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LETTER TO THE EDITOR

Interface of a Potts chain

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Abstract. The properties of the interface of a q -state Potts chain are calculated exactly. For $q > 2$ and non-zero temperature, non-boundary states are created at the interface. The number of such states is calculated as a function of position, temperature and q .

Consider a system which undergoes a phase transition into several ordered structures. Boundaries or defects may break the symmetry between these structures and favour the formation of domains. For systems with discrete symmetry the properties of walls or interfaces between such domains have been extensively studied, mainly for Ising systems (Widom 1977, Bricmont *et al* 1981). Only recently the interface of a two-dimensional 3-state Potts model has been investigated by Selke and Pesch (1982). Using Monte Carlo simulations they showed that at the interface between domains of, say, states 1 and 2 the third state 3 is generated. Similar to the Ising case (Müller-Hartmann and Zittartz 1977) they found a good approximation of the interface free energy by neglecting overhangs and islands, however, the third layer of state 3 has to be taken into account.

This letter considers interface properties of a q -state Potts chain which are calculated exactly, even for continuous q (for a review of the Potts model, see Wu 1982). Of course, this one-dimensional system has a phase transition at $T_c = 0$ only. However, for a chain of N sites one obtains the behaviour of an ordered phase if the correlation length ξ is larger than the size, N , of the system.

Consider a chain of $N + 1$ sites labelled by $i = 0, 1, 2, \dots, N$ with Hamiltonian

$$\mathcal{H} = -k_B T K \sum_{i=1}^N \delta_{S_{i-1}, S_i} \quad (1)$$

where $S_i = 1, 2, \dots, q$ is a q -state Potts variable. Fixing the boundary to $S_0 = 1$ and $S_N = 2$ we create an interface. The partition sum and expectation values are conveniently obtained from the transfer matrix \mathbf{T} given by

$$\langle i | \mathbf{T} | j \rangle = \exp(K \delta_{S_i, S_j}). \quad (2)$$

A power \mathbf{T}^ν of \mathbf{T} with integer ν has the same structure as \mathbf{T} , namely one has

$$\langle i | \mathbf{T}^\nu | j \rangle = C_\nu \exp(K_\nu \delta_{S_i, S_j}) \quad (3)$$

where C_ν is a constant which does not appear in any expectation values and K_ν is

easily obtained from the ratio t of the two eigenvalues of \mathbf{T}

$$t(K) = \frac{e^K - 1}{e^K + q - 1}. \tag{4}$$

One obtains (see e.g. Kinzel and Domany 1981)

$$e^{K_\nu} = \frac{1 + (q - 1)t^\nu(K)}{1 - t^\nu(K)}. \tag{5}$$

We are interested in the average fraction n_i of states at site i which are different from the boundary values and are created by the interface. n_i is given by

$$n_i = (q - 2)(\langle \delta_{S_i,3} \rangle_{12} - \langle \delta_{S_i,3} \rangle_{11}) \tag{6}$$

where $\langle \dots \rangle_{a,b}$ means the thermal expectation value with boundary fixed to $S_0 = a$ and $S_N = b$. Equation (7) can be evaluated using the transfer matrix \mathbf{T} ; one obtains

$$\langle \delta_{S_i,3} \rangle_{12} = \frac{\langle 1|T^i|3\rangle\langle 3|T^{N-i}|2\rangle}{(q - 2)\langle 1|T^i|3\rangle\langle 3|T^{N-i}|2\rangle + \langle 1|T^i|1\rangle\langle 1|T^{N-i}|2\rangle + \langle 1|T^i|2\rangle\langle 2|T^{N-i}|2\rangle} \tag{7a}$$

$$\langle \delta_{S_i,3} \rangle_{11} = \frac{\langle 1|T^i|3\rangle\langle 3|T^{N-i}|1\rangle}{(q - 1)\langle 1|T^i|3\rangle\langle 3|T^{N-i}|1\rangle + \langle 1|T^i|1\rangle\langle 1|T^{N-i}|1\rangle}. \tag{7b}$$

With equations (3) and (6) n_i is given by ($x_\nu = e^{K_\nu}$, $x_1 = e^K$)

$$n_i = \frac{(q - 2)(x_i - 1)(x_{N-i} - 1)}{(q - 2 + x_i + x_{N-i})(q - 1 + x_i x_{N-i})} \quad i = 1, \dots, N - 1. \tag{8}$$

The x_ν are given by equations (4) and (5). Equations (7a) and (7b) have the same numerator, so the ratio of the left-hand sides is given by

$$\frac{\langle \delta_{S_i,3} \rangle_{12}}{\langle \delta_{S_i,3} \rangle_{11}} = \frac{\langle 1|T^N|1\rangle}{\langle 1|T^N|2\rangle} = x_N = \exp(-f/k_B T). \tag{9}$$

This ratio is independent of site i and diverges at $T \rightarrow 0$. Note that the two matrix elements in equation (9) are just the partition sums with and without interface, respectively. Thus f is just the interface free energy; one has $f = -k_B T K_N$.

Another quantity of interest is the thermal average k_i of the number of 1-2 kinks between site i and $i + 1$. It is given by

$$k_i = \langle \delta_{S_i,1} \delta_{S_{i+1},2} \rangle = \frac{x_i x_{N-i-1}}{x_i x + x x_{N-i-1} + x_1 x_{N-i-1} + 1 + (q - 2)(2 + x_i + x_{N-i-1} + x) + (q - 2)(q - 3)}. \tag{10}$$

As already mentioned, a characteristic temperature T_0 may be defined by the condition $\xi(T_0) = N$. ξ is given by the logarithm of the ratio of the two eigenvalues of \mathbf{T} , therefore $T_0 = 1/K_0$ is given by

$$K_0 = \ln\left(\frac{e^{1/N} + q - 1}{e^{1/N} - 1}\right) \approx \ln(Nq + 1) \tag{11}$$

where the last equality holds for large N . Figure 1 shows the number n_i of non-boundary states for system size $N = 50$ and temperature $T = T_0$. In figure 2 $n = \sum_{i=1}^N n_i$

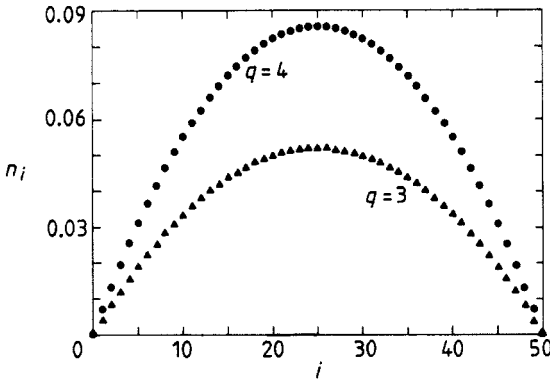


Figure 1. Expectation value n_i of non-boundary states at site i which are created by the interface ($T = T_0$).

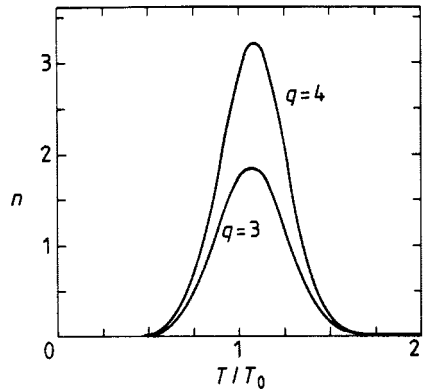


Figure 2. $n = \sum_i n_i$ as a function of temperature. T_0 is defined by $\xi(T_0) = N$.

is shown as a function of temperature. n has a maximum around T_0 . For $T < \frac{1}{2}T_0$ and $T > 1.7 T_0$ there are almost no non-boundary states created by the interface. The total number $k = \sum_{i=1}^{N-2} k_i$ of the 1-2 kinks is shown in figure 3. At $T = 0$ one has obviously $k = 1$. For $q = 2$, i.e. the Ising model, k is related to the energy, thus k increases with T . However, for $q > 2$ 1- a and b -2 kinks are created at $T \neq 0$ with a and b being non-boundary states ($a, b \neq 1, 2$). Figure 3 shows that this reduces the number k of 1-2 kinks. Only for $T \gg T_0$ k increases again to its value at $T = \infty$ which is given by

$$k(T = \infty) = (N - 2)/q^2. \tag{12}$$

Figure 4 shows the q dependence of n and k at $T = T_0(q)$. By increasing the number of Potts states one increases the number $q - 2$ of non-boundary states. Therefore domains of non-boundary states have higher entropy for larger q and are more

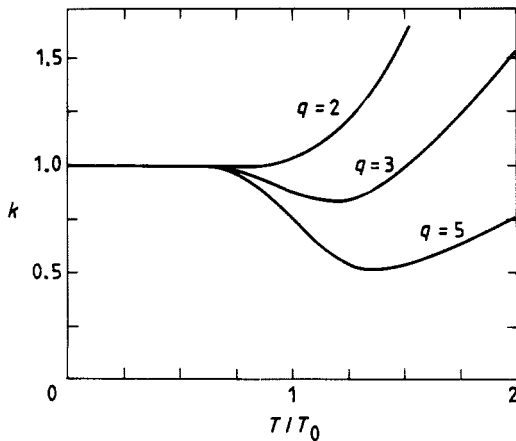


Figure 3. Total number k of (1-2) kinks of a (1-2) interface as a function of temperature.

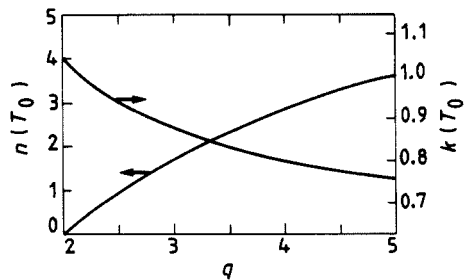


Figure 4. q dependence of the total number n of non-boundary states and k of kinks, for $T = T_0(q)$.

probable. Thus n increases with increasing q . For the same reason $k(T_0)$ decreases with q .

In summary the interface properties of the q -state Potts chain have been calculated exactly. The average number n of non-boundary states which are created by the interface has a sharp maximum around T_0 similar to the results of computer simulations of a two-dimensional 3-state Potts model (Selke and Pesch 1982); there the maximum is just below T_c . The number of kinks of boundary states has a minimum as a function of temperature. $n(T_0)$ increases and $k(T_0)$ decreases with the number q of Potts states.

This shows that the system tries to compensate the energy loss at the interface by a higher entropy in order to keep the free energy as smooth as possible. In the two-dimensional Ising case this entropy is obtained from a rough interface (Gallavotti 1972). For the q -state Potts model with $q > 2$ there is the additional possibility of obtaining entropy by the formation of layers of non-boundary states at the interface. Thus one may speculate that the interface becomes sharp for q large enough. This point clearly deserves further investigations.

The present work may be relevant to interfaces or domain walls for ordered structures of adsorbates on surfaces. For instance the $\sqrt{3} \times \sqrt{3}$ structure of rare gases on graphite or the 3×1 structure of H of Fe(110) both have a three-fold ground state analogous to the $q = 3$ state Potts model (for a recent review with further literature, see Binder *et al* 1982). For lattice gas models for such systems the interface properties are presently being investigated (Rikvold *et al* 1982).

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