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A theory of kinematics for the Potts model

E J S Lage

Laboratório de Física, Faculdade de Ciências, 4000 Porto, Portugal

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Abstract. A master equation formulation of the kinetic, q-state Potts model is presented. It is shown that this formulation reduces to Glauber's dynamics in the Ising limit. The single-spin problem is considered and the properties of its $q-1$, temperature dependent relaxation times are studied. The linear chain problem is much harder than in the Glauber case—a variational method is used to obtain a lower bound for the dynamical critical exponent ($z \geqslant 3$ for $q > 2$). A discussion of these and related problems is presented.

1. Introduction

The simplest generalisation of the Ising model is, perhaps, the Potts model (see, e.g., Wu 1982 for a review). Consider a lattice whose sites are labelled by $i = 1, 2, \ldots, N$. At each site, associate an object (usually called a spin) which can exist in any of q different (orthogonal) states, labelled by $\alpha = 1, 2, \ldots, q$. Let $P_i^{(\alpha)}$ be the projection operator onto the α state of the spin located at site i. In its simplest formulation, the Potts Hamiltonian is

$$\mathcal{H} = -\sum_{(ij)} J_{ij} \bar{P}_i \cdot \bar{P}_j - \sum_i \bar{H}_i \cdot \bar{P}_i. \tag{1}$$

Here, the first term describes a pair interaction and the dot product is an abbreviated notation for $\Sigma_\alpha P_i^{(\alpha)} P_j^{(\alpha)}$—hence, spins couple only if they are in the same state. The last term represents an applied field.

It is easy to show that for $q = 2$ one recovers the Ising model; also, the limit $q = 1$, taken in a convenient way, is equivalent to the percolation model (other limits are discussed by Wu 1982). In zero field and for nearest-neighbour interaction, the q-state Potts model presents a great variety of transitions which depend both on q and d, the space dimensionality.

In $d = 1$ (any q), the transition occurs at zero temperature; the model is trivially solved and the correlation length ξ is found:

$$\xi^{-1} = -\log \frac{e^{\beta J} - 1}{e^{\beta J} + q - 1} \approx q\, e^{-\beta J} \tag{2}$$

where β is the inverse temperature and the last expression applies in the limit $T = 0$.

In higher dimensionalities the transition occurs at finite temperature and a line $q_c(d)$ is found above which the transition is first order. Certainly, $q_c(2) = 4$ and $q_c(d) = 2$ for $d > 4$. Also, the infinite range model is easily solved and it does show a first-order transition for $q > 2$.

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The critical behaviour strongly depends on d and q. The q dependence arises from the underlying permutation group of the order parameter.

The equilibrium properties of the Potts model are, therefore, reasonably well understood, although they still form the subject of very active research. The situation is, however, completely different with respect to the dynamical behaviour of the Potts model—leaving aside Monte Carlo simulations and the Ising model dynamical studies, it appears that there is just one analytical work related to the dynamical properties of the q-state Potts model (Forgacs *et al* 1980). (This work will be discussed below.) Obviously, the study of the dynamical properties should prove to be very interesting, namely the way critical dynamics depends on q and d, the behaviour of transport properties near the different types of phase transitions the model exhibits, etc. Besides, comparison with Monte Carlo or experimental results should prove a crucial test of the model or its approximations.

It is the purpose of this paper to present a Glauber-like approach (Glauber 1963) to the dynamics of the Potts model. It must be stressed, at this point, that even in its simplest formulation there is no unique way to generalise Glauber's dynamics for $q > 2$. The choice we made was based on the criterion of simplicity and the requirement that Glauber's equation should be recovered for $q = 2$. As an illustration of our theory, we study the relaxation of a single spin under a constant field (§ 3): for general field direction, there are $q-1$ relaxation times and even in the particular case of a field pointing in one of the Potts directions, we find different longitudinal and transverse relaxation times. The one-dimensional model (§ 4), which is trivially solved for $q = 2$, is much more complicated for $q > 2$; we were unable to find an explicit solution and we just present a variational calculation which yields a lower bound for the critical dynamical exponent ($z \geqslant 3$ for $q > 2$). Finally, we discuss the results (§ 5) and comment on further lines of research.

2. Basic theory

In this section, we shall introduce the necessary formalism and discuss the requirements for the establishment of a master equation for the Potts model.

We have already introduced the projection operators $P^{(\alpha)}$; from their definition, the following properties are easily established:

$$P^{(\alpha)}P^{(\beta)} = \delta_{\alpha\beta}P^{(\alpha)} \qquad \sum_{\alpha} P^{(\alpha)} = \mathbb{1}, \qquad \operatorname{Tr} P^{(\alpha)} = 1. \tag{3a, b, c}$$

We shall below have to use a related, traceless operator

$$\pi^{(\alpha)} = P^{(\alpha)} - q^{-1}. \tag{4}$$

Notice that

$$\operatorname{Tr} \pi^{(\alpha)}\pi^{(\beta)} = \delta_{\alpha\beta} - q^{-1}. \tag{5}$$

These operators act on the kets $|\alpha\rangle$ defining the space of the states. It will be sometimes preferable to define equivalent operators which act on functions $F(\alpha) = \langle\alpha|F\rangle$ of the states—such operators will be denoted by the same letter with a hat, e.g.,

$$\hat{P}^{(\alpha)}F(\beta) = \delta_{\alpha\beta}F(\alpha).$$

We now introduce operators that change the states. They are obviously unique for $q=2$ but the choice is no longer unique for $q>2$; as we said earlier, our choice is dictated by simplicity and we define shift operators $\psi^{(r)}(r=0,\ldots,q-1)$ by

$$\psi^{(r)}|\alpha\rangle=|\alpha-r\rangle. \tag{6}$$

In here, it is understood that the labels α and $\alpha+q$ denote the same state. We also define the associated operators $\hat{\psi}^{(r)}$:

$$\hat{\psi}^{(r)}F(\alpha)=F(\alpha+r). \tag{7}$$

It then follows that

$$\sum_{\alpha}\hat{\psi}^{(r)}F(\alpha)=\sum_{\alpha}F(\alpha) \tag{8}$$

independent of the shift operator.

The set of operators $\psi^{(r)}$ forms an Abelian group:

$$\psi^{(0)}=\mathbb{1} \tag{9a}$$

$$[\psi^{(r)}]^{-1}=\tilde{\psi}^{(r)}=\psi^{(q-r)}. \tag{9b}$$

Finally we introduce the scalar product of two state functions

$$(\varphi,\theta)=\sum_{\alpha}\varphi(\alpha)\theta(\alpha). \tag{10}$$

We shall only consider real functions.

Now, we require the master equation to be a first-order differential (with respect to time) equation, without any memory effects (stochastic process); to conserve probabilities and to accept the Boltzmann equilibrium distribution as the only static solution; to generate a decay to equilibrium from any initial distribution; and, finally, to reduce to Glauber's equation for $q=2$. We present it as a '*fait accompli*':

$$\frac{\partial}{\partial t}|\mathcal{P}(t)\rangle=\sum_{i}\left(\sum_{r}W_r\psi_i^{(r)}-\sum_{r}W_r\right)M_i|\mathcal{P}(t)\rangle. \tag{11}$$

In here, the first summation is over the spins and $\psi_i^{(r)}$ acts only on the space of the spin located at site i. The set of real parameters W_r $(r=0,\ldots,q-1)$ represents single-spin relaxation times and they are subjected to conditions indicated below; notice, however, that W_0 is irrelevant, since it is added and subtracted in (11). Therefore, there are really $q-1$ relaxation times, only. Finally, M_i is an operator, defined by

$$M_i=\mathrm{e}^{\beta\mathcal{H}}/\mathrm{Tr}_{(i)}\,\mathrm{e}^{\beta\mathcal{H}}\equiv\mathrm{e}^{\beta\mathcal{H}}/Z_i \tag{12}$$

where H is the spin Hamiltonian and Z_i is, in general, still an operator obtained by tracing over the spin i.

If we use the distribution function:

$$\mathcal{P}(\alpha_1,\ldots,\alpha_N;t)=\langle\alpha_1,\ldots,\alpha_N|\mathcal{P}(t)\rangle$$

we can write (11) in the alternative form

$$\frac{\partial}{\partial t}\mathcal{P}(\alpha;t)=\sum_{i}\left(\sum_{r}W_r\hat{\psi}_i^{(r)}-\sum_{r}W_r\right)\hat{M}_i\mathcal{P}(\alpha;t). \tag{13}$$

It is now easy to see that (8) implies both the conservation of probability and a static

solution defined by the equilibrium distribution

$$\mathscr{P}_{\text{eq}}(\alpha; t) = Z^{-1}\langle \alpha_1 \dots \alpha_N | \, \mathrm{e}^{-\beta\hat{\mathscr{H}}} | \alpha_1 \dots \alpha_N \rangle = Z^{-1} \exp(-\beta E(\alpha)) \tag{14}$$

where $Z(\beta)$ is the partition function:

$$Z(\beta) = \sum_{\alpha} \exp(-\beta E(\alpha)) = \operatorname{Tr} \exp(-\beta\hat{\mathscr{H}}). \tag{15}$$

We may rewrite (13) in the form

$$(\partial/\partial t)\mathscr{P}(\alpha; t) = \hat{L}\mathscr{P}(\alpha; t) \tag{16}$$

which defines the Liouville operator $\hat{L}$. Now, let

$$\mathscr{P}'(\alpha; t) = \exp(\beta\hat{\mathscr{H}}/2)\mathscr{P}(\alpha; t) \tag{17a}$$

so that

$$\partial\mathscr{P}'/\partial t = \hat{L}'\mathscr{P}' \tag{17b}$$

where

$$\hat{L}' = \exp(\beta\hat{\mathscr{H}}/2)\hat{L}\exp(-\beta\hat{\mathscr{H}}/2)$$

$$= \sum_i \frac{\exp(\beta\hat{\mathscr{H}}/2)}{\sqrt{\hat{Z}_i}} \left(\sum_r W_r \hat{\psi}_i^{(r)} - \sum_r W_r \right) \frac{\exp(\beta\hat{\mathscr{H}}/2)}{\sqrt{\hat{Z}_i}}. \tag{18}$$

To obtain (18) we used (12) together with the fact that the operator $\hat{Z}_i$ commutes with the shift operators $\hat{\psi}_i^{(r)}$. Now, we require $\hat{L}'$ to be Hermitian; from (9*b*), this demands

$$W_r = W_{q-r} \qquad (r = 0, q, \dots, q-1). \tag{19a}$$

We can now easily show that $\hat{L}'$ is a non-positive operator. Consider $(\varphi, \hat{L}'\varphi)$ where φ is any state function. Using (18) and defining

$$\varphi_i = (\exp(\beta\hat{H}/2)/\sqrt{\hat{Z}_i})\varphi$$

we obtain

$$(\varphi, \hat{L}'\varphi) = \sum_i \left[\sum_r W_r(\varphi_i, \hat{\psi}_i^{(r)}\varphi_i) - \left(\sum_r W_r \right)(\varphi_i, \varphi_i) \right].$$

Using the definition (7) and Schwarz's inequality, one obtains

$$(\varphi_i, \hat{\psi}_i^{(r)}\varphi_i) \leqslant (\varphi_i, \varphi_i).$$

This implies $\hat{L}'$ to be non-positive, provided

$$\sum_r W_r > 0. \tag{19b}$$

We have not been able to prove that the equilibrium distribution is the only static solution. We shall accept that the relaxation times obey other necessary conditions to ensure such property.

Finally, it is easy to show that (13) does reduce to Glauber's for $q = 2$. For that purpose, it is better to label the spin states by $\sigma = \pm 1$ (instead of $\alpha = 1, 2$) and notice that

$$\hat{\pi}_i^{(1)} = -\hat{\pi}_i^{(2)} = \tfrac{1}{2}\hat{\sigma}_i \tag{20}$$

where $\hat{\sigma}_i$ is the usual Pauli matrix. Also,

$$M_i = \frac{1}{2}\left[1 - \sigma_i \tanh\left(\beta \sum_j J_{ij}\sigma_j\right)\right] \tag{21}$$

which is enough to convert (13) into Glauber's equation. Finally, we remark that Forgacs *et al* (1980) work presents a different choice for the dynamical rates—however, for $q = 2$, one does not recover Glauber's equation and, for general q, it is not obvious that their Liouvillian is, or can be reduced to, a non-positive operator. Therefore, any comparison between their work and the present one should be exercised with care.

3. Relaxation of a single spin subjected to a constant field

In this section, we consider a simple application of the previous theory which has pedagogical interest and also yields some useful conclusions. To simplify the algebra, we assume $W_r = W > 0$. The main results are derived in appendix 1.

In general field direction, we find $q-1$ temperature dependent relaxation times (given by (A1.5)); this result should be contrasted with the Ising limit ($q = 2$) for which there is just one, temperature independent, relaxation time.

For the particular choice of a field pointing along a specified direction in Potts space, we obtain one relaxation time associated with the relaxation of the longitudinal component of the distribution function and another relaxation time, with a degeneracy $q-2$ (and, hence, with zero weight for $q = 2$), associated with the relaxation of the transverse components of the distribution function.

4. Critical dynamics in the linear chain

The Glauber model is trivially solved in one dimension. This is due to the simple form that (21) takes in that case—it generates a linear equation for the evolution of the magnetisation.

The situation is, unfortunately, much more complicated for $q > 2$. Indeed, the form which M_i now assumes introduces nonlinear terms, even in one dimension. This can easily be seen from the following identity

$$M_i = \frac{\exp[-\beta J\bar{P}_i \cdot (\bar{P}_{i-1} + \bar{P}_{i+1})]}{\mathrm{Tr}_{(i)} \exp[-\beta J\bar{P}_i \cdot (\bar{P}_{i-1} + \bar{P}_{i+1})]} = \frac{1}{q} - \bar{B}_i \cdot \bar{\pi}_i \tag{22}$$

where

$$B_i^{(\kappa)} = \frac{v(q-3v+v^2)}{(q-2v)(q-2v+v^2)}\left(\pi_{i-1}^{(\kappa)} + \pi_{i+1}^{(\kappa)} - \frac{qv}{q-3v+v^2}\pi_{i-1}^{(\kappa)}\pi_{i+1}^{(\kappa)}\right) \tag{23}$$

with

$$v = 1 - e^{-\beta J}. \tag{24}$$

Notice that the last term in (23), when inserted in (22), cancels exactly for $q = 2$—this is the enormous simplification which, however, only occurs for the Ising model.

Since we can no longer solve exactly the model, we turn to a variational method (Haake and Thol 1980) which yields a lower bound for the dynamical exponent

(Halperin and Hohenberg 1969). The calculation is outlined in appendix 2; here, we comment on the main results.

First, we obtain $z > 3$ for $q > 2$ and $z \geqslant 2$ for $q = 2$; this last result is consistent with the exact one ($z = 2$ for $q = 2$). It is tempting to conjecture $z = q$ for the linear chain, but we believe the more correct guess to be $z = 3$ for $q \neq 2$, the result for $q = 2$ appearing accidentally. Indeed, the method we used in appendix 2 shows clearly that the different result we obtain for $q = 2$ is due to a cancellation, which only occurs for $q = 2$, in the denominator of (A2.9) which is, essentially, the same as in (23) and which, therefore, has its origin in (22).

The numerator of this equation just decouples spin i from the other spins, thus breaking the chain into two independent chains with two less interactions. These introduce a factor ξ^{-2}, and an additional factor ξ^{-1} arises from the denominator of the variational quotient. Therefore, at least for the trial function we used, the case $q = 2$ is distinguished from the others because of the peculiar behaviour the form of the operator M_i takes for $q = 2$—and we recall that this form is imposed by detailed balance.

Now, one may use other trial functions (still orthogonal to $P_{eq}(\alpha)$—other choices have failed to reveal a different lower bound. Also, we have been unable to provide an upper bound for the dynamical exponent.

Finally, we remark that these results seem to contradict the statement of Forgacs *et al* (1980) that $z = 2$ for $q \neq 2$. Unfortunately, these authors do not give details of their calculation—it is possible that the discrepancy arises from the different, non-equivalent formulation of the master equation or the choices for the dynamical rates.

5. Discussion

We have presented a master equation formulation of the kinetic Potts model which reduces to Glauber's dynamics in the Ising limit. Although there is no unique way to generalise the Ising results, we have taken the simplest approach—yet, the results obtained show how special the Ising limit really is.

The isolated spin subjected to an external field shows, in general, $q - 1$ relaxation times with explicit temperature dependence.

The linear chain is no longer trivially soluble. A variational calculation showed that the critical dynamical exponent z is not smaller than 3 for $q > 2$, in contrast with $z = 2$ for the Ising limit. We give some arguments to suggest that $z = 3$ for general $q > 2$, although we could not prove it. It appears that the case $q = 2$ is accidentally an exception because of an exact cancellation of the dynamical matrix. If it is an accident, we should conclude that there is just a universality class for one-dimensional Potts dynamics, as there is for statics.

Of course, the situation should, very likely, be completely different in higher dimensions. The equilibrium properties already depend critically on the number of Potts states—we should expect the dynamics to show similar dependence. It is therefore interesting to investigate within the present approach these higher-dimensional models and, in particular, the effect of changing the order of the transition. Another interesting possibility arises in connection with recent generalisations of Glauber dynamics (Haake and Thol 1980), which already show different dynamical universality classes for the Ising case.

Finally, we must mention that consideration of gauge couplings, random fields or impurities show how rich the kinetic formulation of the clock model can be once it is put to work.

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Appendix 1. Solution of the single-spin problem

We first notice that we can always impose, upon the components H_α of the field, the condition

$$\sum_\alpha H_\alpha = 0. \tag{A1.1}$$

This does not restrict the problem: it is obvious from (1) and (3*b*) that the substitution H_α by $H_\alpha + c$, just adds a constant to the Hamiltonian. Thus, we can always choose c so as to guarantee (A1.1).

The operator M (equation (12)), can always be written as

$$M = \frac{\exp(-\beta \bar{H} \cdot \bar{P})}{\operatorname{Tr} \exp(-\beta \bar{H} \cdot \bar{P})} = \bar{B} \cdot \bar{P} \tag{A1.2}$$

where

$$B_\alpha = \frac{\operatorname{Tr} \exp(-\beta \bar{H} \cdot \bar{P}) P_\alpha}{\operatorname{Tr} \exp(-\beta \bar{H} \cdot \bar{P})}. \tag{A1.3}$$

Therefore

$$\sum_\alpha B_\alpha = 1.$$

For the single-spin problem, these quantities are positive numbers:

$$B_\alpha = \exp(-\beta H_\alpha) / \sum_\gamma \exp(-\beta H_\gamma). \tag{A1.4}$$

Inserting (A1.2) into the master equation and using (8) we obtain

$$\frac{\partial}{\partial \tau} \mathcal{P}(\alpha, \tau) = \sum_\beta \Omega_{\alpha\beta} \mathcal{P}(\beta, \tau)$$

where $\tau = wt$ and

$$\Omega_{\alpha\beta} = B_\beta - qB_\alpha \delta_{\alpha\beta}.$$

Obviously, the eigenvalues of this matrix are the relaxation rates Ω_λ (with the opposite sign). It is easy to find that these are the solutions of

$$\sum_\alpha \frac{B_\alpha}{qB_\alpha - \Omega_\lambda} = 1. \tag{A1.5}$$

In view of (A1.3), one root is always zero, corresponding to the equilibrium distribution.

A graphical method then shows all other roots to be positive, since, from (A1.3), $B_\alpha > 0$. Thus, there are, in general, $q-1$ independent, temperature dependent, relaxation times.

We consider the particular case of a field H oriented along a particular direction in Potts space—say, $H_1 = H > 0$ and $H_\alpha = -H/(q-1)$, $\alpha > 1$. We easily solve (A1.5) and, besides the trivial solution, obtain

$$\Omega_1 = \{\exp(\beta H) + (q-1)\exp[-\beta H/(q-1)]\}/\{(q-1)\exp(\beta H) + \exp[-\beta H/(q-1)]\} \tag{A1.6}$$

$$\Omega_2 = q\exp(\beta H)/\{(q-1)\exp(\beta H) + \exp[-\beta H/(q-1)]\}. \tag{A1.7}$$

The first expression gives the relaxation rate for the longitudinal component. The other root, which is $q-2$ degenerated, is associated with the relaxation of the transverse components ($\alpha > 1$) of the distribution function. Indeed, if we denote

$$\mathscr{P}'(\alpha, t) = \mathscr{P}(\alpha, t) - \mathscr{P}_{eq}(\alpha)$$

we obtain:

$$\mathscr{P}'(1, t) = \mathscr{P}'(1, 0)\exp(-\Omega_1 \tau)$$

$$\mathscr{P}'(\alpha, t) = \left[\mathscr{P}'(\alpha, 0) + \frac{\mathscr{P}'(1,0)}{q-1}\right]\exp(-\Omega_2\tau) - \frac{\mathscr{P}'(1,0)}{q-1}\exp(-\Omega_1\tau) \qquad (\alpha > 1).$$

For general q, both Ω_1 and Ω_2 are temperature dependent. However, for $q = 2$ $\Omega_1 = 1$ and although Ω_2 has a limiting form it disappears completely from the distribution function: the term in brackets in the above equation vanishes identically for $q = 2$.

Appendix 2. Variational method for the linear chain (zero field)

From equation (17*b*), we notice that the long-time behaviour of the relaxation function is determined by the smallest (in absolute value) non-zero root $(-\lambda)$ of the eigenvalue equation for the Liouville operator $\hat{L}'$. Since this is non-positive, any trial function (orthogonal, however, to the eigenfunction with zero eigenvalue, that is, the equilibrium distribution) will certainly yield a lower bound, that is,

$$-\lambda \geqslant (\psi, \hat{L}'\psi)/(\psi, \psi). \tag{A2.1}$$

We shall take $\psi(\alpha)$ of the form:

$$\psi(\alpha) = \exp(-\beta\hat{H}/2)\psi'(\alpha)$$

and specify $\psi'(\alpha)$ later. Now, using (18) and the definition of scalar product, we get

$$\begin{aligned}(\psi, \hat{L}'\psi) &= (\psi', \hat{L}\exp(-\beta\hat{H})\psi') \\ &= \sum_i \left[\psi', \left(\sum_r W_r\hat{\psi}_i^{(r)} - \sum_r W_r\right)\hat{M}_i\exp(-\beta\hat{H})\psi\right] \\ &= \sum_i \left[\exp(-\beta\hat{H})\hat{M}_i\psi', \left(\sum_r W_r\hat{\psi}_i^{(r)} - \sum_r W_r\right)\psi'\right].\end{aligned} \tag{A2.2}$$

Also

$$(\psi, \psi) = (\exp(-\beta\hat{H})\psi', \psi'). \tag{A2.3}$$

Now, we choose

$$\psi'(\alpha)=\frac{1}{\sqrt{N}}\sum_i C_{\alpha_i} \tag{A2.4}$$

where the C_α's are q-real, variational parameters. They will form the components of a vector $\boldsymbol{c}$ in Potts space. Since

$$P_{\mathrm{eq}}(\alpha)=\mathrm{e}^{-\beta E(\alpha)}/Z(\beta)$$

we obtain

$$\begin{aligned}(P_{\mathrm{eq}},\psi)&=\frac{1}{Z(\beta)}\sum_\alpha \exp(-3\beta E(\alpha)/2)\frac{1}{\sqrt{N}}\sum_i C_{\alpha_i}\\&=\frac{Z(3\beta/2)}{Z(\beta)}\frac{1}{\sqrt{N}}\sum_i\langle \boldsymbol{c}\cdot\boldsymbol{P}_i\rangle\end{aligned}$$

where the last line follows from the properties (equations (3)) of the projection operators. Since, in one dimension $\langle P_i^{(\alpha)}\rangle=1/q$ for any finite temperature, it follows that orthogonality is guaranteed if we require

$$\sum_\alpha C_\alpha=0. \tag{A2.5}$$

Using this property, we can now obtain

$$\begin{aligned}(\psi,\psi)&=\frac{1}{N}\sum_{ij}\sum_\alpha \exp(-\beta E(\alpha))C_{\alpha_i}C_{\alpha_j}=\frac{Z(\beta)}{N}\sum_{ij}\langle \bar{C}\cdot\bar{\pi}_i\bar{C}\cdot\bar{\pi}_j\rangle\\&=Z(\beta)\frac{|\bar{C}|^2}{q}\left(1+\frac{2}{q}(\exp(\beta J)-1)\right)\end{aligned} \tag{A2.6}$$

where we have used well known results for one-dimensional correlations. In a similar way, we can write (A2.2) as:

$$\begin{aligned}(\psi,\hat{L}'\psi)&=\frac{1}{N}\sum_{ijk}\sum_\alpha \exp(-\beta E(\alpha))M_i(\alpha)C_{\alpha_j}\left[\sum_r W_r\hat{\psi}_i^{(r)}-\left(\sum_r W_r\right)\right]C_{\alpha_i}\\&=\frac{1}{N}\sum_{ij}\sum_\alpha \exp(-\beta E(\alpha))M_i(\alpha)C_{\alpha_j}\left[\sum_r W_rC_{\alpha_i+r}-\left(\sum_r W_r\right)C_{\alpha_i}\right]\end{aligned}$$

where the second line follows from (8). If, for the moment, we write

$$C_\alpha^{(r)}=C_{\alpha+r}$$

we obtain

$$\begin{aligned}(\psi,\hat{L}'\psi)&=\frac{1}{N}\sum_{ij}\exp(-\beta E(\alpha))M_i(\alpha)C_{\alpha_j}\left[\sum_r W_rC_{\alpha_i}^{(r)}-\left(\sum_r W_r\right)C_{\alpha_i}\right]\\&=\frac{Z(\beta)}{N}\sum_{ij}\left\langle M_i\left[\sum_r W_r\bar{C}^{(r)}\cdot\bar{\pi}_i-\left(\sum_r w_r\right)\bar{C}\cdot\bar{\pi}_i\right]\bar{C}\cdot\bar{\pi}_j\right\rangle\\&=Z(\beta)\sum_{\alpha\gamma}\left[\sum_r C_{\alpha+r}C_\gamma W_r-C_\alpha C_\gamma\left(\sum_r W_r\right)\right]\frac{1}{N}\sum_{ij}\langle M_i\pi_i^{(\alpha)}\pi_j^{(\gamma)}\rangle.\end{aligned} \tag{A2.7}$$

We may calculate the required thermal average, using (22) and recalling the equilibrium value of the correlation of several spin operators. Instead, we shall use another route which, although only adequate for the linear chain, is easier and sheds more light onto the final result. Substituting from (22), we obtain

$$\langle M_i \pi_i^{(\alpha)} \pi_j^{(\gamma)} \rangle = \frac{1}{Z_N(\beta)} \mathrm{Tr}\left(\exp(-\beta H) \frac{\exp[-\beta J \bar{P}_i \cdot (\bar{P}_{i-1} + \bar{P}_{i+1})]}{Z_i} \pi_i^{(\alpha)} \pi_j^{(\gamma)} \right) \tag{A2.8}$$

where

$$\frac{1}{Z_i} = (\mathrm{Tr}_{(i)} \exp[-\beta J \bar{P}_i \cdot (\bar{P}_{i-1} + \bar{P}_{i+1})])^{-1}$$

$$= \frac{q - 2v + v^2(1 - 1/q)}{(q-2v)(q-2v+v^2)} \left(1 - \frac{v^2}{q - 2v + v^2(1-1/q)} \bar{\pi}_{i-1} \cdot \bar{\pi}_{i+1} \right). \tag{A2.9}$$

In equation (A2.8) we labelled the partition function with the number N of spins on the line. Now, equation (A2.8) clearly shows that the spin i becomes totally decoupled from the other spins. Hence, the trace over i can immediately be performed (using equation (5)):

$$\langle M_i \pi_i^{(\alpha)} \pi_j^{(\gamma)} \rangle = \left(\delta_{\alpha\gamma} - \frac{1}{q} \right) \delta_{ij} \frac{1}{Z_N(\beta)} \mathrm{Tr}\left(\prod_{k=1}^{i-2} \rho(k, k+1) \frac{1}{Z_i} \prod_{k=i+1}^{N-1} \rho(k, k+1) \right)$$

where $\rho(k, k+1) = \exp(\beta J \bar{P}_k \cdot \bar{P}_{k+1})$. The linear chain has been split into two disjoint chains. Using (A2.9) we obtain

$$\langle M_i \pi_i^{(\alpha)} \pi_j^{(\gamma)} \rangle = \delta_{ij} \left(\delta_{\alpha\gamma} - \frac{1}{q} \right) \frac{Z_{i-1} Z_{N-i}}{Z_N} \frac{q - 2v + v^2(1-1/q)}{(q-2v)(q-2v+v^2)}.$$

Since

$$Z_N = q[e^{\beta J} + q - 1]^{N-1} \tag{A2.10}$$

we finally obtain

$$(\psi, \hat{L}'\psi) = Z(\beta) \left[\sum_r W_r \sum_\alpha C_{\alpha+r} C_\alpha - \left(\sum_r W_r \right) |\bar{C}|^2 \right]$$

$$\times \frac{q}{[\exp(\beta J) + q - 1]^2} \frac{q - 2v + v^2(1-1/q)}{(q-2v)(q-2v+v^2)}.$$

Using this result and (A2.6) into (A2.1), we obtain

$$\lambda \leqslant \left(\sum_r W_r - \sum_r W_r \frac{\sum_\alpha C_\alpha C_{\alpha+r}}{|\bar{C}|^2} \right) F(q, T) \tag{A2.11}$$

where

$$F(q, T) = q^2 \left(1 - \frac{v^2}{q(q-2v+v^2)} \right) \frac{1}{q-2v} \frac{1}{(\exp(\beta J) + q - 1)^2} \frac{1}{1 + (2/q)(\exp(\beta J) - 1)}. \tag{A2.12}$$

Using (24) and (2), we may cast the limit $T = 0$ in the form

$$F(q, T) = \tfrac{1}{2} \left[1 - \frac{q}{q(q-1)} \right] \frac{1}{q-2} \xi^{-3}.$$

We thus obtain:

$$z \geqslant 3 \qquad \text{for} \qquad q > 2.$$

For $q = 2$, however, the factor $q - 2v$ vanishes (like ξ^{-1}) and we get

$$F(q, T) \propto \xi^{-2}$$

consistent with the exact result.

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