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Nota Científica 02/83

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DEPARTAMENTO DE FÍSICA

Março 1983

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DILUTE POTTS CHAIN IN A MAGNETIC FIELD*

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ABSTRACT. The Potts lattice gas in presence of a uniform magnetic field is solved exactly in one dimension. For negative values of the exchange parameter, the magnetization curve exhibits two or three steps, depending on the concentration of vacancies. These steps arise as a result of the competition between the exchange interaction and the magnetic field, being associated to different structural distribution of vacancies and to the magnetic ordering of one or both sublattices.

RESUMO. A solução exata do modelo de Potts diluido em presença de um campo magnético uniforme em uma dimensão é apresentada. Para valores negativos do parâmetro de exchange a curva de magnetização exibe dois ou três degraus, dependendo da concentração de vacâncias. Estes degraus aparecem como resultado da competição entre a interação de exchange e o campo magnético, estando associados a diferentes distribuições de vacâncias e ordenamentos magnéticos.

* Work partially supported by FINEP, CNPq and CAPES.

1. INTRODUCTION

The annealed (site) dilute Potts model or Potts Lattice Gas (PLG) has been introduced in connection with adsorbed gases on substrates (1) and later shown to be relevant to elucidate the nature of the transition of the pure Potts model (2). Since then it has been under current investigation (3) (see also (4) and references therein).

The hamiltonian for the PLG reads

$$\mathcal{H}_0 = - \sum_{<ij>} J'(r\ \delta_{\sigma_i \sigma_j} - 1) t_i t_j - \sum_i \Delta'(1-t_i)$$

where the variable $t_i = 0,1$ indicates the occupancy of site i, Δ' controlling the number of vacancies. An occupied site may be in one of the r states $\sigma_i = 1,2,\ldots,r$, the interaction between two neighbouring spins being characterized by the coupling constant J'.

The exact solution of this model in one dimension (d=1) has been presented elsewhere[2]. In this paper we consider in addition, the effect of a magnetic field, say, in "direction" σ=1 and now

$$\mathcal{H} = \mathcal{H}_0 - H' \sum_i (r\ \delta_{\sigma_i,1} - 1) t_i \qquad [1.1]$$

In section 2, using a recursion relation method similar

[2] R. Riera and C.M. Chaves, to appear.

to the one presented before[2], we show that the model is still exactly soluble in d=1.

When J'<0, the presence of the field introduces new features into the problem. These are essentially due to the existence of critical fields that drive structural changes in the distribution of occupied sites and vacancies and order magnetically the system. These points are analyzed in section 3.

The pure Potts chain in a magnetic field[3] is recovered when $\Delta = -\infty$ and the results presented in (5) for the dilute Ising model are also reproduced.

2. THE RECURSION RELATION METHOD

From [1.1], the gran-partition function for an open chain $Z_N = Z_N(J,\Delta,H,r)$ is

$$Z_N = \sum_{\{t_i,\sigma_i\}} \left\{ \prod_{i=1}^{N-1} \exp\left[J(r\ \delta_{\sigma_i\sigma_{i+1}} - 1)\, t_i t_{i+1}\right] \prod_{i=1}^{N} \exp\left[\Delta(1-t_i)\right] \prod_{i=1}^{N} \exp\left[H(r\ \delta_{\sigma_i,1} - 1)\, t_i\right] \right\} \qquad [2.1]$$

where $J = \beta J'$, $\Delta = \beta\Delta'$, $H = \beta H'$ and $\beta = \frac{1}{k_B T}$. k_B is the Boltzmann constant and T, the temperature. The $\{\sigma_i\}$ summation is performed only over occupied sites.

We rewrite [2.1] as

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

[3] C.M.Chaves, S.L.A. de Queiroz and R.Riera, 'Exact solution of the r-state Potts chain in a magnetic field', Rio, 1981, unpublished.

$$* \exp\left[J(r\,\delta_{\sigma_{N-1},\sigma_N}-1)\,t_{N-1}\,t_N\right]\Bigg\} \qquad [2.2]$$

We have introduced the notation $Z_L(t_k,\sigma_k)$ to denote the partition function of an L-site chain in which the variables associated to site k have fixed but arbitrary values t_k and σ_k. When these variables assume particular values, say $t_k=1$ and $\sigma_k=2$, we write $Z_L(t_k=1,\sigma_k=2)$. Analogously we define $Z_L(t_k)$ or $Z_L(t_k=1)$ for example, if only the t_k variable is specified.

The following equalities hold

$$Z_N = Z_N(t_N=0) + Z_N(t_N=1)$$

$$Z_N(t_N=1) = Z_N(t_N=1,\sigma_N=1) + (r-1)Z_N(t_N=1,\sigma_N=q) \qquad [2.3]$$

where q denotes an arbitrary fixed state different from one.

But from [2.2]

$$Z_N(t_N=0) = e^{\Delta}\Big[Z_{N-1}(t_{N-1}=0) + Z_{N-1}(t_{N-1}=1,\sigma_{N-1}=1) + (r-1)Z_{N-1}(t_{N-1}=1,\sigma_{N-1}=q)\Big] \qquad [2.4a]$$

$$Z_N(t_N=1,\sigma_N=1) = e^{H(r-1)}\Big[Z_{N-1}(t_{N-1}=0) + e^{J(r-1)}Z_{N-1}(t_{N-1}=1,\sigma_{N-1}=1) + e^{-J}\,Z_{N-1}(t_{N-1}=1,\sigma_{N-1}=q)\Big] \qquad [2.4b]$$

$$Z_N(t_N=1,\sigma_N=q) = e^{-H}\Big[Z_{N-1}(t_{N-1}=0) + e^{-J}\,Z_{N-1}(t_{N-1}=1,\sigma_{N-1}=1) + \left(e^{J(r-1)}+(r-2)e^{-J}\right)\,Z_{N-1}(t_{N-1}=1,\sigma_{N-1}=q)\Big] \qquad [2.4c]$$

$$\text{Defining} \quad \bar{Z}_N = \begin{pmatrix} Z_N(t_{N=0}) \\ Z_N(t_{N-1}=1,\sigma_N=1) \\ Z_N(t_{N=1},\sigma_N=q) \end{pmatrix} ,$$

[2.4] can be put in matrix form $\bar{Z}_N = T\,\bar{Z}_{N-1}$ and, by iteration $\bar{Z}_N = T^{N-1}\,\bar{Z}_1$. Diagonalizing the T-matrix we arrive at the following secular equation

$$\lambda^3 - (\lambda_h^+ + \lambda_h^- + e^{\Delta})\lambda^2 + \left[\lambda_h^+ \lambda_h^- + e^{\Delta}(\lambda_h^+ + \lambda_h^-) - e^{\Delta}(e^{H(r-1)} + (r-1)e^{-H}\right]\lambda$$

$$- e^{\Delta}\left[\lambda_h^+ \lambda_h^- - r\, e^{H(r-2)}(e^{J(r-1)} - e^{-J})\right] = 0 \qquad [2.5]$$

with

$$\lambda_h^{\pm} = \frac{1}{2}\left\{(A_1+A_2) \pm \left[(A_1-A_2)^2 + 4\,A_3A_4\right]^{1/2}\right\} \qquad [2.6]$$

where

$$A_1 = e^{(H+J)(r-1)} \qquad A_2 = e^{-H}\left(e^{J(r-1)} + (r-2)e^{-J}\right)$$

$$A_3 = (r-1)e^{-J+H(r-1)} \qquad A_4 = e^{-(H+J)}$$

Now, if Λ is the diagonal representation of T and P the transformation matrix

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

Both P and $\bar{Z}_1$ can be easily calculated and from [2.3] we obtain Z_N. In the thermodynamic limit, the free energy per site is

$$g(J,\Delta,H,r) = k_B\,T\,\ln\lambda^+ \qquad [2.7]$$

where λ^+ is the highest eigenvalue of T.

The results for the pure Potts model ($\Delta = -\infty$) in a magnetic field[3] follows immediately from [2.5], the non-zero eigenvalues of the corresponding T-matrix being $\lambda_h^{\pm}$.

3. RESULTS AND DISCUSSIONS

From the results of section 2 many thermodinamic properties of the chain can be obtained. Here we will be interested in the situation where the concentration $p = \langle t_i \rangle$ of occupied sites is held constant. Let us consider the magnetization per site "parallel" to the field

$$M = \frac{1}{(r-1)} \langle (r\ \delta_{\sigma_i,1} - 1) t_i \rangle$$

Figure 1 shows a plot of M against H/J for fixed $T \neq 0$ and $J' > 0$. More interesting is the behaviour of the system when $J' < 0$ (see figures 2 and 4). M exhibits two or three steps depending on the value of p.

The steps arise as a result of the competition between J' and H', the first favouring the clustering of occupied sites in an "antiferromagnetic" arrangement whereas the latter favours the alignment of occupied sites in state $\sigma = 1$.

At $T = 0^0$K for $p = 1$ and small H', the ground state will then be ...$1\bar{1}1\bar{1}$..., where $\bar{1}$ denotes an occuppied site in any state different from one. This gives $M_1 = \frac{(r-2)}{2(r-1)}$, the value of the first step in the magnetization curve. A magnetic field, however small, is enough to order one sublattice, lifting partially the degeneracy of the ground-state, and so $H'_{c0} = 0$ is a critical field.

If $p<1$ it is energetically favourable to segregate vacancies and occupied sites, the latter being distributed again in a sublattice arrangement of the form $...1\bar{1}1\bar{1}$ and thus this step has $M = p\, M_1$ in fig.2. This corresponds to having coexistence between the phases with $p=0$ (to be denoted by ...0000...) and with $p=1$. The phase diagram in the $(p,H/|J|)$ plane is shown in fig.3.

Given that one sublattice (of occupied sites) is already "saturated", the system remains in the above state as the magnetic field increases, until another critical field (H_{c1}) is reached. For $0<p<1$ it is convenient to the system to exchange vacancies and sites of type $\bar{1}$ and then "to flip" the latter. For each exchange, the first operation costs $2|J'|$ while the second gives $H'r$ and so $H_{c1} = \frac{2|J|}{r}$. For $H' \geq H'_{c1}$ the condition of minimum energy is equivalent to the maximization of the number of clusters of occupied sites.

In our notation, the phase for $p=1/2$, is denoted by ...010101... . If $1/2<p<1$, the maximum number of clusters is $(1-p)$. The ground state is formed by $(1-p)$ isolated sites with $\sigma=1$ (like in the $p=1/2$ phase) and the remaining $(2p-1)$ sites condensed as $...1\bar{1}1\bar{1}...$. This regime (denoted by $...1010\ 1\bar{1}1\bar{1}...$ in figure 3) thus results from the coexistence of the two phases with $p=1/2$ and $p=1$. This step has $M_2 = \frac{r-2p}{2(r-1)}$.

For $p<1/2$, again two phases coexist (those with $p=0$ and $p=1/2$). As the number of vacancies between two sucessive occupied sites is arbitrary, the resulting phase is disordered.

At H'_{c1}, the magnetic field then causes a change in the spatial distribution of vacancies and occupied sites, decreasing the degree of structural order but increasing at the same time the magnetic order.

The last critical field (H_{c2}) is strong enough to orient every occupied site in state 1, keeping the tendence of alternance of vacancies and occupied sites. Clearly, $H_{c2} = 2|J|$ (This field is critical only for $p>1/2$, the system being already "saturated" by H_{c1} for $p\leq 1/2$).

For $\frac{1}{2}<p<1$ and $H'>H'_{c_2}$ again two phases coexist, those corresponding to $p=1/2$ and $p=1$, and now $M=p$.

The above discussion applies for $T=0^0K$. At higher temperatures the change of regime is more smooth (see fig.4).

In fig.5 we show the entropy versus H at fixed temperature, for several ranges of p. As expected, the entropy has peaks at the critical fields, corresponding to an increase in the degeneracy of the states as those fields are approached.

Acknowledgement

We want to acknowledge Dr. A.N. Berker for several usefull discussions about the Potts lattice gas during his recent visit to our Department.

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Figure Captions

Figure 1: Typical plot of magnetization versus H/J for constant p and $T \neq 0^0 K$, when $J' > 0$.

Figure 2: Magnetization versus $H/|J|$ at $T = 0^0 K$ for several ranges of p, when $J' < 0$. $M_1 = \frac{-(r-2)}{2(r-1)}$ and $M_2 = \frac{r-2p}{2(r-1)}$.

Figure 3: Phase diagram of the one-dimensional Potts Lattice gas with $J' < 0$ at $T = 0^0 K$. $\underline{0}$ denotes a vacancy, $\underline{1}$ an occupied site in state $\sigma = 1$ and $\bar{1}$ an occupied site with $\sigma \neq 1$.

Figure 4: An illustration of the dependence of the magnetization on magnetic field for $J' < 0$, $T \neq 0^0 K$ for several values of p. Here $J = -10.0$ and $r = 3$.

Figure 5: Entropy versus magnetic field for $J' < 0$ and $T \neq 0^0 K$ for several value of p. Here $J = -10.0$ and $r = 3$.

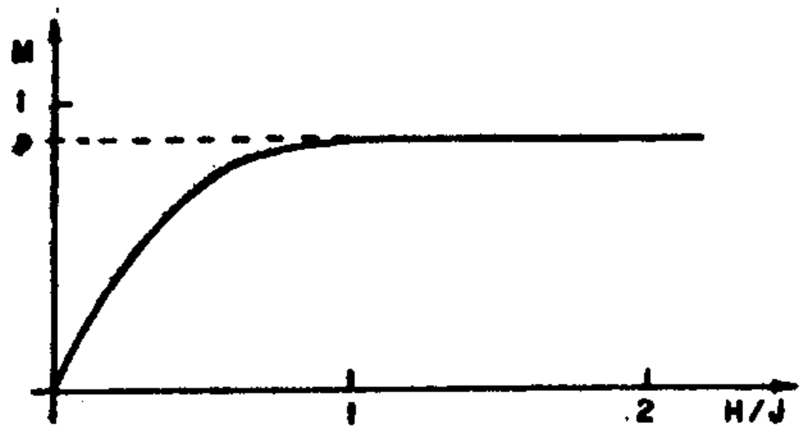

Figure 1

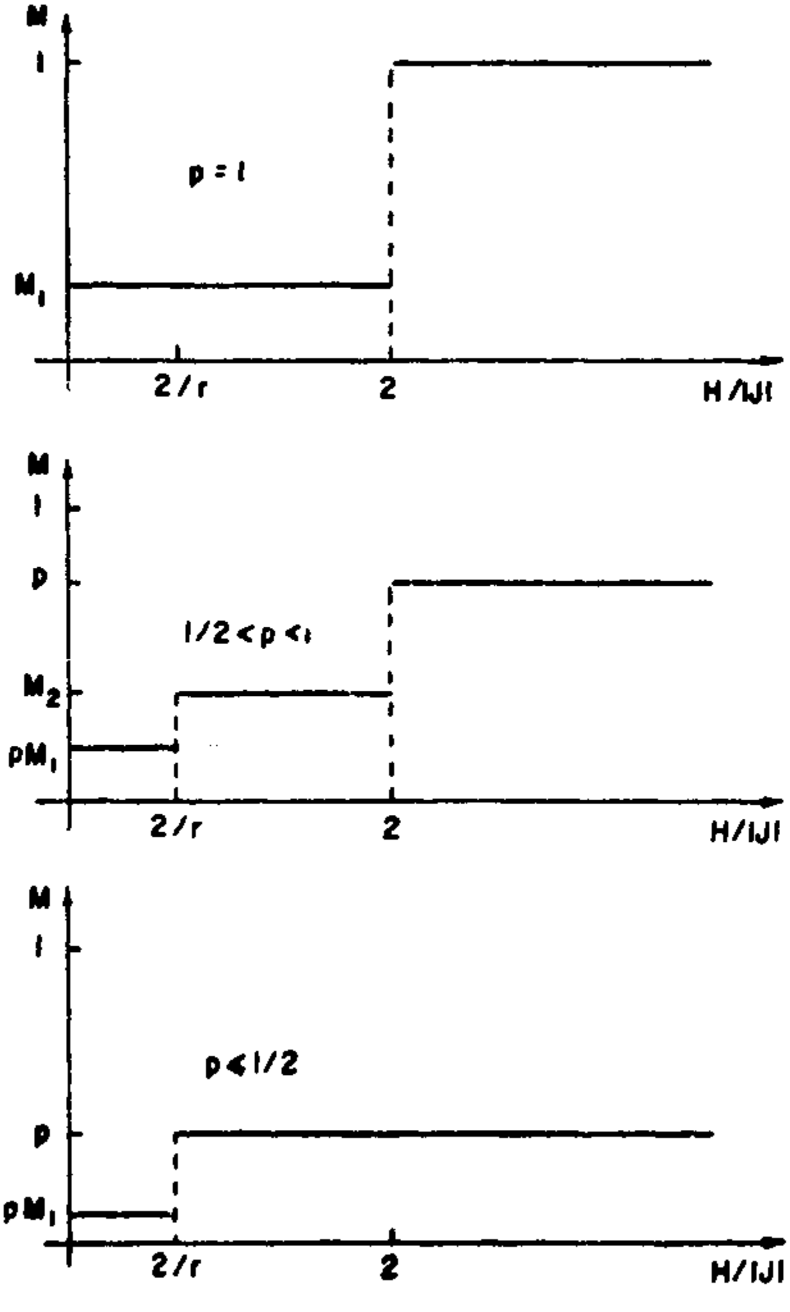

Figure 2

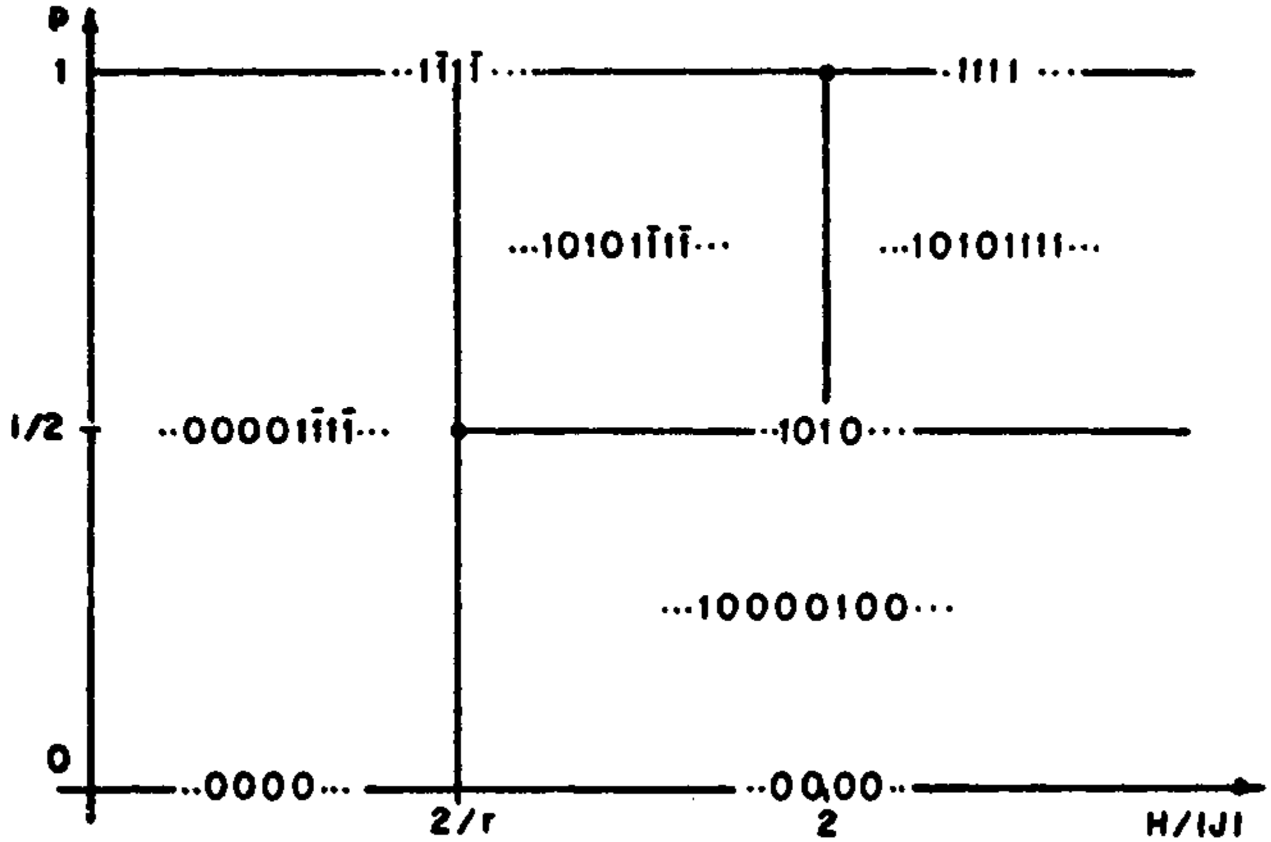
P
1
1/2
0
...1̄1̄1̄...
...1111 ...
...10101̄1̄1̄...
...10101111...
...00001̄1̄1̄...
...1010...
...10000100...
...0000...
...0000...
2/r
2
H/|J|

Figure 3

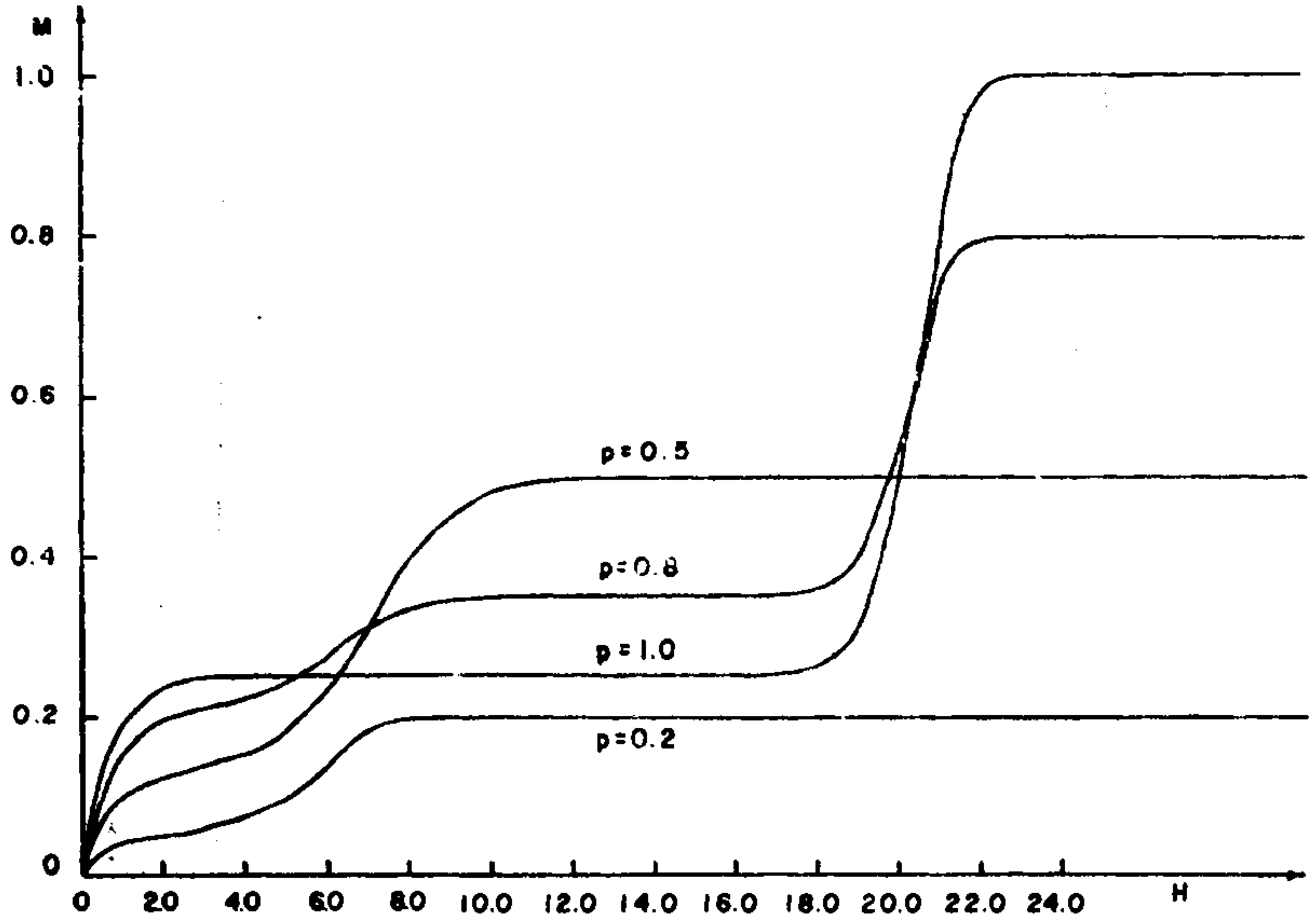
M
1.0
0.8
0.6
0.4
0.2
0
p=0.5
p=0.8
p=1.0
p=0.2
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
22.0
24.0
H

Figure 4

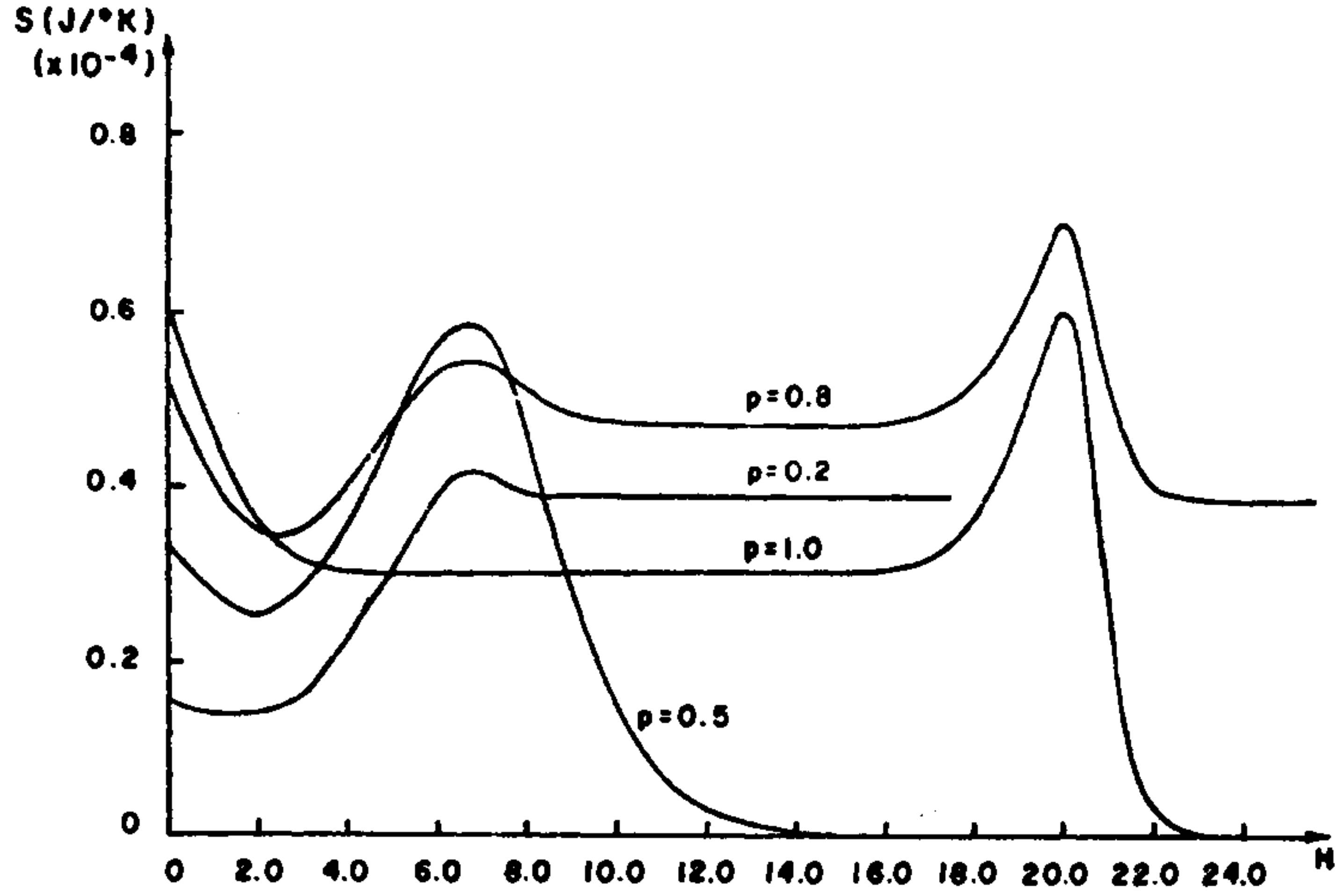
S(J/°K)
(x10^-4)
0.8
0.6
0.4
0.2
0
p=0.8
p=0.2
p=1.0
p=0.5
0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
22.0
24.0
H

Figure 5