbol{R})=\frac{1}{\Omega^{1/2}}\sum_{\boldsymbol{k}\in\mathrm{BZ}}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\theta_{\boldsymbol{k}} \tag{7}$$

where Ω is the number of sites in the system. The sum is over the first Brillouin zone sketched in figure 3. We can then write the Hamiltonian as

$$-\beta H=-\frac{J}{2}\sum_{\boldsymbol{k}}|\theta_{\boldsymbol{k}}|^2\left(6+4\sum_{n=1}^{3}\cos(\boldsymbol{k}\cdot\boldsymbol{\varepsilon}_n)\right). \tag{8}$$

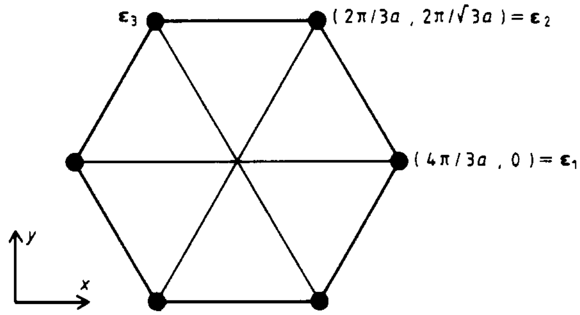

Figure 3. The reciprocal lattice unit cell of the lattice of lattice constant 'a' is shown.

The lattice vectors $\boldsymbol{\varepsilon}_n$ are sketched in figure 4. The Gaussian Green function $(1/J)g_{\mathrm{D}}(\boldsymbol{R}-\boldsymbol{R}')=\langle\theta(\boldsymbol{R})\theta(\boldsymbol{R}')\rangle$ is then easily calculated to be

$$\frac{1}{J}g_{\mathrm{D}}(\boldsymbol{R}-\boldsymbol{R}')=\frac{1}{\Omega^{1/2}}\sum_{\boldsymbol{k}\in\mathrm{BZ}}\exp[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')]\langle|\theta_{\boldsymbol{k}}|^2\rangle \tag{9}$$

$$=\frac{v}{J}\int_{\mathrm{BZ}}\frac{\mathrm{d}^2\boldsymbol{k}}{(2\pi)^2}\frac{\exp[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')]}{[6+4\sum_{n=1}^{3}\cos(\boldsymbol{k}\cdot\boldsymbol{\varepsilon}_n)]} \tag{10}$$

where $v=\sqrt{3}a^2/2$ is the area of the unit cell in real space. The integrand has poles

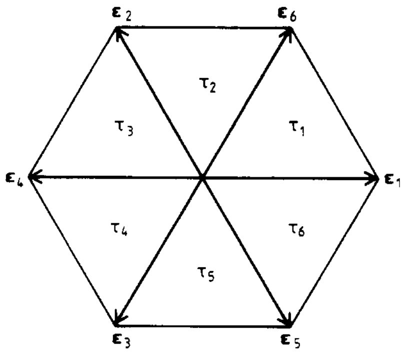

Figure 4. There are six equivalent elementary lattice vectors of the triangular lattice labelled $\varepsilon_1, \ldots, \varepsilon_6$. With each site '$i$', there are associated six plaquettes. There is a minus sign associated with τ_n when n is odd and a plus sign when n is even.

whenever the equality

$$F(\boldsymbol{k}) = 6 + 4 \sum_{n=1}^{3} \cos(\boldsymbol{k} \cdot \boldsymbol{\varepsilon}_n) = 0 \tag{11}$$

is valid. This condition occurs in the six corners of the first Brillouin zone at the vectors generated by 30° rotations of the vector $[4\pi/(3a), 0]$. But, because each corner is split between three zones, there are in fact only two poles per Brillouin zone. Expanding $F(\boldsymbol{k})$ around these poles, one finds

$$F(\boldsymbol{k}_0 + \boldsymbol{\delta}) \simeq \tfrac{3}{2} a^2 \boldsymbol{\delta}^2 + \dots \tag{12}$$

where $\boldsymbol{k}_0$ corresponds to any corner of the Brillouin zone. Since $C_2(\boldsymbol{R} - \boldsymbol{R}')$ is given in the Gaussian approximation as

$$C_2(\boldsymbol{R} - \boldsymbol{R}') = \exp[\langle \theta(\boldsymbol{R}) \theta(\boldsymbol{R}') \rangle - \langle \theta^2(\boldsymbol{R}) \rangle] = \exp[g_D(\boldsymbol{R} - \boldsymbol{R}') - g_D(\boldsymbol{0})]$$

the correlation function $C_2(\boldsymbol{R} - \boldsymbol{R}')$ is non-zero when $g_D(\boldsymbol{R} - \boldsymbol{R}') - g_D(\boldsymbol{0})$ is finite. This occurs when the condition

$$\exp[\mathrm{i}\boldsymbol{k}_0 \cdot (\boldsymbol{R} - \boldsymbol{R}')] = 1 \tag{13}$$

is valid. This is equivalent to the requirement that $\boldsymbol{R}$ and $\boldsymbol{R}'$ be on the same triangular sublattice. The $C_2(\boldsymbol{R} - \boldsymbol{R}')$ is given by

$$C_2(\boldsymbol{R} - \boldsymbol{R}') \simeq \exp\left(\frac{\sqrt{3}}{2} \frac{a^2}{J} 2 \int_{|\boldsymbol{\delta}| < 1/a} \frac{\mathrm{d}^2 \boldsymbol{\delta}}{(2\pi)^2} \frac{\{\exp[\mathrm{i}\boldsymbol{\delta} \cdot (\boldsymbol{R} - \boldsymbol{R}')] - 1\}}{\tfrac{3}{2} a^2 \boldsymbol{\delta}^2} \right) \tag{14}$$

$$\propto \exp\left[-\frac{1}{\sqrt{3}\pi J} \ln\left(\frac{|\boldsymbol{R} - \boldsymbol{R}'|}{a} \right) \right] \tag{15}$$

$$= \left(\frac{|\boldsymbol{R} - \boldsymbol{R}'|}{a} \right)^{-1/\sqrt{3}\pi J}. \tag{16}$$

If $\boldsymbol{R}$ and $\boldsymbol{R}'$ are not on the same sublattice, the result is zero.

Using a similar analysis, we can calculate the three-point correlation

$$C_3(\boldsymbol{R}_1, \boldsymbol{R}_2, \boldsymbol{R}_3) = \langle \exp\{\mathrm{i}[\theta(\boldsymbol{R}_1) + \theta(\boldsymbol{R}_2) + \theta(\boldsymbol{R}_3)]\} \rangle. \tag{17}$$

This has a non-zero value only if the equality

$$\exp(\mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{R}_1) + \exp(\mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{R}_2) + \exp(\mathrm{i}\boldsymbol{k}_0 \cdot \boldsymbol{R}_3) = 0 \tag{18}$$

is valid. This is true if and only if $\boldsymbol{R}_1$, $\boldsymbol{R}_2$ and $\boldsymbol{R}_3$ belong to the three different sublattices. The condition has obvious analogues for higher-order correlation functions.

4. Conversion to Coulomb gas and duality transformations

Let us return to the original Hamiltonian, but instead of the cosine interaction in equation (3), we take the Villain potential. This is given by

$$-\beta V_J(\theta) = -\ln\left(\sum_{n=-\infty}^{\infty} \exp[-\tfrac{1}{2} J (\theta - 2\pi n)^2] \right). \tag{19}$$

The partition function can then be written as

$$Z = \mathrm{Tr}\,\exp\Big(-\sum_{\langle t\rangle} \tfrac{1}{2}J(\theta_t - 2\pi N_t)^2\Big) \tag{20}$$

where

$$\mathrm{Tr} = \sum_{\{N_t\}} \prod_{\boldsymbol{R}} \int \mathrm{d}\theta(\boldsymbol{R}). \tag{21}$$

Thus there are plaquette variables N_t and site variables $\theta(\boldsymbol{R})$. When $\theta(\boldsymbol{R}) = 2\pi n/p$, the theory is self-dual. As previously calculated (Alcaraz and Jacobs 1982b), the self-dual point is given by

$$1/T_c = \beta_c = p/2\pi. \tag{22}$$

A dual transformation can be made when $p = \infty$. In this case we generate a Coulomb gas, and the rest of this section describes this calculation.

Using the Poisson summation formula, the partition function Z can be rewritten as

$$Z = \mathrm{Tr}\,\exp\Big(-\tfrac{1}{2}J\sum_{\langle t\rangle}(\theta_t - 2\pi\phi_t)^2 + 2\pi\mathrm{i}\sum_{\langle t\rangle} N_t\phi_t\Big) \tag{23}$$

where

$$\mathrm{Tr} = \prod_{\langle \boldsymbol{R}\rangle}\Big(\int \mathrm{d}\theta(\boldsymbol{R})\Big)\prod_{\langle t\rangle}\Big(\int \mathrm{d}\phi_t\Big)\prod_{\langle t'\rangle}\Big(\sum_{N_{t'}=-\infty}^{\infty}\Big). \tag{24}$$

Note that we have defined $\theta_t = \theta(\boldsymbol{R}) + \theta(\boldsymbol{R}') + \theta(\boldsymbol{R}'')$ with $\boldsymbol{R}, \boldsymbol{R}', \boldsymbol{R}''$ defined by the triplet t. Thus $\theta(\boldsymbol{R})$ is defined on *sites* of the triangular lattice, while there is a configurational sum over the ϕ_t. The variables ϕ_t and integers N_t live on the plaquettes.

The integral over ϕ_t can now be done to give

$$Z = \mathrm{Tr}\,\exp\Big(-\frac{1}{2J}\sum_{\langle t\rangle} N_t^2 + \mathrm{i}\sum_{\langle t\rangle} N_t\theta_t\Big) \tag{25}$$

where

$$\mathrm{Tr} = \prod_{\langle \boldsymbol{R}\rangle}\Big(\int \mathrm{d}\theta(\boldsymbol{R})\Big)\prod_{\langle t\rangle}\Big(\sum_{N_t=-\infty}^{\infty}\Big). \tag{26}$$

The integral over $\mathrm{d}\theta(\boldsymbol{R})$ can now be performed. This gives a delta function over the sum of all integers $\{N_{t_l}\}$ such that the triplets t_l surround the site $\boldsymbol{R}$ (see figure 3). Thus the partition function can be rewritten as

$$Z = \mathrm{Tr}\,\exp\Big(-\frac{1}{2J}\sum_{\langle t\rangle} N_t^2\Big)\prod_{\langle \boldsymbol{R}\rangle}\delta\Big(\sum_{l} N_{t_l}\Big). \tag{27}$$

We now define the variable τ_t to be $(+1)$ on 'up' triangles (Δ) on the lattice and to be (-1) on the 'down' triangles (∇). This enables us to define a new integer-valued field $M(\boldsymbol{R})$ associated with the site $\boldsymbol{R}$ on the original lattice by

$$N_t = \tau_t \sum_{\boldsymbol{R}_t} M(\boldsymbol{R}_t) \tag{28}$$

where $\boldsymbol{R}_t$ label the sites surrounding the triplet 't'. The integers N_t so defined satisfy the delta function constraint in equation (27) so that the partition function can be rewritten without a constraint as

$$Z = \mathrm{Tr}\exp\left(-\frac{1}{2J}\sum_{R}(M_t)^2\right). \tag{29}$$

Here again $M_t = M(\boldsymbol{R}) + M(\boldsymbol{R}') + M(\boldsymbol{R}'')$ where $\boldsymbol{R}, \boldsymbol{R}', \boldsymbol{R}''$ label the sites associated with the triplet t and an overall harmless constant has been dropped. Using the Poisson summation formula again, we can rewrite this as

$$Z = \mathrm{Tr}\exp\left(-\frac{1}{2J}\sum_{t}(\phi_t)^2 + 2\pi\mathrm{i}\sum_{\boldsymbol{R}}\phi(\boldsymbol{R})N(\boldsymbol{R})\right) \tag{30}$$

where

$$\mathrm{Tr} = \prod_{\boldsymbol{R}}\left(\sum_{N(\boldsymbol{R})=-\infty}^{\infty}\right)\prod_{\boldsymbol{R}'}\left(\int \mathrm{d}\phi(\boldsymbol{R}')\right) \tag{31}$$

and the variable is the sum over the three-site variables of the triplet 't':

$$\phi_t = \phi(\boldsymbol{R}) + \phi(\boldsymbol{R}') + \phi(\boldsymbol{R}''). \tag{32}$$

Thus the original problem has been converted to an explicitly Gaussian model with integer 'vortex' charges $N(\boldsymbol{R})$. These are the analogues of the vortex charges in the ordinary XY model and reflect the periodicity of the interactions in the original Hamiltonian.

It might be of interest to draw a vortex configuration in this model. The vorticity is the sum of θ_t around each vertex, counting each 'down' triangle with a minus sign and each 'up' triangle with a plus sign. The angle θ_t is defined to be between $-\pi$ and π. When the spin configuration is a conventional plus vortex on sublattice 'a', a minus vortex on sublattice 'b' and nothing on lattice 'c', the vorticity in the triplet model is zero everywhere except at the point a in figure 5. This is therefore an elementary vortex configuration.

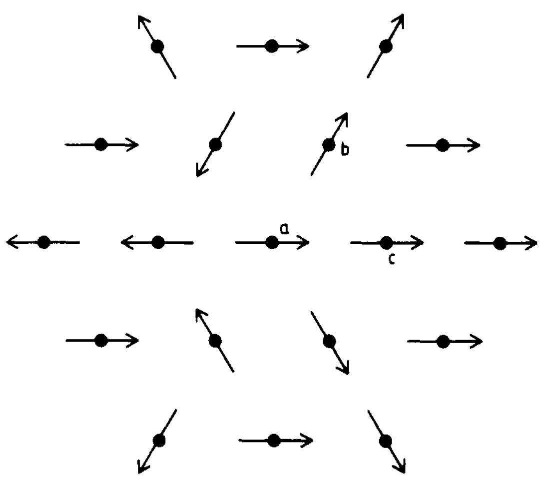

Figure 5. The core region of a vortex centred at the point a on the a sublattice. This configuration is specified by $\theta_a = a$, $\theta_b = \phi$, $\theta_c = -\phi$, where ϕ is the polar angle.

Using the results from §2, we can integrate over $\phi(\boldsymbol{R})$ to find an interaction between the vortex charges $N(\boldsymbol{R})$:

$$Z = \operatorname{Tr} \exp\Big(-(2\pi)^2 J \sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} N(\boldsymbol{R}) N(\boldsymbol{R}') g_{\mathrm{D}}(\boldsymbol{R}-\boldsymbol{R}')\Big) \tag{33}$$

where $g_{\mathrm{D}}(\boldsymbol{R}-\boldsymbol{R}')$ is given in equation (10) and each distinct pair $\langle \boldsymbol{R}, \boldsymbol{R}'\rangle$ is counted once. The definition of the trace is

$$\operatorname{Tr} = \prod_{\boldsymbol{R}} \Big(\sum_{N(\boldsymbol{R})=-\infty}^{\infty} \Big). \tag{34}$$

Expanding about the poles of $F(\boldsymbol{k})$, we find the following expression for $g_{\mathrm{D}}(\boldsymbol{R})$:

$$g_{\mathrm{D}}(\boldsymbol{R}-\boldsymbol{R}') = \frac{N^2}{\sqrt{3}} \Big(\frac{1}{6} \sum_{\boldsymbol{k}_0} \exp[\mathrm{i}\boldsymbol{k}_0 \cdot (\boldsymbol{R}-\boldsymbol{R}')]\Big) \int \frac{\mathrm{d}^2 k}{(2\pi)^2} \frac{\exp[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')]}{k^2}. \tag{35}$$

The lattice sum $P(\boldsymbol{R}-\boldsymbol{R}')$ is defined by

$$P(\boldsymbol{R}-\boldsymbol{R}') = \tfrac{1}{6} \sum_{\boldsymbol{k}_0} [\exp(\mathrm{i}\boldsymbol{k}_0 \cdot (\boldsymbol{R}-\boldsymbol{R}')]. \tag{36}$$

This sum is simply one if $\boldsymbol{R}$ and $\boldsymbol{R}'$ are on the same sublattice a, b or c and is $-\frac{1}{2}$ otherwise. Thus $g(\boldsymbol{R}-\boldsymbol{R}')$ defined by

$$g(\boldsymbol{R}-\boldsymbol{R}') = g_{\mathrm{D}}(\boldsymbol{R}-\boldsymbol{R}') - P(\boldsymbol{R}-\boldsymbol{R}') g_{\mathrm{D}}(\boldsymbol{0}) \tag{37}$$

is finite. In order to incorporate this more elegantly and to gain some insight we define the vector charges $\boldsymbol{m}(\boldsymbol{R})$ by

$$\boldsymbol{m}(\boldsymbol{R}) = N(\boldsymbol{R}) \boldsymbol{\varepsilon}_j \tag{38}$$

where $j = 1, 2$ or 3 respectively if $\boldsymbol{R}$ is on sublattice a, b or c. The vectors $\boldsymbol{\varepsilon}_j$ are shown in figure 4. We can then rewrite the Hamiltonian as

$$H = -(2\pi)^2 J \Big(\sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} \boldsymbol{m}(\boldsymbol{R}) \cdot \boldsymbol{m}(\boldsymbol{R}') g(\boldsymbol{R}-\boldsymbol{R}') + \sum_{\langle \boldsymbol{R},\boldsymbol{R}'\rangle} g_{\mathrm{D}}(\boldsymbol{0}) \boldsymbol{m}(\boldsymbol{R}) \cdot \boldsymbol{m}(\boldsymbol{R}') \Big). \tag{39}$$

Use has been made of the fact that the dot product of the vectors $\boldsymbol{\varepsilon}_j \cdot \boldsymbol{\varepsilon}_k$ is either 1 or $-\frac{1}{2}$. Note that the last term is divergent unless the vector charge neutrality condition

$$\sum_{\boldsymbol{R}} \boldsymbol{m}(\boldsymbol{R}) = 0 \tag{40}$$

is valid. We have thus mapped our original problem exactly onto a vector Coulomb gas of the form studied by several authors (Nelson and Halperin 1979, Young 1979). This Coulomb gas lacks an angular coupling of the relative orientation of the separation vector and the vector charge. This model was discussed (Nelson 1978) as a special case of the model analysed by Young (1979). In the context of a replica calculation, this model was also analysed by Cardy and Ostlund (1982) and is related to the *XY* model in a random symmetry breaking field.

In order to make progress in the next section, it is useful to obtain the constant term 'C' in $g(\boldsymbol{R}-\boldsymbol{R}')$:

$$g(\boldsymbol{R}-\boldsymbol{R}') \sim \frac{1}{\sqrt{3}\pi} \ln\Big(\frac{|\boldsymbol{R}-\boldsymbol{R}'|}{a}\Big) + C. \tag{41}$$

This constant can be approximately evaluated quite easily, since

$$g(\boldsymbol{\varepsilon}_r) = g_{\rm D}(\boldsymbol{\varepsilon}_r) + \tfrac{1}{2}g_{\rm D}(\mathbf{0}) = \tfrac{1}{12}\left(4\sum_{n=1}^{3} g_{\rm D}(\boldsymbol{\varepsilon}_n) + 6g_{\rm D}(\mathbf{0})\right). \qquad (42a, b)$$

It is easily seen that $g(\boldsymbol{\varepsilon}_n) = \frac{1}{12}$, when this expression is used with equation (10). Hence the complete Hamiltonian in equation (39) can be rewritten as

$$-\beta H = -\frac{4\pi J}{\sqrt{3}} \sum_{\langle \boldsymbol{R}, \boldsymbol{R}'\rangle} \boldsymbol{m}(\boldsymbol{R}) \cdot \boldsymbol{m}(\boldsymbol{R}') \ln\left(\frac{|\boldsymbol{R}-\boldsymbol{R}'|}{a}\right) + \ln y \sum_{\langle \boldsymbol{R}\rangle} \boldsymbol{m}^2(\boldsymbol{R}) \qquad (43)$$

where $y = \exp(-\pi^2 J/3)$.

5. Renormalisation group

Having mapped our three-spin model into a Coulomb gas, we can take over the renormalisation group equations analysed by Nelson (1978) and Young (1979). We find that

$$\mathrm{d}J/\mathrm{d}l = -8\sqrt{3}\pi^3 J^2 y^2, \qquad \mathrm{d}y/\mathrm{d}l = (2 - 2\pi J/\sqrt{3})y + 2\pi y^2. \qquad (44a, b)$$

We may also introduce a symmetry breaking field into the problem:

$$-\beta H = \sum_{t} V_J(\theta_t) + \sum_{\langle \boldsymbol{R}\rangle} V_{h_p}(\theta(\boldsymbol{R})). \qquad (45)$$

When $h_p = \infty$, this Hamiltonian corresponds to the $Z_p \times Z_p$ model. By using the Poisson summation formula on the partition function defined by (45) we can rewrite the partition function as

$$Z = \mathrm{Tr}\exp\left(\sum_{\langle t\rangle} V_J(\theta_t^{\cdot}) + \mathrm{i}p\sum_{\boldsymbol{R}} [\tilde{N}(\boldsymbol{R})\theta(\boldsymbol{R}) - h_p^{-1}\tilde{N}^2(\boldsymbol{R})]\right). \qquad (46)$$

Thus the interaction between the dual charged $\tilde{N}(\boldsymbol{R})$ and the equivalent dual vector charges $\underset{\sim}{\boldsymbol{m}}(\boldsymbol{R})$ is precisely of the form in equations (38)–(40) with $\tilde{N}(\boldsymbol{R})$ replacing $N(\boldsymbol{R})$, $\underset{\sim}{\boldsymbol{m}}(\boldsymbol{R})$ replacing $\boldsymbol{m}(\boldsymbol{R})$ and $(2\pi p)^2/J$ replacing J. Therefore we can identify the complete renormalisation group to lowest order in y and $y_p = \exp(-h_p^{-1})$ as

$$\mathrm{d}J/\mathrm{d}l = 2\sqrt{3}\pi p^2 y_p^2 - 8\sqrt{3}\pi^3 J^2 y^2, \qquad (47a)$$

$$\mathrm{d}y_p/\mathrm{d}l = [2 - p^2/(2\sqrt{3}\pi J)]y_p + 2\pi y_p^2, \qquad (47b)$$

$$\mathrm{d}y/\mathrm{d}l = (2 - 2\pi J/\sqrt{3})y + 2\pi y^2. \qquad (47c)$$

This form reduces to the correct renormalisation group equations when $y = 0$ and $y_p = 0$. The renormalisation group flows for $h_p = 0$ are shown in figure 6. When $J < \sqrt{3}/\pi$, vortices are unbound and we have a paramagnetic phase.

It is of interest to compute the critical value of J for the $U_1 \times U_1$ Villain model. At infinite length scales, J then renormalises to $\sqrt{3}/\pi$. In order to do this, we linearise the equations in the variable J. Defining $x = 2 - 2\pi J/\sqrt{3}$, and $Y = 2\pi y$, we find

$$\mathrm{d}x/\mathrm{d}l = -12Y^2, \qquad \mathrm{d}Y/\mathrm{d}l = xY + Y^2. \qquad (48a, b)$$

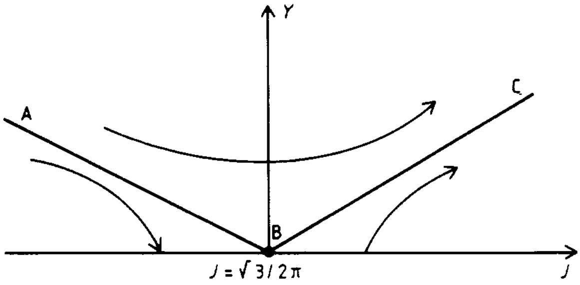

Figure 6. The renormalisation group flows for the reduced fugacity variable $Y = 2\pi y$ against J are shown. The incident separatrix has slope $-\frac{1}{4}$, and the outgoing separatrix slope $\frac{1}{3}$. For starting points below the line AB, the renormalisation flows onto the axis $Y = 0$, corresponding to a Gaussian phase. Otherwise, flows to large Y occur, indicating the possibility of a paramagnetic phase.

The solutions $Y = mx$ exist for $m = +\frac{1}{3}$ or $-\frac{1}{4}$. The solution of $-\frac{1}{4}$ corresponds to the incident separatrix to the point $y = 0$, $J = \sqrt{3}/\pi$, so that we have the equation

$$-\tfrac{1}{4}(2 - 2\pi J_c^0/\sqrt{3}) = 2\pi \exp(-\pi^2 J_c^0/3) \tag{49}$$

that gives an estimate for the critical value J_c^0 for the Villain $U_1 \times U_1$ model. We can use the estimate for J_c^0 to estimate an upper bound for p so that for $p > p_c$ the $Z_p \times Z_p$ model has a Gaussian phase.

In the appendix we show inequalities (A14) and (A 20) which state that correlation functions of order (disorder) variables are weaker (stronger) in the $U_1 \times U_1$ model than in the self-dual $Z_p \times Z_p$ discrete Villain model for a given value of the coupling constant J. Assume that the $Z_p \times Z_p$ Villain model has only two phases, so that the phase transition is given at the self-dual point: $J_{SD} = p/2\pi$. Therefore, for $J < J_{SD}$, the phase must be disordered. But if $J > J_c^0$, inequality (A14) implies that the discrete Villain model must be ordered or massless. We therefore have a contradiction if $p > p_c = 2\pi J_c^0$. The transition cannot then be given by the self-dual point, hence three phases must occur, the intermediate phase being ordered or massless. This intermediate phase cannot be ordered because in this case the inequality (A 20) will be contradicted. If this intermediate phase is ordered the self-dual nature of the intermediate phase implies that the LHS of (A20) must be non-zero in this phase, but the RHS corresponds to the disordered high temperature phase of the model (29). Since this is zero, it contradicts the inequality. Using the value of $J_c^0 \simeq 0.90$ obtained by equation (49), we have proved that for $p > p_c = 2\pi J_c^0 \simeq 5.68$ all discrete models will exhibit an intermediate massless phase between the high and low temperature phases.

6. Phase diagrams

When $h_p = 0$ we have the $U_1 \times U_1$ model; for $J > J_0^c$ there is a Gaussian-like low temperature massless phase with power law decay of correlation with distance according to equation (16). At the critical temperature, the correlation length diverges as

$$l \propto \exp(t^{-\bar{\nu}}) \tag{50}$$

where $\bar{\nu} = \frac{2}{5}$ and the exponent η in $C_2(\boldsymbol{R}) \propto |\boldsymbol{R}|^{-\eta}$ has the value $\frac{1}{3}$. The value for $\bar{\nu}$ is a consequence of the analysis of the renormalisation group equations by Young (1979), and we do not discuss the details here.

When $h_p \neq 0$, a phase diagram as shown in figures 7(*a*)–(*c*) results. We know from the renormalisation group that if $p > 2\sqrt{3}$, the Gaussian phase extends away from the axis $h_p = 0$. However, Monte Carlo results suggest that the Gaussian phase is absent for $p < 5$ in the $Z_p \times Z_p$ model, that corresponds to the limit $h_p = \infty$, whereas it seems to be present for $p \geq 5$. This is also consistent with our estimate of $p_c \leq 5.7$. Thus we believe that a global phase diagram as in figure 7(*a*) for $p \geq 5$ is likely. When $p = 4$, we believe that a phase diagram as shown in figure 7(*b*) is likely, although it is conceivable that slow relaxation in the Monte Carlo calculation induced hysteresis for $p = 4$ and caused Alcaraz and Jacobs (1982a) to conclude that the $Z_4 \times Z_4$ model did not have a massless phase. The validity of their conclusions is not contradicted by the estimate for p_c.

Finally for $p = 2$ or 3, both the renormalisation group analysis and Monte Carlo calculations are consistent with the phase diagram shown in figure 7(*c*).

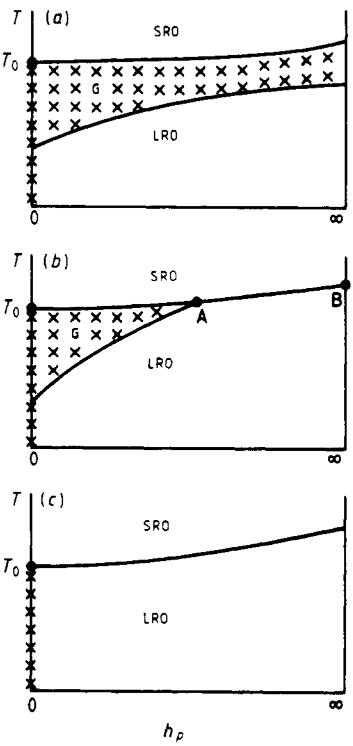

Figure 7. The phase diagram that we believe to be likely for the U(1)×U(1) model with a p-fold symmetry breaking field of strength h_p is shown as a function of $T = 1/J$. The vertical axis $h_p = \infty$ corresponds to the $Z_p \times Z_p$ model and $h_p = 0$ corresponds to the U(1)×U(1) model that has a massless phase for $T < T_0 = 1/J_0^c$. There are three types of phases, an ordered p^2-fold (LRO) degenerate phase, a Gaussian massless phase (G), and a paramagnetic phase (SRO). The points represented by × denote the region that is Gaussian (massless). (*a*) $p \geq 6$. (*b*) $2\sqrt{3} < p \leq 5.7$. For weak values of h_p a Gaussian phase exists, whereas this phase is suppressed for sufficiently large values of h_p. The line AB is probably a line of first-order phase transitions. (*c*) $p < 2\sqrt{3}$. There is no Gaussian phase except on the line $h_p = 0$.

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Appendix

This appendix shows that the correlations in the $Z_p \times Z_p$ Villain model are weaker than the correlations in the $U(1)\times U(1)$ Villain model for the same value of the coupling constant J. This fact is used in the text to estimate p_c so that for $p > p_c$ the $Z_p \times Z_p$ Villain model has a massless phase.

Let us consider the m-point correlation function for the $Z \times Z_p$ model:

$$C_p(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_m) = \left\langle \cos\left(\sum_{i=1}^{m} \theta(\boldsymbol{r}_i) \right) \right\rangle \tag{A1}$$

where $\theta(\boldsymbol{r}) = (2\pi/p) q(\boldsymbol{r})$ ($q(\boldsymbol{r}) = 0, 1, \ldots, p-1$) are Z_p-variables. For the Vaillain potential this correlation function is given by

$$C_p^{\mathrm{V}}(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_m) = \frac{1}{Z_p^{\mathrm{V}}} \sum_{\{\theta(r)=0\}}^{2\pi(p-1)/p} \sum_{\{N_t=-\infty\}}^{\infty} \exp\left(-\frac{\beta}{2} \sum_t (\theta_t - 2\pi N_t)^2 \right) \times \exp\left(\sum_{\boldsymbol{r}'} Q(\boldsymbol{r}')\theta(\boldsymbol{r}') \right) \tag{A2}$$

where Z_p^{V} is the partition function, θ_t the triangular variable defined in equation (3) and

$$Q(\boldsymbol{r}') = \sum_{i=1}^{m} \delta_{\boldsymbol{r}', \boldsymbol{r}_i}. \tag{A3}$$

By using the Poisson summation formula, we introduce an integer field l_t defined on the triangles; then performing the $\theta(\boldsymbol{r})$ summation, we obtain

$$C_p^{\mathrm{V}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_m) = \frac{1}{Z_p^0} \sum_{l_t=-\infty}^{\infty} \exp\left(-\sum_t \frac{l_t^2}{2\beta} \right) \prod_{\boldsymbol{r}'} \delta_p[l_t^*(\boldsymbol{r}') + Q(\boldsymbol{r}')] \tag{A4}$$

in which $\delta_p[l_t^*(\boldsymbol{r}') + Q(\boldsymbol{r}')]$ is a Kronecker delta modulo p, and $l_t^*(\boldsymbol{r}')$ is the sum of the l_t variables that has $\boldsymbol{r}$ as a corner and Z_p^0 is the numerator with $Q = 0$. We can write the above expression in terms of a normal Kronecker delta by introducing an integer field $m(\boldsymbol{r})$ defined on sites so that

$$C_p^{\mathrm{V}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_m) = \frac{1}{Z_p^0} \sum_{\{l_t=-\infty\}}^{\infty} \sum_{\{m(r')=-\infty\}}^{\infty} \times \prod_{\boldsymbol{r}'} \delta[l_t^*(\boldsymbol{r}') + Q(\boldsymbol{r}') + pm(\boldsymbol{r}')] \exp\left(-\frac{1}{2\beta} \sum_t l_t^2 \right). \tag{A5}$$

For the U(1) case we reach a similar result, only differing in that already in (A4) we obtain a normal Kronecker delta, thus

$$C_\infty^{\mathrm{V}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_m) = \frac{1}{Z_\infty^0} \sum_{l_t=-\infty}^{\infty} \prod_{\boldsymbol{r}'} [\delta(l_t^*(\boldsymbol{r}') + Q(\boldsymbol{r}')] \exp\left(-\frac{1}{2\beta} \sum_t l_t^2 \right). \tag{A6}$$

Following Elitzur *et al* (1979) we define the interpolating function

$$C_H^{\rm V}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_m)=\frac{1}{Z_H^0}\sum_{\{l_t=-\infty\}}^{\infty}\sum_{\{m(\boldsymbol{r}')=-\infty\}}^{\infty}\prod_{\boldsymbol{r}'}\delta[l_t^*(\boldsymbol{r}')+Q(\boldsymbol{r}')+pm(\boldsymbol{r}')]$$
$$\times\exp\left(-\frac{1}{2\beta}\sum_t l_t^2-\frac{1}{H}\sum_{\boldsymbol{r}'}m^2(\boldsymbol{r})\right) \tag{A7}$$

with Z_H^0 being the same function of the denominator with $Q=0$. This function has the desired properties that for $H=0$ the $m(\boldsymbol{r})$ field must be zero so that we obtain the correlation for the U(1) case; otherwise when $H\to\infty$ the $m(\boldsymbol{r})$ field has a fugacity y equal to 1 so that we have the correlation for the Z_p case.

We want to show that for a given temperature, as we decrease H the correlation decreases; i.e.

$$\partial C_H^{\rm V}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_m)/\partial H\geqslant 0. \tag{A8}$$

Taking the derivative of (A7) we have

$$\frac{\partial}{\partial H}C_H^{\rm V}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_m)$$
$$=\frac{1}{(HZ_H^0)^2}\sum_{\{l_t=-\infty\}}^{\infty}\sum_{\{m(\boldsymbol{r}')=-\infty\}}^{\infty}\sum_{\{l'_t=-\infty\}}^{\infty}\sum_{\{m'(\boldsymbol{r}')=-\infty\}}^{\infty}$$
$$\times\prod_{\boldsymbol{r}'}\{\delta[l_t^*(\boldsymbol{r}')+Q(\boldsymbol{r}')+pm(\boldsymbol{r}')]\delta[l_t'^*(\boldsymbol{r}')+pm'(\boldsymbol{r}')]\}$$
$$\times\exp\left(-\frac{1}{2\beta}\sum_t(l_t^2+l_t'^2)-\frac{1}{H}\sum_{\boldsymbol{r}'}(m^2(\boldsymbol{r}')+m'^2(\boldsymbol{r}'))\right)\sum_{\boldsymbol{r}''}(m^2(\boldsymbol{r}'')-m'^2(\boldsymbol{r}'')). \tag{A9}$$

We now make the following convenient change of variables in the triplet variables:

$$\rho_t=l_t+l'_t,\qquad \rho'_t=l_t-l'_t \tag{A10a,b}$$

and in the site variables

$$\mu(\boldsymbol{r})=m(\boldsymbol{r})+m'(\boldsymbol{r}),\qquad \mu'(\boldsymbol{r})=m(\boldsymbol{r})-m'(\boldsymbol{r}). \tag{A10c,d}$$

This transformation has the virtue of making symmetric the δ-requirements in (A9)

$$\delta[\rho_t^*(\boldsymbol{r}')+Q(\boldsymbol{r})+p\mu(\boldsymbol{r})]\delta[\rho_t'^*(\boldsymbol{r})+Q(\boldsymbol{r})+p\mu'(\boldsymbol{r})]. \tag{A11}$$

However the new variables ρ_t, ρ'_t and μ, μ' are not independent; they must be even or odd simultaneously (same parity). We can make them independent if we multiply by the term

$$\prod_t\tfrac{1}{2}[1+(-1)^{\rho_t+\rho'_t}]\prod_{\boldsymbol{r}'}\tfrac{1}{2}[1+(-1)^{\mu(\boldsymbol{r}')+\mu'(\boldsymbol{r}')}]. \tag{A12}$$

We can expand the above product of triangles (lattice points) in terms of a general subset of triangles T (of lattice points L); so that we finally obtain

$$\frac{d}{dH} C^{V}_{H} = \frac{1}{(Z^0_H H)^2} \sum_{r''} \sum_{L} \sum_{T} \bigg\{ \bigg[\sum_{\rho_t, \mu} \prod_{r'} \delta[\rho^*_t(r') + p\mu(r') + Q(r')] \times \mu(r'') \exp\Big(-\frac{1}{4\beta} \sum_t \rho_t^2 - \frac{1}{2H} \sum_{r'} \mu^2(r') \Big) (-1)^{\{\sum_{t\in T} \rho_t + \sum_{j\in L} \mu(j)\}} \bigg] \times \bigg[\sum_{\rho'_t, \mu'} \prod_{r'} \delta[\rho'_t(r') + p\mu'(r') + Q(r')] - \mu'(r'') \times \exp\Big(-\frac{1}{4\beta} \sum_t \rho'^2_t - \frac{1}{2H} \sum_r \mu^2(r) \Big) (-1)^{\{\sum_{t\in T} \rho'_t + \sum_{j\in L} \mu'(j)\}} \bigg] \bigg\}. \tag{A13}$$

It is now clear that the quantity in brackets is positive so that (A8) is proved. This implies that at a given temperature

$$\Big\langle \cos\Big(\sum_{i=1}^{m} \theta(r_i) \Big) \Big\rangle^{V}_{p} \geqslant \Big\langle \cos\Big(\sum_{i=1}^{m} \theta(r_i) \Big) \Big\rangle^{V}_{U(1)}. \tag{A14}$$

We can also consider correlation functions of disorder variables

$$D(r_1, r_2, \ldots, r_m) = \Big\langle \cos\Big(\sum_{i=1}^{m} \frac{2\pi}{p} \phi(r_i) \Big) \Big\rangle \tag{A15}$$

with $(2\pi/p)\phi(r_i)$, $(0, 1, \ldots, p-1)$ being the dual Z_p variable at the site r_i.

In a similar way to that in which (A7) was analysed we introduce the interpolating function

$$D^{V}_{H}(r_1, r_2, \ldots, r_m) = \frac{1}{Z^0_H} \sum_{\{\phi(r) = -\infty\}}^{\infty} \sum_{s_t = -\infty}^{\infty} \exp\Big(-\frac{1}{2\beta} \sum_t (\phi_t - ps_t)^2 \Big) \times \exp\Big(-\frac{1}{H} \sum s_t^2 \Big) \cos\Big(\frac{2\pi}{p} \sum_{r'} Q(r)\phi(r) \Big) \tag{A16}$$

with Z^0_H being a normalising constant and $Q(r)$ as defined in (A3). As before, in the limit $H \to 0$ ($H \to \infty$) the field s_t must be zero (assume whatever integer value) so that we have the correlation in the U(1) (Z_p) case.

Let us now consider the derivative

$$\frac{\partial}{\partial H} D^{V}_{H}(r_1, \ldots, r_m) = \frac{1}{(HZ^0_H)^2} \sum_{\{\phi(r)\}} \sum_{\{s_t(r)\}} \sum_{\{\phi'(r)\}} \sum_{\{s'_t(r)\}} \times \exp\Big(-\frac{1}{2\beta} \sum_t [(\phi_t - ps_t)^2 + (\phi'_t - ps'_t)^2] - \frac{1}{H} \sum_t (s_t^2 + s'^2_t)^2 \Big) \times \Big(\sum_t (s_t^2 - s'^2_t) \Big) \cos \frac{2\pi}{p} \sum_r Q(r)\phi(r). \tag{A17}$$

We can symmetrise the above expression over prime and non-prime variables by replacing $\cos(2\pi/N)\,\Sigma_r\, Q(\boldsymbol{r})\phi(\boldsymbol{r})$ by

$$\frac{1}{2}\left(\cos\frac{2\pi}{p}\sum_r Q(\boldsymbol{r})\phi(\boldsymbol{r})-\cos\frac{2\pi}{p}\sum_r Q(\boldsymbol{r})\phi'(\boldsymbol{r})\right)$$

$$=-\sin\left(\frac{\pi}{p}\sum_r Q(\boldsymbol{r})[\phi(\boldsymbol{r})+\phi'(\boldsymbol{r})]\right)\sin\left(\frac{\pi}{p}\sum_r Q(\boldsymbol{r})[\phi(\boldsymbol{r})-\phi'(\boldsymbol{r})]\right). \tag{A18}$$

It is convenient to make the change of variables

$$\mu(\boldsymbol{r})=\phi(\boldsymbol{r})+\phi'(\boldsymbol{r}),\qquad \mu'(\boldsymbol{r})=\phi(\boldsymbol{r})-\phi'(\boldsymbol{r}),$$
$$\rho_t=s_t+s'_t,\qquad \rho'_t=s_t-s'_t. \tag{A19}$$

Of course ρ, ρ' and μ, μ' are not independent, but we can restore their independence by adding a term like (A12). Then replacing the new variables, and expanding the term (A12) in terms of a subset of triangles (T) and sites, we obtain

$$\frac{\partial}{\partial H}D_H^{\mathrm{V}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_m)$$
$$=-\frac{1}{(Z_H^0 H)^2}\sum_t\sum_L\sum_T$$
$$\times\left\{\left[\sum_{\mu,\rho_{t'}}\exp-\sum_{t'}\left(\frac{1}{4\beta}(\mu-p\rho_{t'})^2+\frac{1}{2H}\rho_{t'}'^2\right)\rho_t\sin\frac{\pi}{p}\sum_r Q(\boldsymbol{r})\mu(\boldsymbol{r})\right]\right.$$
$$\left.\times\left[\sum_{\mu'\rho_{t'}}\exp-\sum_{t'}\left(\frac{1}{4\beta}(\mu'-p\rho'_{t'})^2+\frac{1}{2H}\rho_{t'}'^2\right)\rho'_t\sin\frac{\pi}{p}\sum_r Q(\boldsymbol{r})\mu'(\boldsymbol{r})\right]\right\}.$$

The term in brackets is clearly positive so that

$$\partial D_H^{\mathrm{V}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_m)/\partial H\leqslant 0.$$

Hence

$$D_p^{\mathrm{V}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_m)\leqslant D_{\mathrm{U}(1)}^{\mathrm{V}}(\boldsymbol{r}_1,\ldots,\boldsymbol{r}_m). \tag{A20}$$

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