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Exact Results on the One-Dimensional Potts Lattice Gas

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Abstract We present an exact calculation of the Potts Lattice Gas inone dimension. Close to $T=0^0K$, the uniform susceptibility presents an essential singularity, when the exchange parameter is positive, and a power law behaviour with critical exponent $\gamma=1$, when this parameter is negative.

1. INTRODLICTION

The pure r-state Potts model has been extensively investigated in recent years[1]. The annealed (site) dilute Potts model or Potts lattice gas is also of interest in relation to adsorbed gases on substrates[2,3,4]. In the latter, each of the N sites of a d-dimensional lattice may be occupied ($t_i=1$) or not ($t_i=0$), the vacancies being controlled by a chemical potential A'. An occupied site may be in one of the r states, $\sigma_i = 1,...r$ and two neighbouring occupied sites interact through the Potts hamiltonian, the coupling constant being J'. Thus

$$H = - \sum_{<ij>} J'(r\delta_{\sigma_i,\sigma_j} - 1) t_i t_j - \sum_i \Delta'(1-t_i) \qquad (1)$$

The grand-canonical partition function $Z_N = Z_N(J,\Delta,r)$ is then

$$Z_N = \sum_{\{t_i\}} \sum_{\{\sigma_i\}}' \left\{ \prod_{<ij>} \exp\left[J(r\delta_{\sigma_i,\sigma_j} - 1) t_i t_j\right] \prod_i \exp\Delta(1-t_i) \right\} , \qquad (2)$$

where $J=\beta J'$, $\Delta=\beta\Delta'$ and $\beta=1/k_BT$. k_B is the Boltzmann constant and T, the temperature. The prime on $\sum_{\{\sigma_i\}}'$ implies a summationonly overoccupied sites.

This model is also relevant in the polymer gelation[5] and in the site-bond percolation problems[6]. Furthermore, the dilute Ising ($r=2$) and the pure Potts (A' = $-\infty$) limits[7] follows immediately.

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2. EXACT CALCULATION OF $Z_n(J, \Delta, r)$ IN ONE DIMENSION

We rewrite eq. (1) for the open chain as:

$$Z_N = e^{\Delta} \sum_{T_N, \sigma_N} e^{-\Delta t_N} \left\{ \sum_{t_{N-1}, \sigma_{N-1}} Z_{N-1}(t_{N-1}, \sigma_{N-1}) \right.$$

$$\left. \times \exp\left[J(r\delta_{\sigma_{N-1}, \sigma_N} - 1) t_{N-1} t_N\right] \right\} \tag{3}$$

$Z_{N-1}(t_{N-1}, \sigma_{N-1})$ is the partition function for an open chain with $N-1$ sites, with fixed values of t_{N-1} and σ_{N-1}.

But, clearly

$$Z_N = Z_N(t_{i=0}) + Z_N(t_i=1) \tag{4}$$

$$Z_N(t_i=1) = r\, Z_N(t_i=1, \sigma_i=q) \tag{5}$$

where q denotes an arbitrarily given state that the variable σ_N can assume. From eqs. (3), (4) and (5) it follows that

$$Z_N(t_{N=0}) = e^{\Delta} Z_{N-1}(t_{N-1}=0) + e^{\Delta} Z_{N-1}(t_{N-1}=1) \tag{6}$$

$$Z_N(t_{N=1}) = r\, Z_{N-1}(t_{N-1}=0) + \lambda_0\, Z_{N-1}(t_{N-1}=1) \tag{7}$$

with

$$\lambda_0 = e^{J(r-1)} + (r-1)e^{-J} \tag{8}$$

Defining

$$\bar{Z}_N = \begin{Bmatrix} Z_N(t_{N=0}) \\ Z_N(t_{N=1}) \end{Bmatrix}$$

allows us to condense eqs. (6) and (7) in

$$\bar{Z}_N = T\, \bar{Z}_{N-1}$$

and, by iteration

$$\bar{Z}_N = T^{N-1}\, \bar{Z}_1$$

The eigenvalues of the T-matrix are

$$\lambda^{\pm} = \frac{1}{2}\left[(e^{\Delta}+\lambda_0) \pm \alpha\right] \tag{9}$$

where

$$\alpha = \left[(\lambda_0-e^{\Delta})^2 + 4r\ e^{\Delta}\right]^{1/2} \tag{10}$$

From these and from the elgenvectors we can easily find

$$Z_N(t_{N=0}) = e^{\Delta}\alpha^{-1}\left[(r-e^{\Delta}A^-)(\lambda^+)^{N-1} - (r-e^{\Delta}A^+)(\lambda^-)^{N-1}\right] \tag{11}$$

$$Z_N(t_{N=1}) = e^{\Delta}\alpha^{-1}\left[(r-e^{\Delta}A^-)A^+(\lambda^+)^{N-1} - (r-e^{\Delta}A^+)A^-(\lambda^-)^{N-1}\right] \tag{12}$$

and thus from eq. (4)

$$Z_N(J,\Delta,r) = \alpha^{-1}\left[(r-e^{\Delta}A^-)(\lambda^+)^N - (r-e^{\Delta}A^+)(\lambda^-)^N\right] \tag{13}$$

with

$$e^{\Delta}A^{\pm} = \lambda^{\pm} - e^{\Delta}$$

3. THERMODYNAMICS OF THE DILUTE POTTS CHAIN

From eq. (13) many thermodynamic properties of the chain can be obtained. For example, the free energy per site, in the thermodynarnic limit, is

$$g(J,\Delta) = k_B T\ \ln\ \lambda^+ \tag{14}$$

The entropy per site is given by

$$S(J,\Delta) = k_B\ \ln\ \lambda^+ - \frac{k_B}{2\alpha\lambda^+}\left[(r-1)\lambda_0^-\ J\{(\lambda_0-e^{\Delta}) + \alpha\}\right.$$

$$\left. + e^{\Delta}\Delta\{(e^{\Delta}-\lambda_0) + 2r + \alpha\}\right] \tag{15}$$

where

$$A^- = e^{J(r-1)} - e^{-J} \tag{16}$$

We define the correlation function by $\Gamma_\ell(J,\Gamma) = \langle(r\delta_{\sigma_i\sigma_{\ell+i}} - 1)t_i\ t_{\ell+i}\rangle$; it is shown in the Appendix that:

$$\Gamma_\ell(J,\Delta) = \frac{e^{\Delta}A^+}{\lambda^+}\ (r-1)\left(\frac{\lambda_0^-}{\lambda^+}\right)^\ell \tag{17}$$

From this result and the fluctuation-dissipation theorem we

can compute the zero field uniform susceptibility

$$\chi(J,\Delta) = \frac{e^{\Delta_A^+}}{\lambda^+} \frac{(r-1)}{k_B T} \left[\frac{\lambda^+ + \lambda_0^-}{\lambda^+ - \lambda_0^-}\right] \tag{18}$$

We now discuss the physical picture emerging from the above results. When $J'>0$, two situations are possible according to the relative magnitude of Δ' and J'. When $\Delta'<J'(r-1)$, the ground state ($T=0^0K$) has energy $E_0 = -(N-1)J'(r-1)$ and corresponds to a r-fold degenerate ferromagnetic order without vacancies, the entropy per site being zero in the thermodynamic limit. As the temperature approaches 0^0K, the uniform susceptibility eq.(18) exhibits an essential singularity

$$\chi \sim \frac{2}{k_B T} \frac{(r-1)}{r} e^{Jr}$$

which is characteristic of the pure ferromagnetic Ising model. Clearly this holds for the pure ferromagnetic Potts model as well.

The average number of vacancies per site is

$$q_s = \langle 1-t_i \rangle = \frac{e^{\Delta}(r+e^{\Delta}-\lambda^-)}{\alpha \lambda^+} \tag{19}$$

Figure I-a illustrates the dependence of q_s upon T. As $T \to \infty$, $q_S^m = 1/(1+r)$ as can be seen using eq.(19) or remembering that each site can be in $(1+r)$ states (vacant or in r occupied states). Thus $q_s < 1/2$ whenever $r > 1$, for any temperature, and occupied sites are more favorable than vacancies. At $T=0^0K$, the energy is reduced by occupyingevery lattice site; as T raises, vacancies are created.

In figure I-a we plot also

$$p_0 = \langle t_i t_{i+1} \rangle = \frac{\lambda_0 (\lambda^+ - e^{\Delta})}{(\lambda^+)} \tag{20}$$

the probability of having a neighbouring pair of occupied sites and

$$p_{0v} = \langle t_i (1-t_{i+1}) + (1-t_i) t_{i+1} \rangle = 2(1-q_s-p_0) \tag{21}$$

the probability for a neighbouring pair vacancy-occupied site. It's easily seen on physical grounds or using eqs.(20) and (21) that, as $T\to\infty$, $p_0^\infty = r^2/(1+r)^2 = (1-q_s^\infty)$ and $p_{0v}^\infty = 2r/(1+r)^2 = 2\, q_s^\infty (1-q_s^\infty)$.

In the one-dimensional system, the introduction of a vacancy in the interior of a cluster of occupied sites splits the cluster and at

the same time creates two vacancy-occupied site pairs. The total number of clusters (clusters of vacancies plus clusters of occupied sites) increases by two. The quantity p_{0v} thus counts the number of clusters per site and in some sense plays the role of a disorder parameter.

Once the probabilities q_s and p_{0v} are both less than 1/2 (see fig.1a), there is a tendency of the system to segregate or to form clusters of occupied sites.

If $\Delta' > J'(r-1)$, at $T=0^0K$, $E_i=-NA'$ and every site is ernpty. Thus S=O and $\chi=0$. In fig.1-b we plot q_s, p_0 and p_{0v} against T.

The qualitative behavlour of the entropy with temperature is irrespective of the relative value of A' and J' ($J'>0$), and is shown in fig.2 (lower curve). When $T\to\infty$, $S_\infty=k_B \ln (1+r)$, as expected in physical grouncls.

We consider now $J'<0$. Again two situations are possible. If $\Delta' > |J'|$, the results are the same as those for $J'>0$ and $A' > J'(r-1)$. More interesting is the behaviour of the system when $\Delta' < |J'|$ (this includes the pure Potts model with $J'<0$). As the temperature approaches 0^0K, the uniform susceptibility eq. (18) has now a power law singularity

$$\chi \sim \frac{(r-1)(r-2)}{r\, k_B T}$$

which defines the exponent $\gamma=1$. At $T = 0^0K$, the system becomes pure. In order to understand the nature of this transition, let us applya small uniform megnetic field, say, in "direction" $q=1$. The system then orders in the following way: in alternate sites of the lattice (say, sublattice A_1) the atoms are in the same state q=l and the sites on the other sublattice (say, A_2) are distributed among the remaining (r-l) states (the degeneracy is $(r-1)^{N/2}$).

Clearly, this kind of order is only possible for $r \geq 3$. For $r=2$, it is an usual antiferrornagnetic phase. Of course, we can also have "true" antiferromagnetic phases in the Potts model, but we expect these to show up in the corresponding wave vector dependent susceptibility.

At zero magnetic field the above configurations have the same energy as those obtained by partitioning the lattice in up to sublattices, where at least one is ordered. There are still many other degenate configurations with no ordered sublattice. Counting all them, we end up with $r(r-1)^{N-1}$ possibilities. Thus, at $T=0^0K$, in the ground

state, whose energy is $E_s = -(N-1)|J'|$, the entropy per site is given by $S_0 = k_B \ln (r-1)$, as can also be seen by performing the appropriate limit in eq. (15). The entropy versus temperature is shown in fig. 2 (upper curve).

The discussion on the probabilities q_s, p_0 and p_{0v} follows analogously as in the case $J'>0$, $\Delta'<J'(r-1)$. (See fig. 1-a).

The hamiltonian eq. (1) corresponds to a particular case of a more general Potts lattice gas hamiltonian†

$$\beta H = -\sum_{<ij>} \left[K\delta_{\sigma_i,\sigma_j} + K'\right] t_i t_j - \sum_i \Delta(1-t_i) \qquad (22)$$

with $K=Jr$ and $K' = -J$. Nevertheless, eq. (22) can be treated by the same methods developped before giving the same results, except that now

$$A_+ = e^{K+K'} + (r-1)eK'$$

and

$$A_- = e^{K+K'} - e^{K'}$$

The discussion of this section still applies but now the comparison must be made between $K'+K$ and Δ (for $K>0$) and between K' and Δ (for $K<0$).

APPENDIX

We derive here the expression eq. (17) for the correlation function

$$\Gamma_\ell(J,\Delta) = <(r\,\delta_{\sigma_1\,\sigma_{\ell+1}} - 1) t_1 t_{\ell+1}>$$

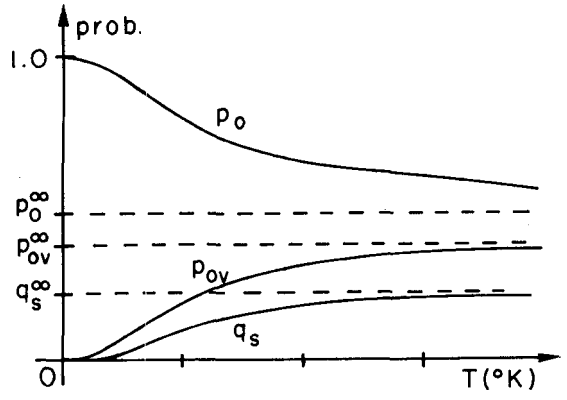
Let

$$\delta_{\sigma_i\sigma_j;q} = \begin{cases} 1 & \text{if } \sigma_i=\sigma_j=q \quad , \quad q=1,\ldots r \\ 0 & \text{otherwise} \end{cases}$$

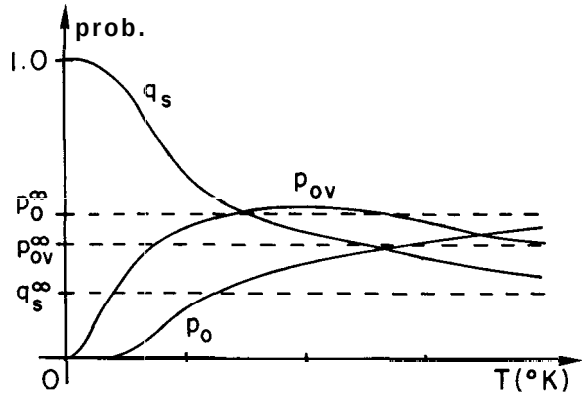
Then

$$<\delta_{\sigma_1\sigma_{\ell+1}}\, t_1 t_{\ell+1}> = r < \delta_{\sigma_1\sigma_{\ell+1};q}\, t_1 t_{\ell+1}>$$

† However, hamiltonian eq. (22) has an additional symmetry not presented in eq. (1); when $2K=2K'=\Delta$ the former reduces, in $d=1$, to the $(r+1)$--state Potts rnodel.



(1a)



(1b)

Fig.1-Plots of the average number of vacancies per site (q_s), of the probability of a neighbouring pair of occupied sites (p_0) and of the probability of a neighbouring pair occupied site-vacancy (p_{0v}) versus temperature. For $T \to \infty$ $q_s^\infty = 1/(1+r)$, $p_0^\infty = 2r/(1+r)^2$ and $p_{0v} = 2r/(1+r)^2$ **a)** $J'>0$ and $\Delta' < J'(r-1)$ or $J'<0$ and $\Delta' \lesssim |J'|$ b) $J' > 0$ and $\Delta' > J'(r-i)$ or $J' < 0$ and $\Delta' > |J'|$.

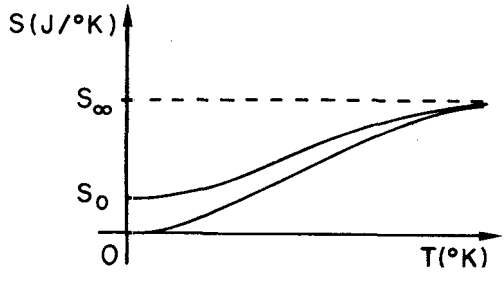


Fig.2 - Entropy per sites versus temperature. Lower curve: $J'>0$ or $J'<0$ and $A > |J'|$; Upper curve: $J'<0$ and $A \lesssim |J'|$; $S_0 = k_B \ln(r-1)$, $S_\infty = k_B \ln(r+1)$.

and so,

$$\Gamma_{\ell}(J,\Delta) = r^2 \langle \delta_{\sigma_1\sigma_{\ell+1};q}\, t_1 t_{\ell+1} \rangle - \langle t_1 t_{\ell+1} \rangle \tag{A1}$$

But

$$\langle t_1 t_{\ell+1} \rangle = \lim_{N\to\infty} Z_N(t_1=1,\ t_{\ell+1}=1)\ /Z_N \tag{A2}$$

$$\langle \delta_{\sigma_1\sigma_{\ell+1};q}\, t_1 t_{\ell+1} \rangle = \lim_{N\to\infty} Z_N(t_1=1,\ \sigma_1=q;\ t_{\ell+1}=1,\ \sigma_{\ell+1}=q)/Z_N \tag{A3}$$

Divide a N-site chain in two others with $\ell+1$ and $N-\ell$ sites,such that the $\ell+1$ site is in a fixed spin-state q. It follows that

$$Z_N(t_{\ell+1}=1,\ \sigma_{\ell+1}=q) = Z_{\ell+1}\ (t_{\ell+1}=1,\ \sigma_{\ell+1}=q).\ Z_{N-\ell}(t_1=1,\sigma_1=q) \tag{A4}$$

Note that the $\ell+1$ site of the original lattice is now the first one of the $(N-\ell)$-site lattice. Also

$$Z_N(t_1=1,\sigma_1=q;t_{\ell+1}=1,\sigma_{\ell+1}=q) = Z_{\ell+1}(t_1=1,\sigma_1=q;t_{\ell+1}=1,\sigma_{\ell+1}=q)$$

$$\times\ Z_{N-\ell}(t_1=1,\sigma_1=q) \tag{A5}$$

Using eqs. (5) and (A4) we have

$$Z_N(t_1=1;t_{\ell+1}=1) = \frac{1}{r}\, Z_{\ell+1}(t_1=1;t_{\ell+1}=1) Z_{N-\ell}(t_1=1) \tag{A6}$$

The calculations of $Z_{\ell+1}(t_1=1;t_{\ell+1}=1)$ and $Z_{\ell+1}(t_1=1,\sigma_1=q,\ t_{\ell+1}=1,\sigma_{\ell+1}=q)$ are carried out by a shaightforward generalization of the procedures leading from eqs. (6) to (13)

$$Z_{\ell+1}(t_1=1;\ t_{\ell+1}=1) = r\alpha^{-1}\left[e^{\Delta}A^{+}(\lambda^{+})^{\ell} - e^{\Delta}A^{-}(\lambda^{-})^{\ell}\right] \tag{A7}$$

$$Z_{\ell+1}(t_1=1,\sigma_1=q;t_{\ell+1}=1,\sigma_{\ell+1}=q) =$$

$$= (r\alpha)^{-1}\left[(r-1)\alpha(\lambda_0^{-})^{\ell} + e^{\Delta}A^{+}(\lambda^{+})^{\ell} - e^{\Delta}A^{-}(\lambda_0^{-})^{\ell}\right] \tag{A8}$$

with $\lambda^{\pm}$, a ,$A^{\pm}$ and λ_0^{-} defined in section 2.

Using eq. (12) to evaluate $Z_{N-\ell}(t_1=1)$ in eq. (A6), we obtain

$$\langle t_1 t_{\ell+1} \rangle = \frac{e^{\Delta_A^+}}{\alpha\lambda^+} \left[e^{\Delta_A^+} - e^{\Delta_A^-} \left(\frac{\lambda^-}{\lambda^+}\right)^{\ell} \right] \qquad \text{(A9)}$$

Note that this reduces to expression eq. (20), when R=1.

Expressions eqs. (5) and (12) allow us to evaluate $Z_{N-\ell}(t_1=1, \sigma_1=q)$ in eq. (A5) and thus

$$\langle \delta_{\sigma_1 \sigma_{\ell+1};q} t_1 t_{\ell+1} \rangle = \frac{e^{\Delta_A^+}}{r^2 \alpha \lambda^+} \left[(r-1)\,\alpha \left(\frac{\lambda_0^-}{\lambda^+}\right)^{\ell} - e^{\Delta_A^-} \left(\frac{\lambda^-}{\lambda^+}\right)^{\ell} + e^{\Delta_A^+} \right] \qquad \text{(A10)}$$

Finally, from eqs. (A9), (A10) and (A1), eq. (17) follows.

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Resumo

Propõe-se um método que permite o cálculo exato do modelo de Potts diluído em uma dimensão. Para parâmetro de troca positivo, a susceptibilidade uniforme apresenta uma singularidade essencial, quando a temperatura tende a $0^{\circ}K$; para parâmetro de troca negativo, é obtido um comportamento em lei de potência, com expoente crítico $\gamma=1$.