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NUMERICAL EXPERIMENTS ON LATTICE GAS MODELS

by

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Acknowledgements

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1. Introduction

The two dimensional Ising Model has never been solved in a finite field. The critical point exponents,[1] however, have all been inferred from the exact solution of Onsager[2] in zero field or determined by series expansions.[8] It remains to determine the magnetization $m(H,T)$ for finite H. Recently Mattis and Plischke[3] derived rigorous analytic lower bounds to $m(H,T)$ in terms of the zero field internal energy $u(0,T)$ and the spontaneous magnetization of Yang[4] $m_0(T)$. As the zero field susceptibility could not be rigorously incorporated into this expression the response to small fields was much too weak and these analytic bounds do not lie very close to the correct answer.

In this chapter we present the results of numerical computations giving a lower bound to $m(H,T)$ which, except for a small region of the H-T plane, lies within .1% of the correct answer. This lower bound is obtained by dividing the infinite lattice into strips of infinite length and width N spins. This is achieved by removing ferromagnetic bonds and can only lower the magnetization as has been shown by Griffiths.[5] The Kramers-Wannier transfer matrix for such a strip is a $2^N \times 2^N$ matrix whose largest eigenvalue, as well as the corresponding eigenvector, we obtain by a simple iterative process described in Section II.

In Section III we introduce a new approximation to the transfer matrix, solvable in zero field, which reproduces completely the critical point behavior of the full Ising Model in zero field. This pseudo transfer matrix has a feature which makes it easier to study numerically.

2. Hamiltonian and Transfer Matrix

The Hamiltonian for the isotropic Ising ferromagnet on a two dimensional M x N lattice is

$$\mathcal{H} = -J \sum_{i=1}^{M} \sum_{j=1}^{N} \{\sigma_{ij}\sigma_{i,j+1} + \sigma_{ij}\sigma_{i+1,j}\} - H \sum_{ij} \sigma_{ij} \qquad (1)$$

where $\sigma_{ij} = \mp 1$.

The partition function is

$$Z = \sum_{\sigma_{11}=\mp 1} \sum_{\sigma_{12}=\mp 1} \cdots \sum_{\sigma_{MN}=\mp 1} e^{-\beta\mathcal{H}} = tr\, V^M \qquad (2)$$

where V is a 2^N x 2^N matrix called the transfer matrix. For a derivation of this matrix see, for example, reference 9.

$$V = (V_2V_3)^{\frac{1}{2}} V_1 (V_2V_3)^{\frac{1}{2}} \qquad (3)$$

where

$$\begin{aligned} V_1 &= (2\sinh 2K)^{N/2} \exp(-K^* \sum_{j=1}^{N} \sigma_j^x) \\ V_2 &= \exp(K \sum_{j=1}^{N} \sigma_j^z \sigma_{j+1}^z) \\ V_3 &= \exp(\beta H \sum_{j=1}^{N} \sigma_j^z) \end{aligned} \qquad (4)$$

where σ^x, σ^z are the Pauli spin matrices, $K = J/kT$, $K^* = -\frac{1}{2}\log(\tanh K)$ and where the lattice is wrapped on a torus in that $\sigma_{N+1}^z = \sigma_1^z$.

If the lattice is M spins long then, as $M \to \infty$, the thermodynamics of the system are completely contained in the largest eigenvalue and the corresponding eigenvector of V. In particular

$$f = F/MN = -1/N\ kT \log \Lambda_{max}(N,H,T) \tag{5}$$

where f is the free energy per spin and Λ_{max} is the largest eigenvalue of V.

$$m(H,T) = 1/N \langle \psi_0 | \sum_{j=1}^{N} \sigma_j^x | \psi_0 \rangle \tag{6}$$

where m(H,T) is the magnetization per spin and $|\psi_0\rangle$ is the eigenvector belonging to Λ_{max}. At H = 0 the transfer matrix may be diagonalized exactly as was first done by Onsager.[2] Other methods have been developed since then, and we will illustrate one of them in the derivation of the thermodynamic properties of the pseudo model in Section III. The zero field solution has the following properties:

$$kT_c = 2J/\log(1+\sqrt{2}) \doteq 2.269185J$$

$$u(0,T_c) = -\sqrt{2}J$$

$$c(0,T) \cong A \log(T-T_c)/T_c \qquad |T - T_c| \ll 1$$

$$m_0(T) = \left\{1 - (1 - \tanh^2 K)^4/(16\tanh^4 K)\right\}^{1/8} \qquad T < T_c$$

$$= 0 \qquad T \geq T_c$$

In the critical region $m_0(T) \cong (T_c - T)^{1/8}$. The formula for $m_0(T)$ was first revealed by Onsager and subsequently derived by Yang.[4] The derivation of $m_0(T)$ is not rigorous but Griffiths[6] has shown that $m_0(T)$ is a lower bound to the true spontaneous magnetization m(0,T) of the Ising Model. The following critical point properties have also been established:

$$\chi(0,T) \cong |T - T_c|^{-7/4} \quad \text{for} \quad |T - T_c| \ll 1$$

by Fisher,[7] and

$$m(H,T_c) \cong H^{1/15} \qquad \text{for} \quad H \ll 1$$

by Gaunt,[8] the latter by numerical studies.

3. Calculational Procedure and Results

We obtain the largest eigenvalue of V and the corresponding eigenvector by the following simple iterative process. Begin with any trial vector ϕ_0 in the direct product representation. If ϕ_0 is not orthogonal to the ground state vector ψ_0 we may write

$$\phi_0 = \alpha_0 \psi_0 + \sum_{j=1}^{2^N-1} \alpha_j \psi_j \tag{1}$$

where the ψ_j's are eigenstates of V.

$$\begin{aligned} V\psi_0 &= \Lambda_{max}\psi_0 \\ V\psi_j &= \Lambda_j \psi_j \qquad \Lambda_j < \Lambda_{max} \end{aligned} \tag{2}$$

Apply V n times.

$$\phi_n = V^n \phi_0 = \Lambda_{max}^n \left\{ \alpha_0 \psi_0 + \sum_{j>0} \alpha_j \left(\frac{\Lambda_j}{\Lambda_{max}}\right)^n \psi_j \right\} \tag{3}$$

If we normalize ϕ_n it is clear that

$$V\phi_n \to \Lambda_{max}\phi_n \quad \text{as} \quad n \to \infty \tag{4}$$

Moreover $\phi_n \to \phi_0$ as $n \to \infty$

In practice convergence of this process is very rapid. Except for small magnetic fields it rarely takes more than five iterations, starting from the completely aligned state, to arrive at six figure accuracy in the eigenvalue.

There are several ways of testing the convergence of the numerical solution. If one is primarily interested in the largest eigenvalue of V then there exists a criterion of absolute convergence. Given an $\varepsilon > 0$ and a number σ such that

$$\| V\phi_n - \sigma\phi_n \|_2 \leq \varepsilon \| V\phi_n \|_2 \equiv \varepsilon \| \phi_{n+1} \|_2 \tag{5}$$

then

$$\left| 1 - \frac{\sigma}{\Lambda_{max}} \right| \leq \varepsilon \tag{6}$$

Here $\sigma = \dfrac{\langle \phi_n | V | \phi_n \rangle}{\langle \phi_n | \phi_n \rangle}$ and $\| \quad \|_2$ is the Euclidean norm. Proof of this theorem may be found in reference 15.

Since our primary interest, in this chapter, is the calculation of m(H,T), which is a more sensitive function of the eigenstate than Λ_{max} we test on successive values of the quantity $\langle \phi_n | \sum_{j=1}^{N} \sigma_j^z | \phi_n \rangle$. This has the advantage that, while very few multiplications of a trial vector by V will produce the eigenvalue to within the accuracy of the machine (6 figures), the eigenvector, and other averages taken over it, may still be changing. In general we stop iterating when successive multiplication of the trial vector by V does not change m by more than one part in 10^4. This does not give any absolute criterion of the accuracy to which we know m but we feel that, except at a singular point (H = 0), m is accurate to one part in 10^3 at least.

From the largest eigenvalue we obtain the free energy of a strip N spins wide and infinitely long.

$$f(N,H,T) = - kT/N \log \Lambda_{max}(N,H,T) \qquad (7)$$

The thermodynamic functions u(N,H,T), m(N,H,T) may be obtained from f by numerical differentiation or by computation of the appropriate correlation functions in the ground state. In particular

$$m(N,H,T) = -\frac{\partial}{\partial H} f(N,H,T)\Big|_T = \frac{1}{N}\langle \psi_0 | \sum_{j=1}^{N} \sigma_j^z | \psi_0 \rangle \qquad (8)$$

We have computed m(N,H,T) as a function of H for several temperatures for strips between 2 and 10 spins wide. In Figure 1 we plot m(N,H,T) vs. $\tanh \beta H$ for $T = .61T_c$, $T = .927T_c$, $T = T_c$, $T = 1.83T_c$. These curves correspond to the lower bounds of reference 3 and were obtained from strips of width 6 spins, 8 spins, 9 spins, and 6 spins respectively. For $T \neq T_c$ these curves lie within .1% of the limiting curve for an infinite lattice. At $T = T_c$ these results are accurate to within .1% for $H \geq .1J$ and accurate to 1% for $H \geq .05J$. In all cases the strips were wrapped on a torus. It might be argued that this destroys the lower bounds in that it is not possible to arrive at these toroidal strips by a removal of ferromagnetic bonds. However, we have found experimentally that the magnetization of a toroidal strip increases monotonically with the circumference, and we henceforth assume it to approach the magnetization of the infinite lattice from below.

A noteworthy feature of the curves is that for $T < T_c$ our

computor solution exhibits a non zero spontaneous magnetization. This is due to the fact that the solution was iterated only a finite number of times. The solution at $H = 0$ for $T < T_c$ is metastable and a sufficient number of iterations will reduce the zero field magnetization to zero. However, the same curves may be obtained by the following procedure, which, nevertheless, guarantees a lower bound. Since the zero field magnetization of Yang, $m_0(T)$, is a lower bound to the spontaneous magnetization of the Ising Model[6] and since $m(H,T)$ is a concave function of H[14] any straight line drawn between the point $m(0,T)$ and the nearest accurate value at another point, $m(H_1,T)$, where $m(H_1,T)$ is, moreover, known to be a lower bound, will provide a lower bound to the magnetization over the entire range $0 \leq H \leq H_1$. Taking successively smaller values of H_1 one effectively generates the curves shown in figure 1 for $T < T_c$, as a lower bound to the exact result.

In tables 1-3 we show the magnetization $m(H,T)$ as a function of H for $T = .9T_c$, $T = T_c$, $T = 2T_c$ for $N = 8,10,6$ respectively. Again for $T \neq T_c$ the results are correct to .1%. For $T = T_c$ the magnetizations are correct to .1% for $H > .05J$ and accurate to .5% for $H > .025J$. The critical region behavior $m = A(H/J)^{1/15}$ extends to $H/J \approx .3$. The coefficient $A = 1.00 \mp .01$. This was previously determined by Gaunt[8] to be 1.002, consistent with our result.

From the Ising Model one can also obtain the thermodynamics of the classical lattice gas. The correspondence is[13]

$$p \leftrightarrow -(f + H + 2J)$$
$$v \leftrightarrow 2/(1 - m(H,T)) \qquad (9)$$

In this chapter we deal only with attractive forces $J > 0$. In figure 2 we plot the isotherms of the lattice gas for temperatures $T = .8T_c$, $T = .927T_c$, $T = T_c$, and $T = 1.5T_c$ along with the boundary of the two phase region as determined from the exact solution of Onsager.[2] Again, except for $T = T_c$, the curves are accurate to .1%. At high temperatures the isotherms approach those of the hard core, $J = 0$, lattice gas given by

$$p/kT = \log(v/(v-1)) \tag{10}$$

4. Pseudo Ising Model

We arrive at the 'pseudo Ising Model' by combining exponents in the transfer matrix, neglecting all Baker-Hausdorff corrections. Thus

$$V_p = (2\sinh 2K)^{N/2} \exp\left\{K\sum_{j=1}^{N-1}\sigma_j^z\sigma_{j+1}^z - K^*\sum_{j=1}^{N}\sigma_j^x + \beta H\sum_{j=1}^{N}\sigma_j^z\right\} \tag{1}$$

where we have not imposed boundary conditions yet. At $H = 0$ this matrix may be diagonalized in the same way as the full Ising Model transfer matrix except that slightly less algebra is necessary. It is clear that we need only determine the largest eigenvalue of the matrix in the exponent.

$$V_p' = K\sum_{j=1}^{N-1}\sigma_j^z\sigma_{j+1}^z - K^*\sum_{j=1}^{N}\sigma_j^x + \beta H\sum_{j=1}^{N}\sigma_j^z \tag{2}$$

This property makes the pseudo model useful for the study of the three dimensional Ising Model in that the matrix is 'sparse' in the product representation, i.e. it has a large number of zeros. This decreases the amount of storage required and allows

the treatment of larger finite strips or parallelepipeds. To verify that this pseudo transfer matrix reproduces the correct critical point behavior at least at H = 0 we carry out the calculation of f,u,c,m where

$$f(0,T) = -\,kT/MN \log \mathrm{tr.}\, V_p^M = -\,kT/N \log \Lambda_{max}(N,0,T)$$

$u(0,T) = \frac{\partial}{\partial\beta}(\beta f)$ is the 'internal energy'

$c(0,T)/k = -\beta^2 \frac{\partial u(0,T)}{\partial \beta}$ is the 'specific heat'

$m_0^2(T) = \lim_{|i-j|\to\infty} \langle \sigma_i \sigma_j \rangle$ is the analog of the Yang

magnetization. To do this we follow step by step the procedure of Schultz, Mattis and Lieb[11] and first make a rotation.

$$\sigma^x \longrightarrow \sigma^z$$
$$\sigma^z \longrightarrow -\sigma^x$$

Then we introduce fermion operators via the transformation:

$$\sigma_m^+ = \exp\{\pi i \sum_{j=1}^{m-1} c_j^+ c_j\}\, c_m^+ \qquad (3)$$
$$\sigma_m^- = \exp\{\pi i \sum_{j=1}^{m-1} c_j^+ c_j\}\, c_m$$

where $\{c_j, c_l^+\} = \delta_{jl}$ and $\{c_j, c_l\} = \{c_j^+, c_l^+\} = 0$

With these substitutions the matrix V_p' becomes

$$V_p' = K\sum_{j=1}^{N-1}(c_j^+ - c_j)(c_{j+1}^+ + c_{j+1}) - 2K^*\sum_{j=1}^{N}(c_j^+ c_j - \tfrac{1}{2}) \quad (4)$$

We complete the first term by adding $\sigma_N^x \sigma_{N+1}^x$

$$= e^{\pi i \sum_{j=1}^{N} c_j^+ c_j}(c_M^+ - c_M)(c_{M+1}^+ + c_{M+1}) = (-1)^n (c_M^+ - c_M)(c_{M+1}^+ + c_{M+1}) \quad (5)$$

Now if n is odd we let $C_{M+1} = -C_1 \quad C_{M+1}^+ = -C_1^+$;

if n is even we let $C_{M+1} = C_1 \quad C_{M+1}^+ = C_1^+$

This imposes boundary conditions and gives two types of transfer matrix, $V_p'^{\pm}$, where an acceptable eigenstate of $V_p'^{+}$ must have an even number of fermions, and an eigenstate of $V_p'^{-}$ must have an odd number of fermions. To diagonalize we make the further transformation

$$C_m = \frac{1}{\sqrt{N}} e^{-i\pi/4} \sum_q e^{iqm} \eta_q$$

For V^+ $q = \pm \frac{\pi}{N}, \pm \frac{3\pi}{N}, \cdots \pm \frac{N-1}{N}\pi$

(6)

For V^- $q = 0, \pm \frac{2\pi}{N}, \cdots \pm \frac{N-2}{N}\pi, \pi$

Then $V_q' = 2K\sum_{q>0} \cos q\,(\eta_q^+ \eta_q + \eta_{-q}^+ \eta_{-q}) + 2K^*$ (7)

$$- 2K\sum_{q>0} \sin q\,(\eta_q^+ \eta_{-q}^+ - \eta_q \eta_{-q}) - 2K^*\sum_{q>0}(\eta_q^+ \eta_q + \eta_{-q}^+ \eta_{-q})$$

The terms for $q = 0$, $q = \pi$ are

$$2(K - K_1^*)\left(\eta_0^+ \eta_0 - \tfrac{1}{2}\right)$$

$$-2(K + K_1^*)\left(\eta_\pi^+ \eta_\pi - \tfrac{1}{2}\right)$$

Finally the transformation

$$\eta_q^+ = \cos\phi_q\, \xi_q^+ - \sin\phi_q\, \xi_{-q}$$
$$\eta_{-q}^+ = \cos\phi_{+q}\, \xi_{-q}^+ + \sin\phi_q\, \xi_q \qquad (8)$$

with

$$\cos\phi_q = \frac{1}{\sqrt{2}} \left\{ 1 + \frac{a}{\sqrt{a^2+b^2}} \right\}^{\frac{1}{2}}$$

$$\sin\phi_q = -\frac{1}{\sqrt{2}} \left\{ 1 - \frac{a}{\sqrt{a^2+b^2}} \right\}^{\frac{1}{2}}$$

where $a = K \cos q - K^*$, $b = K \sin q$ diagonalizes V.

In diagonal form V is given by

$$V = -2 \sum_{q \neq 0} \varepsilon_q \left(\xi_q^+ \xi_q + \xi_{-q}^+ \xi_{-q} - 1 \right) \qquad (9)$$

$$\varepsilon_q = \left\{ K^2 + K^{*2} - 2 K K^* \cos q \right\}^{\frac{1}{2}}$$

The $q = 0$, $q = \pi$ terms may be incorporated in the same way with

$$\varepsilon_0 = K^* - K \qquad \varepsilon_\pi = K^* + K$$

From (9) it is clear that the largest eigenvalue is obtained when $\xi_q |\phi\rangle = 0$, i.e. the completely empty state. If $K^* \leq K$ and the singly occupied state of V^- is degenerate with the empty state of V^+. This defines the critical temperature as it is well known that we must have such a degeneracy for long range order to exist. Thus $T_p = T_c$ where T_c is the critical temperature of the full Ising Model.

The free energy is given by

$$f = -kT\left\{\frac{1}{2}\log(2\sinh 2K) + \frac{1}{2\pi}\int_{-\pi}^{\pi} dq\, \varepsilon_q\right\} \qquad (10)$$

The internal energy is

$$u = -J\coth 2K \qquad (11)$$
$$-\frac{J}{2\pi}\int_{-\pi}^{\pi} dq\, \frac{\left(K - \frac{1}{2}K^*\frac{\operatorname{sech}^2 K}{\tanh K}\right) - \left(K^* - \frac{K}{2}\frac{\operatorname{sech}^2 K}{\tanh K}\right)\cos q}{\left\{K^2 + K^{*2} - 2KK^*\cos q\right\}^{\frac{1}{2}}}$$

As $K \to K^*$

$$u \to -J\coth 2K - \frac{J}{2\pi}\,\frac{K\left(1 - \frac{\operatorname{sech}^2 K}{2\tanh K}\right)}{\sqrt{2}\,K}\int_{-\pi}^{\pi} dq\,\sqrt{1-\cos q} \qquad (12)$$

$$= -J\coth 2K - \frac{J}{2\pi\sqrt{2}}\left(1 - \frac{1}{\sinh 2K}\right)\int_{-\pi}^{\pi} dq\,\sqrt{1-\cos q} \qquad (13)$$

Now at T_p

$$\sinh 2K = 1 \qquad U_p(0,T_p) = -J\sqrt{2} = U(0,T_c) \qquad (14)$$

In figure 3 we plot $u_p(0,T)$ and $u(0,T)$ as functions of T. The most divergent term in the specific heat is given by

$$c/k \sim \frac{J^2}{\pi}\,\frac{(1+\sinh 2K)}{\sinh 2K}\int_0^{\pi} dq\,\frac{1}{\sqrt{K^2+K^{*2}-2KK^*\cos q}} \qquad (15)$$

$$\sim \frac{J^2}{\pi}\,\frac{(1+\sinh 2K)}{\sinh 2K}\,\frac{K^*+K}{K^{*2}+K^2}\int_0^{\frac{\pi}{2}} \frac{dq}{\sqrt{1 - \frac{4K^*K}{(K^*+K)^2}\sin^2 q}} \qquad (16)$$

This diverges logarithmically as $K^* \to K$ and we have, after expanding

K, K^* in terms of $T - T_c$

$$c/k \sim -\frac{(J\beta)^2}{\pi}\,\frac{(1+\sinh 2K)}{K \sinh 2K}\,\log\left|\frac{T-T_c}{T_c}\right| \qquad (17)$$

$$\approx -\frac{2}{\pi}\left(\frac{J}{kT_c}\right)\log\left|\frac{T-T_c}{T_c}\right| . \qquad (18)$$

By comparison the specific heat of the full Ising Model is given by[12]

$$c/k \approx -\frac{2}{\pi}\left(\frac{2J}{kT_c}\right)^2 \log\left|\frac{T-T_c}{T_c}\right| \qquad (19)$$

The coefficients differ but the form of the divergence is exactly the same.

The spontaneous magnetization is expressable as a Toeplitz Determinant:[11]

$m_0^2(T) = \det|a_{ij}|$ where

$$a_{ij} = a_{i-j} = -\frac{1}{N}\sum_{l} e^{-il(j-i)}\, e^{i(2\phi_l + l)} \qquad (20)$$

where ϕ_l is the function of l defined in (8). The dimensionality of the determinant is the separation of the spins i,j in the correlation function $\langle \sigma_i \sigma_j \rangle$ and as this becomes infinitely large the determinant may be evaluated to give

$$m_0(T) = (1 - K^{*2}/K^2)^{1/8} \qquad T < T_c$$

$$= 0 \qquad T \geq T_c \qquad (21)$$

Expansion about T_c yields

$$m_0 \approx \left\{\frac{1+\tanh K_c+2K_c}{K_c^2}\right\}^{1/8}\left(\frac{T_c-T}{T_c}\right)^{1/8} \qquad T\approx T_c \qquad (22)$$

The Yang magnetization near T_c behaves as

$$m_y \approx \left(4\cosh 2K_c\right)^{1/8}\left(\frac{T_c-T}{T_c}\right)^{1/8} \qquad T\approx T_c \qquad (23)$$

Again, as with the specific heat, the critical point behavior is the same with the multiplicative constant being different.

We have shown that the pseudo model exhibits the same critical point behavior as the Ising Model in zero field. We have found that

$$T_p = T_c$$

$$u_p(0,T_c) = u(0,T_c)$$

$$m_p(0,T) \sim |T - T_c|^{1/8} \qquad T\lesssim T_c$$

$$c_p(0,T) \sim -\log|T - T_c| \qquad T\approx T_c$$

This leads to the speculation that the critical exponents will be the same in a finite field in two dimensions as well as in three dimensions. The investigation of this will be carried out at a later time.

5. References

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The properties of the lattice gas were evaluated in this book, using relatively crude molecular field theory. We should also note early, accurate results in lattice gases, particularly for $J < 0$, the numerical work by L.K. Runnels, Phys. Rev. Letters 15, 581 (1965) on the hard square lattice gas (the $J \to -\infty$ limit of the present model), and the related work of A. Bellemans in Statistical Mechanics, ed. by T. Bak (W.A. Benjamin, Inc., New York, 1967), p. 373, are to be noted.

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6. Figure Captions

Figure 1 Plot of $M(H,T)$ as function of $\tanh \beta H$ for various temperatures. A) $T = .61T_c$, $N = 6$ B) $T = .8T_c$, $N = 7$ C) $T = .927T_c$, $N = 8$ D) $T = T_c$, $N = 9$ E) $T = 1.83T_c$, $N = 6$. The critical behavior $m(H,T_c) = A(H/J)^{1/15}$ extends to $\tanh \beta H \approx .15$ in curve D.

Figure 2 Plot of isotherms for the lattice gas. A) $T = .8T_c$ B) $T = .927T_c$ C) $T = T_c$ D) $T = 1.5T_c$. Curve E is the boundary of the two phase region as determined from the analytic solution at $H = 0$.

Figure 3 Plot of internal energies of the pseudo model and the Ising model in zero field as function of temperature. A) $U_p(0,T)$ B) $U_I(0,T)$. The deviation from infinite slope at T_c results from inertia in the mechanical plotter, not from any significant computer error.

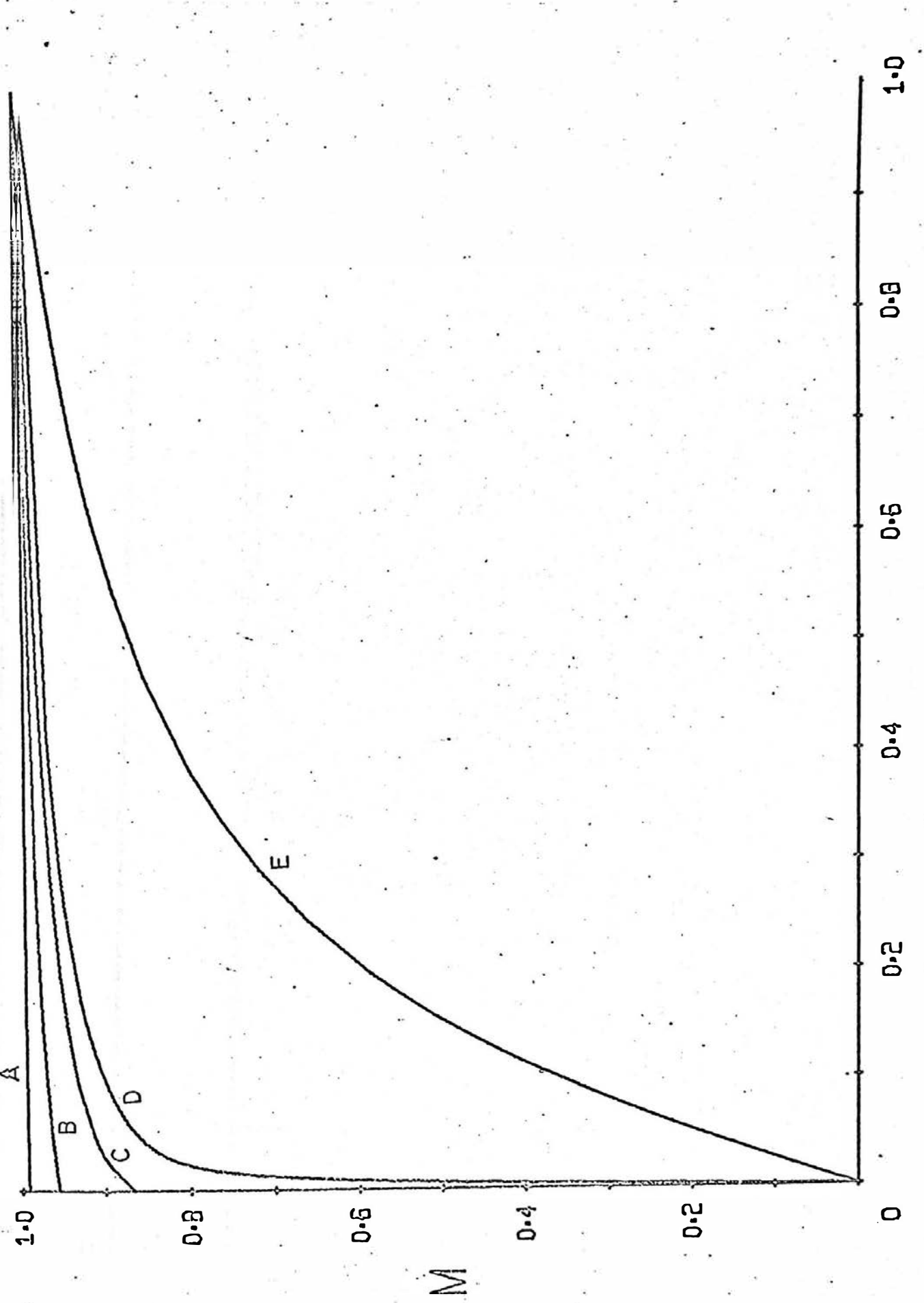

Figure 1

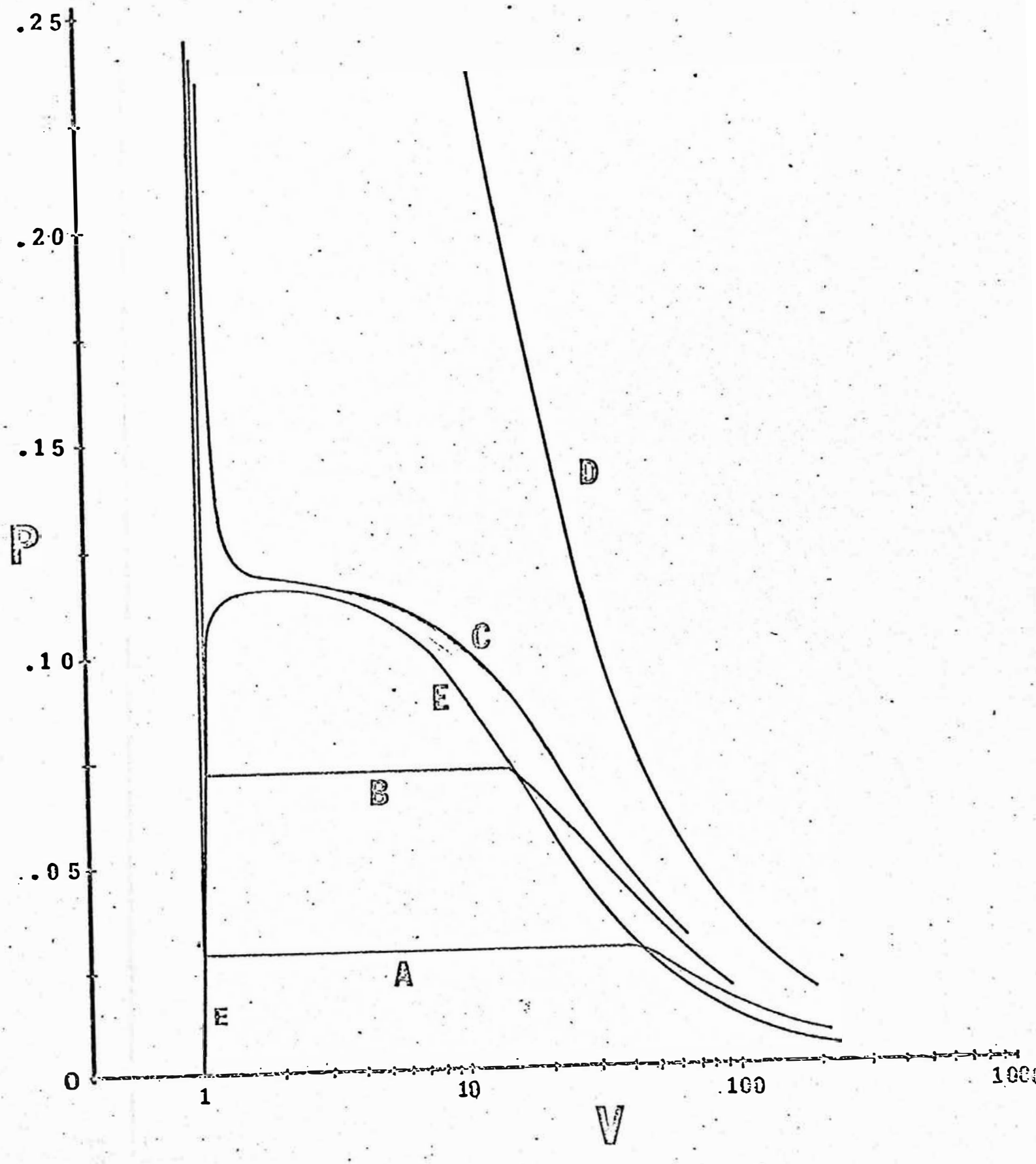

Figure 2

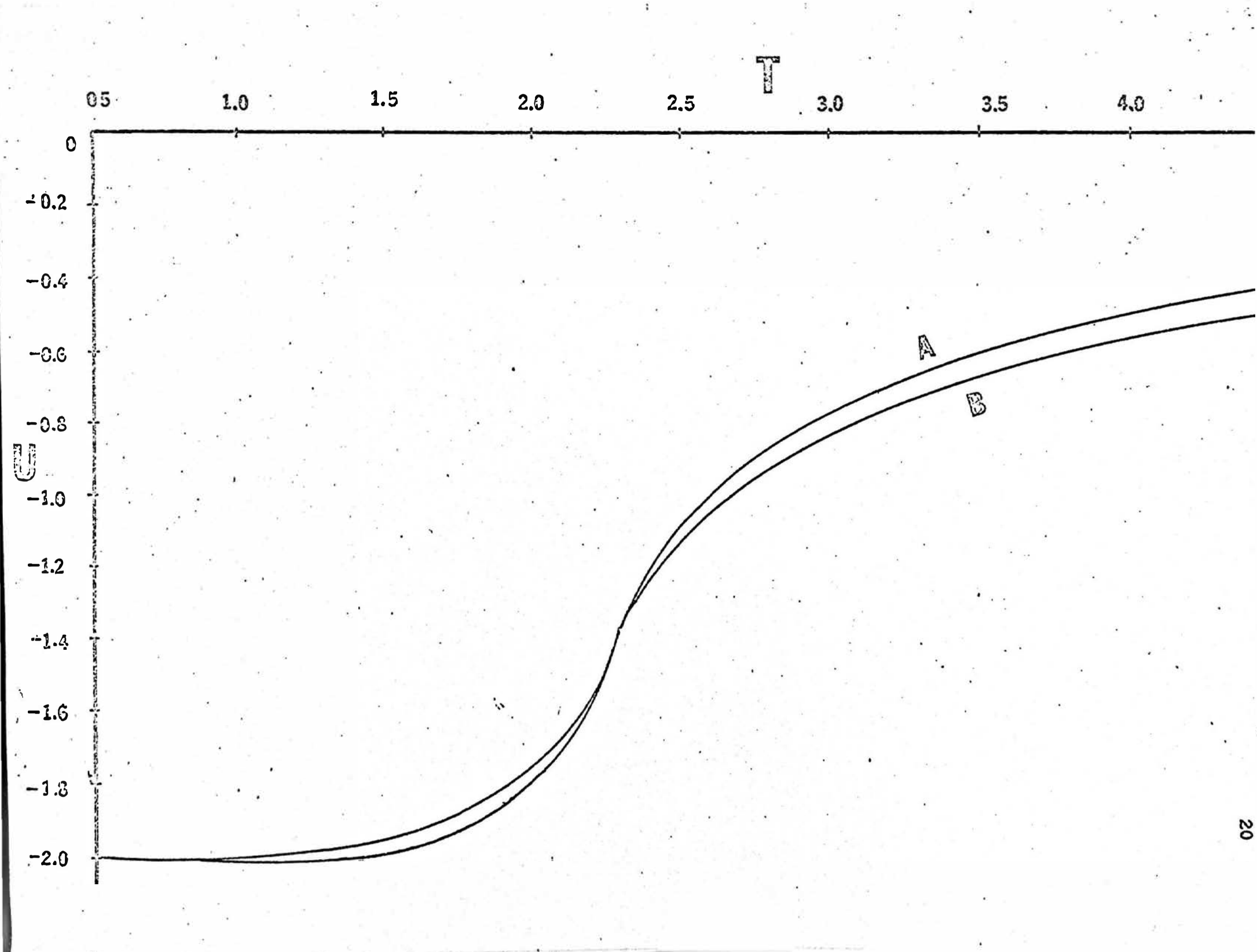
T
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0
-0.2
-0.4
-0.6
-0.8
-1.0
-1.2
-1.4
-1.6
-1.8
-2.0
U
A
B

TABLE 1

M(H) AS FUNCTION OF H FOR $T = 0.90T_c$

H	M(H)
1.0000	0.9818
0.9500	0.9806
0.9000	0.9794
0.8500	0.9781
0.8000	0.9766
0.7500	0.9751
0.7000	0.9734
0.6500	0.9716
0.6000	0.9695
0.5500	0.9673
0.5000	0.9648
0.4500	0.9621
0.4000	0.9590
0.3500	0.9555
0.3000	0.9515
0.2500	0.9469
0.2000	0.9414
0.1800	0.9390
0.1600	0.9362
0.1400	0.9332
0.1200	0.9298
0.1000	0.9261
0.0900	0.9239
0.0800	0.9217
0.0750	0.9205
0.0700	0.9192
0.0600	0.9164
0.0500	0.9131
0.0450	0.9114
0.0400	0.9098
0.0350	0.9081
0.0300	0.9065
0.0250	0.9048
0.0200	0.9031
0.0100	0.8998
0.0090	0.8995
0.0080	0.8992
0.0070	0.8988
0.0060	0.8985
0.0050	0.8982
0.0040	0.8978
0.0030	0.8975
0.0020	0.8972
0.0010	0.8968
0.0000	0.8965

TABLE 2

M(H) AS FUNCTION OF H FOR $T = 1.00T_c$

H	M(H)
1.0000	0.9683
0.9000	0.9642
0.8000	0.9595
0.7000	0.9540
0.6000	0.9473
0.5000	0.9389
0.4500	0.9339
0.4000	0.9281
0.3500	0.9215
0.3000	0.9138
0.2500	0.9045
0.2000	0.8931
0.1900	0.8903
0.1800	0.8875
0.1700	0.8845
0.1600	0.8813
0.1500	0.8775
0.1400	0.8738
0.1300	0.8698
0.1200	0.8655
0.1100	0.8607
0.1000	0.8556
0.0900	0.8499
0.0800	0.8434
0.0700	0.8357
0.0600	0.8274
0.0500	0.8159
0.0450	0.8083
0.0400	0.7995
0.0350	0.7883
0.0300	0.7740
0.0250	0.7548
0.0000	0.0000

TABLE 3

M(H) AS FUNCTION OF H FOR $T = 2.00T_c$

H	M(H)
1.0000	0.5670
0.9500	0.5490
0.9000	0.5299
0.8500	0.5099
0.8000	0.4889
0.7500	0.4667
0.7000	0.4433
0.6500	0.4188
0.6000	0.3931
0.5500	0.3661
0.5000	0.3379
0.4500	0.3084
0.4000	0.2778
0.3500	0.2460
0.3000	0.2131
0.2500	0.1793
0.2000	0.1445
0.1800	0.1304
0.1600	0.1162
0.1400	0.1019
0.1200	0.0875
0.1000	0.0730
0.0900	0.0658
0.0800	0.0585
0.0750	0.0549
0.0700	0.0512
0.0600	0.0439
0.0500	0.0366
0.0450	0.0330
0.0400	0.0293
0.0350	0.0256
0.0300	0.0220
0.0250	0.0183
0.0150	0.0110
0.0100	0.0073
0.0090	0.0066
0.0080	0.0059
0.0070	0.0051
0.0060	0.0044
0.0050	0.0037
0.0040	0.0029
0.0030	0.0022
0.0010	0.0007
0.0000	0.0000

II. LATTICE GASES WITH SOFT CORE REPULSION: ISING ANTIFERROMAGNET

1. Introduction

Our aim is to investigate the properties of lattice gases having a soft core repulsive potential as well as a hard core. The basic system, in magnetic language, is the nearest neighbor Ising antiferromagnet. In zero magnetic field this system has the same thermodynamic properties as the Ising ferromagnet which was solved exactly in two dimensions by Onsager.[1] The antiferromagnet was treated by Garrett[2] using molecular field theory (MFT). He obtained, for $T < T_N$, a second order phase transition at a finite critical field $H_c(T)$ at which the magnetization is continuous but the susceptibility is discontinous. In section 2 of this chapter of this chapter we also use MFT to obtain the properties of the lattice gas. In section 3 we analyze the transfer matrix of the two dimensional antiferromagnet for strips of infinite length but finite width by the same method used in chapter I to treat the ferromagnet. We are able to treat strips up to 10 sites wide and find MFT to be qualitatively correct, with possibly one important exception, discussed below.

In section 4 we consider the antiferromagnet with ferromagnetic interactions between next nearest neighbors. In lattice gas language this is a system with hard cores, soft cores, and a longer range attractive force. Hemmer and Stell[3] have recently treated exactly

a one dimensional continuum fluid with hard core, soft core, and a weak long range attractive potential. They found either a single first order phase transition or two first order transitions depending on certain parameters in their model. They have also argued that if the attractive part of the interaction is capable of producing a first order phase transition in the lattice gas, then the soft core repulsion should bring about two first order phase transitions. In MFT, however, we find that while there are always two phase transitions the nature of these transitions is variable. Notably, there is a temperature $T_1 < T_c$ above which the transitions are second order, whereas the transitions are first order below T_1. These results are expected to hold for an exact calculation as well.

It might be expected that this model would at least qualitatively reproduce the properties of the rare gases, we find in MFT no critical line (or critical point or triple point) even for interactions with more structure than the ones reported on here. In view of the fact that Hemmer and Stell have found the possibility of such a critical line already in one dimension, it seems to us that molecular field theory is the culprit. Thus, the major improvement of an exact transfer matrix solution, in two or three dimensions, over MFT will be the precise delineation of the critical lines and their dependence on the structure of the interactions (depth and width of attractive potentials and radius, as well as gradient, of repulsive core). It is our opinion, from the present calculations, that only a blend of repulsive and attractive forces comparable to the forces between two Argon atoms can yield a thermodynamic phase diagram comparable to the experiments

on Argon. We have not yet found this blend.

In section 5 we apply the transfer matrix method to the antiferromagnet with ferromagnetic interactions along crossed bonds. While at present time we cannot yet verify the existence of the temperature T_1 we present evidence that MFT does indeed give the correct picture concerning the order of the phase transitions.

2. Ising Antiferromagnet: Molecular Field Theory

The Ising antiferromagnet on an isotropic square lattice has the Hamiltonian

$$\mathcal{H} = J \sum_{ij} \left(S_{ij} S_{ij+1} + S_{ij} S_{i+1,j} \right) - H \sum_{ij} S_{ij} \qquad (1)$$

where $S_{ij} = \pm 1$ and $J > 0$. The magnetic properties of the antiferromagnet have been previously derived in MFT by Garrett.[2] Dividing the lattice into A and B sublattices and designating the sublattice magnetizations by m_A and m_B we have

$$\begin{aligned} m_A &= - \tanh \beta (zJm_B - H) = - \tanh(m_B - h)/t \\ m_B &= - \tanh \beta (zJm_A - H) = - \tanh(m_A - h)/t \end{aligned} \qquad (2)$$

where $h = H/zJ$, $t = kT/zJ$, and where z is the number of nearest neighbors. The MFT treatment applies to any lattice which may be divided into two sublattices in such a way that the nearest neighbor of any site on the A sublattice is on the B sublattice and vice versa. In Eq. (1) we wrote the Hamiltonian for a square lattice in view of the transfer matrix treatment of the next

section but the rest of this section applies equally well to the three dimensional simple cubic and body centered cubic lattices; only the parameter z is different.

The free energy per spin is given by

$$f/zJ = -t \log 2 - \tfrac{1}{2} m_A m_B - t/2 \log \cosh(m_B - h)/t - t/2 \log \cosh(m_A - h)/t \qquad (3)$$

The equations (2) admit two types of solution

a) $m_A = m_B$ with free energy f_a

b) $m_A \neq m_B$ with free energy f_b

As was shown by Garrett[2] $f_b < f_a$ whenever the b type solution of equations (2) exists. As the magnetic field is increased at constant temperature $t < 1$ from zero we pass through a critical field $h_c(t)$ at which the b type solution ceases to exist. The sublattice magnetizations m_A, m_B approach each other continuously and the magnetization $m = \frac{1}{2}(m_A + m_B)$ is continuous. The susceptibility $\chi = \left.\frac{\partial m}{\partial h}\right|_t$ is discontinuous and the transition is second order. In figure 4a we show some magnetic isotherms. The temperature dependence of the critical field is given by

$$h_c(t) = \sqrt{1 - t} + t \tanh^{-1}\sqrt{1 - t} \qquad (4)$$

This curve is plotted in figure 5.

The properties of the lattice gas are obtained from the magnetic properties via

$$v = 2/(1 - m(H,T))$$
$$p = - f - H + zJ/2 \qquad (5)$$

Since the magnetization is everywhere continuous the lattice gas can have no discontinuous change in volume and thus no first order phase transition. However, there are two second order phase transitions along each isotherm with $T < T_c = zJ$ and we have three distinct phases in the system. Some isotherms are shown in figure 4b along with the locus of the coexistence curve $p_c(v)$. Note that there is a region where $\left.\frac{\partial p}{\partial T}\right|_v < 0$, in which increasing temperature causes the pressure to decrease. In figure 6 the coexistence curve in the p - T plane is shown. In figure 7a we show the compressibility factor pv/kT as function of 1/v. Note the structure for $t < 1$. At higher temperatures $t > 1$ it is a monotonically increasing function.

The identification of the various phases is as follows:
(b) is degenerate because for any solution $m_A = S$, $m_B = Q$ with $S \neq Q$ we can find a second equally valid solution $m_A = Q$, $m_B = S$. The existence of degeneracy is the sine qua non of long range order, as is well known. Then whenever (b) is the solution, a crystal is formed, having twice the basic lattice parameter of the original lattice.
(a) The solution being unique, there is no long range order. The identification of vapor vs. liquid is merely a question of density.

3. Ising Antiferromagnet: Transfer Matrix Method

The Ising antiferromagnet on a square lattice has the transfer matrix

$$V = (V_2 V_3)^{\frac{1}{2}} V_1 (V_2 V_3)^{\frac{1}{2}} \tag{6}$$

where

$$V_1 = e^{-MK} \prod_{j=1}^{M} (1 + \sigma_j^x e^{2K})$$

$$V_2 = \exp\left(-K \sum_{j=1}^{M} \sigma_j^z \sigma_{j+1}^z\right)$$

$$V_3 = \exp\left(\beta H \sum_{j=1}^{M} \sigma_j^z\right)$$

$K = \beta J$ and σ^x, σ^z are the Pauli matrices. The thermodynamics is given by the partition function

$$Z(M,H,N,T) = Z = \mathrm{tr}\, V^N = \Lambda_{\max}^N (M,H,T) \tag{7}$$

where $\Lambda_{\max}$ is the largest eigenvalue of V. In zero magnetic field the transfer matrix may be exactly diagonalized[1] and the thermodynamic properties are exactly the same as those of the Ising ferromagnet with the same interaction strength. In particular the specific heat is logarithmically infinite at $T = T_N \doteq 2.269185J$.

In chapter I we used a simple iterative process to obtain $\Lambda_{\max}$ and the corresponding eigenvector for the ferromagnet on strips of infinite length and width up to 10 spins. We use this same procedure to analyze the transfer matrix of the antiferromagnet for strips of width 2, 4, 6, 8, and 10 spins. Only strips

with an even number of sites are treated so that, when wrapped on a torus, they may be divided into two sublattices. In figure 8a we plot the magnetization M(H) for several temperatures for the case N = 6. All isotherms are smooth as is to be expected for a lattice which is infinite in only one direction. That a phase transition is developing is indicated, however, by the specific heat $C_H(N,T)$. For strips of width N the specific heat $C_H(N,T)$, which we obtain by numerical differentiation of the internal energy $U_N(H,T)$, has a maximum at a temperature $T_c(N,H)$. As $N \to \infty$, $T_c(N,H) \to T_c(H)$ where $T_c(H)$ is the critical temperature of the infinite two dimensional lattice in field H. We estimate that the numerical differentiation introduces a possible error of 1% in the specific heat. Using T_c for 8 spins we, nevertheless, find that in any field $H < zJ$

$$C_H(N,T_c(8,H)) \sim \log N$$

leading to the conjecture that the infinity which is known to exist at H = 0 persists at finite field. A plot of $C_H(N,T_c(8,H))$ vs log N is whown in figure 13. From the maxima of the specific heat we obtain the curve $h_c(t)$ in successively better approximation. Here we define $t = T/T_c$ (rather than $t = kT/zJ$) and $h \equiv H/zJ$. We plot it in figure 5 for N = 8 together with the MFT version of $h_c(t)$. While convergence is worst near t = 0, it is clear that the initial increase in h_c at t = 0 in MFT is an artifact of the approximation.

In figure 8b we show the lattice gas isotherms corresponding to the magnetizations shown in figure 8a. It will be seen that the essential features of MFT are preserved. The region $\left(\frac{\partial p}{\partial T}\right)_v < 0$ exists

here also.

Various thermodynamic phases can be identified using the degeneracy (or nondegeneracy) of Λ_{max}, following the arguments given at the conclusion of the preceding section. The exact results agree with molecular field theory in the essential qualitative features.

4. Ising Antiferromagnet with Next Nearest Neighbor Ferromagnetic Interactions: Molecular Field Theory

We consider the antiferromagnet with next nearest neighbor ferromagnetic interactions. In anticipation of the transfer matrix treatment we let the ferromagnetic interactions be along crossed bonds:

$$\mathcal{H} = J\sum_{ij}\left(s_{ij}s_{i\,j+1} + s_{ij}s_{i+1\,j}\right) - \alpha J\sum_{ij} s_{ij}\left(s_{i+1\,j+1} + s_{i+1\,j-1}\right) - H\sum_{ij} s_{ij} \qquad (8)$$

Here $\alpha > 0$ is a parameter specifying the strength of the ferromagnetic coupling. In lattice gas language this Hamiltonian describes particles with a hard core, a soft core, and a longer range attraction. If the soft core part of the interaction were not there the attraction would be sufficient to bring about a first order phase transition in the lattice gas in two or more dimensions. Hemmer and Stell[4] have argued that the soft core should then cause the system to undergo <u>two</u> first order phase transitions. In the MFT approximation we find that, while there are always two phase transitions, they are first order only below some temperature $T_1(\alpha) < T_c(\alpha)$. Between T_1 and T_c the transitions are second order and above T_c

there is no transition at all.

Dividing the lattice into A and B sublattices with magnetizations m_A, m_B we obtain the equations

$$\begin{aligned} m_A &= -\tanh \beta (zJm_B - zJm_A - H) = -\tanh(m_B - m_A - h)/t \\ m_B &= -\tanh \beta (zJm_A - zJm_B - H) = -\tanh(m_A - m_B - h)/t \end{aligned} \tag{9}$$

for the magnetizations and

$$\begin{aligned} f = F/zJN = &- t \log 2 - \tfrac{1}{2}m_A m_B + 2/4(m_A^2 + m_B^2) \\ &- t/2 \log \cosh(m_A - m_B - h)/t \\ &- t/2 \log \cosh(m_B - m_A - h)/t \end{aligned} \tag{10}$$

for the free energy. Again $t = kT/zJ$, $h = H/zJ$. The critical temperature $t_c = 1 + \alpha$. The equations (9) admit two types of solution

a) $m = m_A = m_B$ with free energy f_a

b) $m_A \neq m_B$ with free energy f_b

Except at $t = 0$ the (a) state is always a solution with $m \neq 0$. At $t = 0$ we need $h > 1 - \alpha$, for $\alpha < 1$, for the (a) state to exist. At $h = 0$ the (b) state always has the solution $m_A = -m_B \neq 0$ for $t < t_c$. Moreover, at $h = 0$ the (b) state always has the lower free energy. As h is raised we reach a value $h_c(t)$ where $f_a = f_b$. However, unlike the antiferromagnetic case, this does not mean that $m_A = m_B$. The (b) state may continue to be a solution of equations (9) after the free energies have crossed. The situation is illustrated in figure 9a for the case $\alpha = .5$. The dashed curve

is the locus of $f_a(h,t) = f_b(h,t)$ and the solid curve represents the mathematical limit of the (b) state. The two curves merge at a temperature $t_1(\alpha)$. For $t < t_1$, the system switches from the (b) state to the (a) state with a discontinuous change of magnetization. For $t \geqslant t_1$ there is no discontinuity in m and only the kink, familiar from the pure antiferromagnet, remains. In figure 9b $t_1(\alpha)/(1+\alpha)$ is plotted as a function of α. As $\alpha \to \infty$, i.e. the limit of purely ferromagnetic interactions, $t_1 \to \alpha$ which is the critical temperature of a molecular field ferromagnet with interaction strength α. In figure 10 we show m(h,t) as function of h for several values of α for a fixed ratio $t/(1+\alpha) = 0.5$. As $t_1(\alpha)$ becomes greater than 0.5 it can be seen that the magnetization changes from a continuous function to a discontinuous one.

We make the transformation (5) to obtain the properties of the lattice gas. The jump in magnetization at $\pm h_c(t)$ implies two first order phase transitions for the lattice gas. In figure 11a we show some isotherms of the lattice gas for $\alpha = 1.0$. In figure 11b we show the coexistence curve in the p - T plane. We interpret the enclosed region as a solid phase, for regions given in section 2. The lattice spacing (fcc) is twice the length of the basic lattice parameter. The second phase transition takes the system to a liquid phase. In figure 7b we show the compressibility factor pv/kT for $\alpha = 0.5$ at several temperatures as function of 1/v. Again, as in the $\alpha = 0$ case, there is considerable structure for $t < 1 + \alpha$. Moreover, for $t < t_1$ there is a straight line

segment in each region of decrease, corresponding to constant p and discontinuous change in v.

We also find that MFT is incapable of predicting the type of phase diagram found in the rare gases,[5,6] i.e. a triple point at p_t, T_t(A) and a liquid-gas transition line terminating at T_c, p_c(B) as sketched in figure 11b. Assuming that the enclosed region in figure 11b correctly limits the solid phase, we are still missing the liquid-gas transition line extending from A to B. In magnetic language we would need a region $T_t \leq T \leq T_c$ where the critical field $h_c(t)$ is zero, i.e. where the ordering is ferromagnetic rather than antiferromagnetic. In MFT, however, if the ground state is antiferromagnetically ordered then this type of ordering also exists just below the highest critical temperature. This theorem can easily be proved by Fourier transforming the interaction $J(R_{ij})$. We note also that, while the Hamiltonian was written for a two dimensional lattice with the ferromagnetic coupling along crossed bonds, the MFT treatment is for a lattice of any dimensionality with antiferromagnetic interactions between A-B sublattices and ferromagnetic interactions inside a sublattice.

5. Ising Antiferromagnet with Next Nearest Neighbor Ferromagnetic Interaction: Transfer Matrix

We write the transfer matrix for the crossed bond problem with Hamiltonian (8) as

$$V = (V_2 V_3)^{\frac{1}{2}} V_1' (V_2 V_3)^{\frac{1}{2}}$$

V_2 and V_3 are the same as for the antiferromagnet. It is inconvenient to express the matrix V_1' in closed form in terms of Pauli

matrices. This is not required, as we know all the matrix elements of V in the direct product representation. Let $|\mu_i\rangle$ be some configuration of the N spins corresponding to a row. Then

$$\langle \mu_i | V_1' | \mu_j \rangle = \prod_{k=1}^{N} e^{-K\sigma_{ik}\sigma_{jk}} \; e^{\alpha K \sigma_{ik}(\sigma_{jk+1} + \sigma_{jk-1})}$$

where $\sigma_{ik} = \pm 1$ is the orientation of the k^{th} spin in configuration i.

It is clear that the crossed bond coupling supports both ferromagnetism and antiferromagnetism so that at H = 0 we always expect the ordering to predominantly antiferromagnetic. At t = 0 the critical field can be exactly determined to be H = zJ (or h = 1) by examination of the matrix elements of V. Again we compute the largest eigenvalue for strips up to 6 spins wide for several values of α. From the maxima of the specific heat we find that $T_c(\alpha) \cong (1 + \alpha)T_c(0)$ where $T_c(\alpha)$ is the critical temperature. This confirms the molecular field result. We show, in figure 12, the effect of increasing α on the magnetization m(h) at fixed value of $t = T/(1 + \alpha)T_c(0) = 0.5$. The solid curves are the N = 6 isotherms and the dashed curves are the N = 4 isotherms at the same t, α. While the data so far obtained is inconclusive it seems likely that at t = 0.5, $\alpha = 0$ and $\alpha = 0.5$ there is no first order phase transition; whereas, judging from the change in slope of m(h) in going from N = 4 to N = 6 there is a first order transition at $\alpha = 1.0$.

Our results on the transfer matrix are not yet extensive enough to discuss the existence (or lack thereof) of a critical line, or its dependence on the various parameters. We have found

that two repulsive step potentials, of decreasing magnitude, do not give any indication of a triple point or critical line for strips up to 8 sites wide. This may be due to the finite size of the strip or to an inopportune choice of potentials. We hope to report on calculations done on larger strips soon, and plan to study this peculiar problem from other points of view as well.

6. References

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7. Figure Captions

Figure 4a Plot of m(h) obtained from MFT for the simple antiferromagnet at several temperatures.
A) t = .25, B) t = .5, C) t = .75, D) t = 1.0

Figure 4b Plot of some p-v isotherms in the MFT approximation for the antiferromagnet.
A) t = 0, B) t = .25, C) t = 1.0
The dashed curve D is the coexistence curve. Only those crossings of D by an isotherm marked with a dot correspond to phase transitions. See also figure 6.

Figure 5 Plot of the critical field $h_c(t)$ as function of temperature for the antiferromagnet.
A) MFT B) Transfer Matrix for N = 8
For curve B the variable t is defined t = T/2.269185J; for curve A, t = T/zJ.

Figure 6 Coexistence curve for the antiferromagnet in the p-v plane obtained from MFT.

Figure 7a Plot of the compressibility factor pv/kT against 1/v for the lattice gas with only soft core repulsion for several temperatures:
A) t = .25, B) t = .5, C) t = .75, D) t = 1.0

Figure 7b Plot of the compressibility factor pv/kT against 1/v for the lattice gas with soft core repulsion and next nearest neighbor attraction with strength $\alpha = .5$.
A) t = .25, B) t = .5, C) t = .75, D) t = 1.0.
The straight lines in curve A correspond to first order phase transitions.

Figure 8a Plot of some magnetic isotherms for the Ising antiferromagnet obtained by the transfer matrix method for N = 6.
A) t = .25, B) t = .5, C) t = .75, D) t = 1.0.
Here t = T/2.269185J.

Figure 8b Plot of the lattice gas isotherms corresponding to the magnetic isotherms of figure 8a.
A) t = .25, B) t = .50, C) t = .75, D) t = 1.0

Figure 9a The critical field $h_c(t)$ obtained from MFT is plotted against $t/(1 + \alpha)$ for the antiferromagnet with next nearest neighbor ferromagnetic coupling of strength $\alpha = .5$. The dashed curve is the locus of $f_a(h,t) = f_b(h,t)$ and the solid curve is the mathematical limit of the b state for $t < t_1$.

Figure 9b Plot of $t_1/(1 + \alpha)$ as function of α. For $t < t_1$ m(h) has a discontinuity at $h_c(t)$.

Figure 10 Plot of m(h) as function of h to several values of α at fixed $t/(1+\alpha) = .5$.

A) $\alpha = 0$, B) $\alpha = .25$, C) $\alpha = .5$, D) $\alpha = .75$, E) $\alpha = 1.0$

Figure 11a Some lattice gas isotherms in MFT for $\alpha = 1.0$.

A) $t = 0$, B) $t = .5(1+\alpha)$, C) $t = .75(1+\alpha)$, D) $t = 1+\alpha$

Figure 11b Coexistence curve in the p-T plane for the lattice gas at $\alpha = 1.0$. The solid part of the curve corresponds to first order phase transitions along an isotherm. AB is the critical line which is not given by MFT, extending from the triple point A to the critical point B, which should appear in a better theory.

Figure 12 Plot of m(h) against h for several values of α at fixed ratio if $T/2.269185J(1+\alpha) = 0.5$ The solid curves are obtained from a six site transfer matrix, the dashed curves from a four site transfer matrix.

A) $\alpha = 0$, B) $\alpha = 0.5$, C) $\alpha = 1.0$

Figure 13 Plot of $C_H(N, T_c(8,H))$ as function of N on a logarithmic scale.

A) $h = 0$, B) $h = .4$, C) $h = .8$.

The error bars correspond to an estimated error of 1% in C_H.

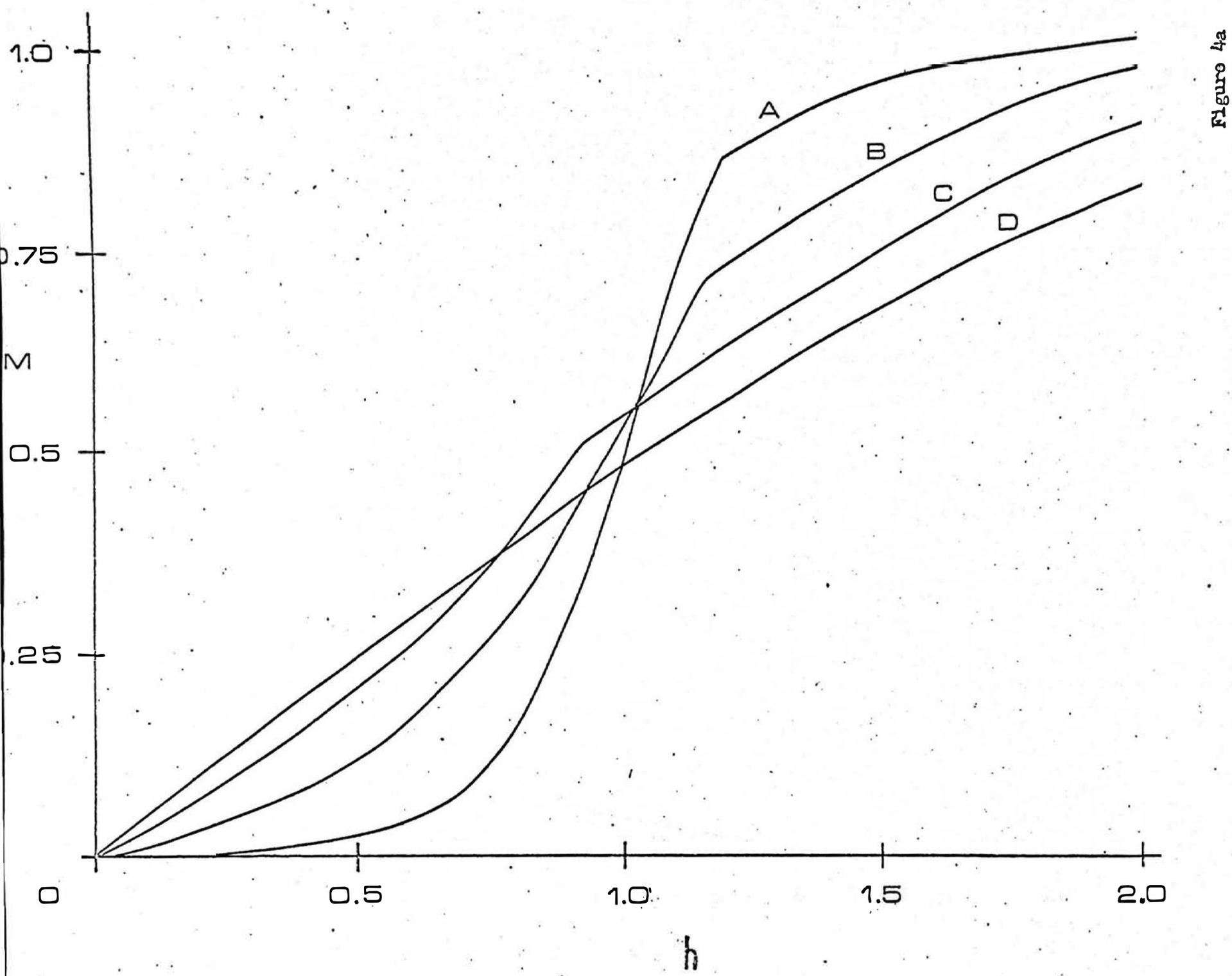

Figure 4a

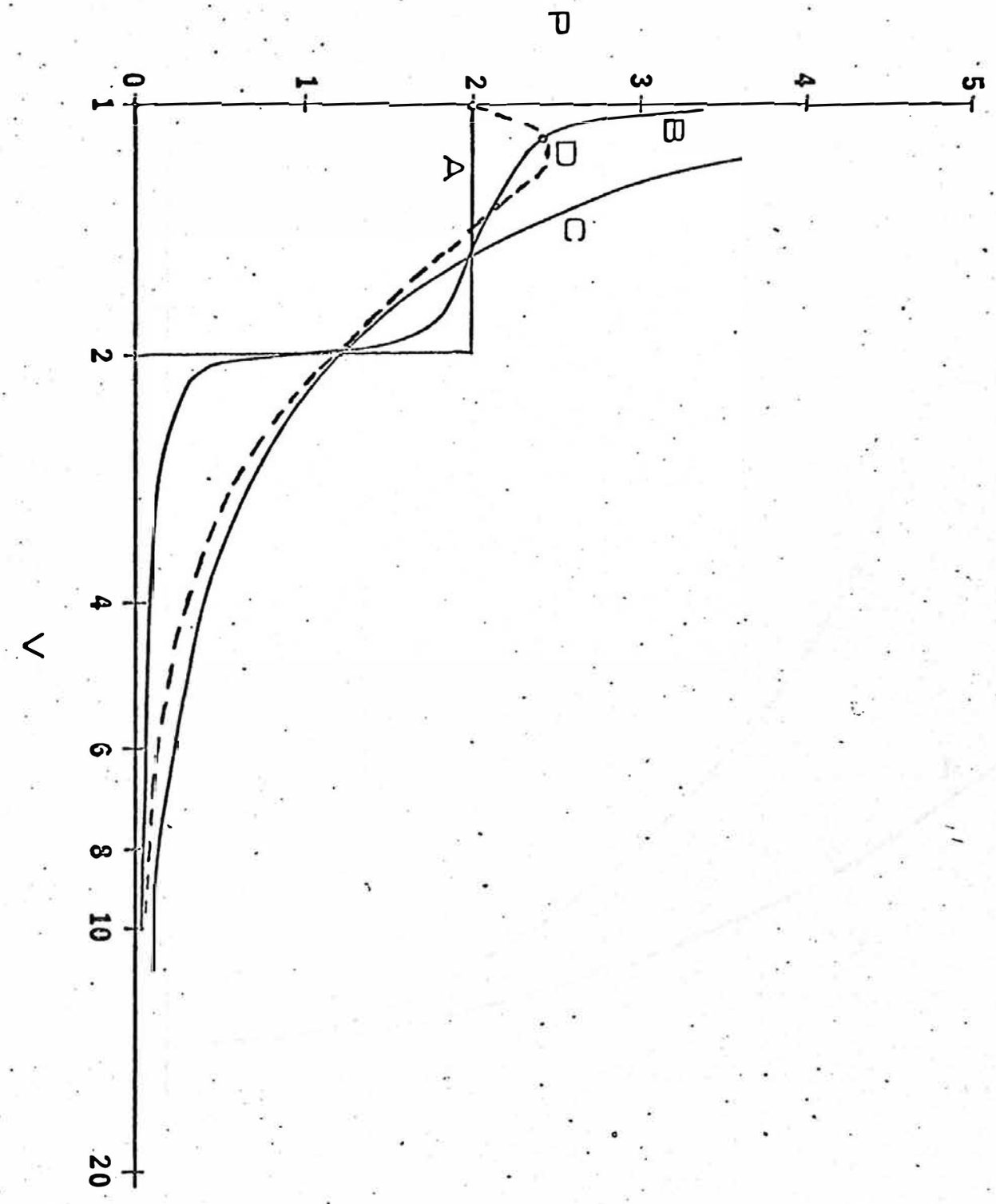

Figure 4b

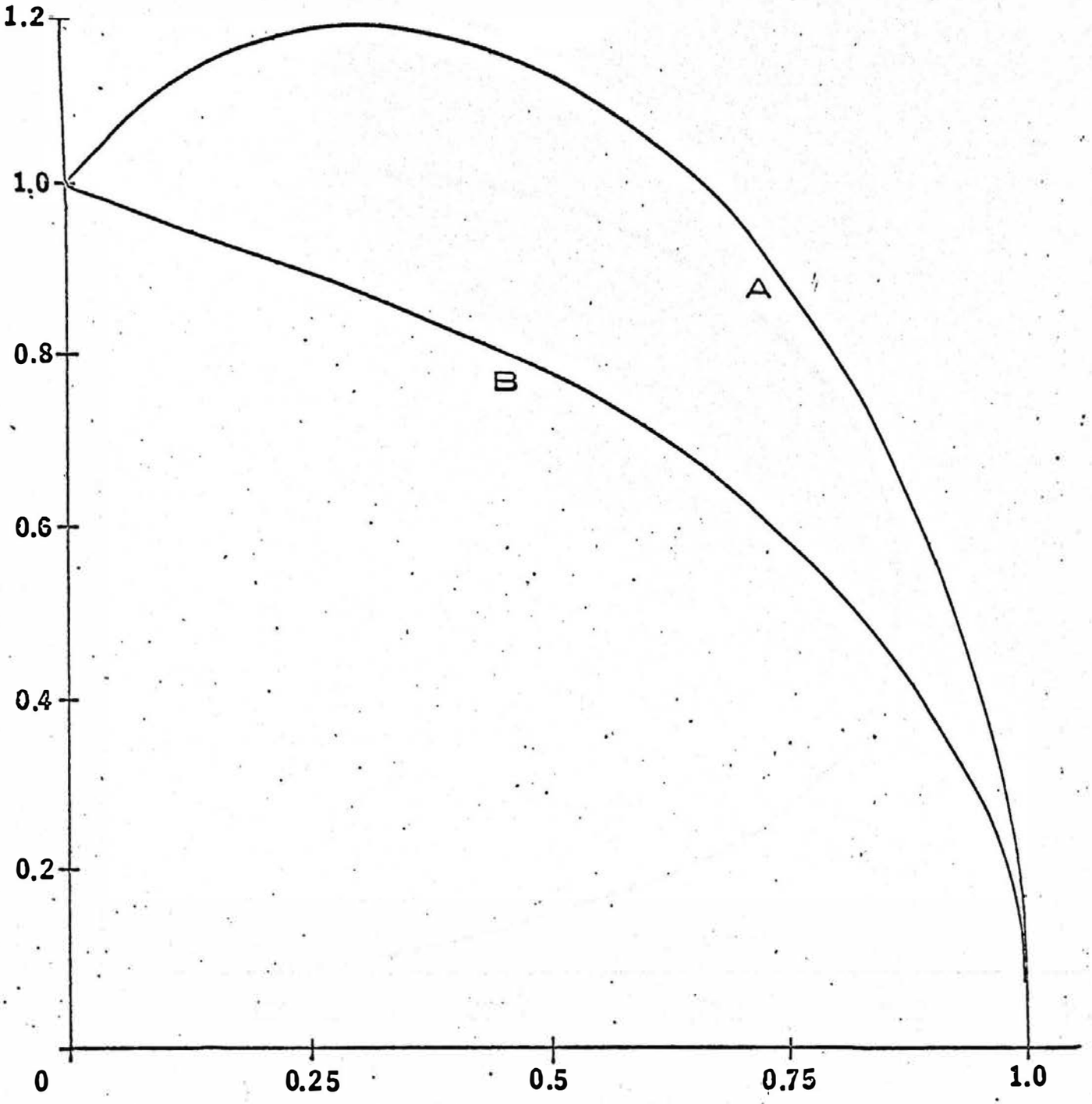

Figure 5

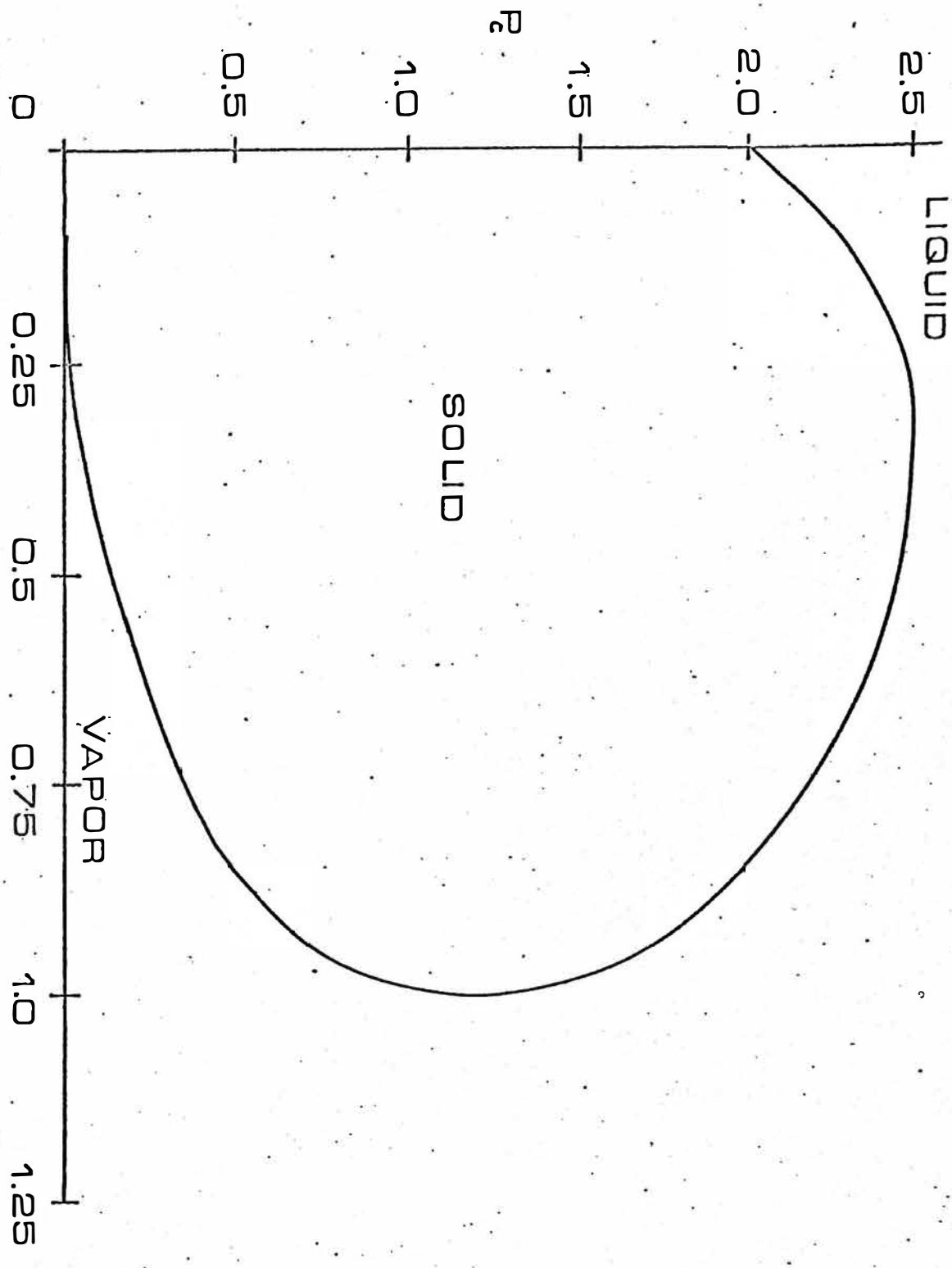

Figure 6

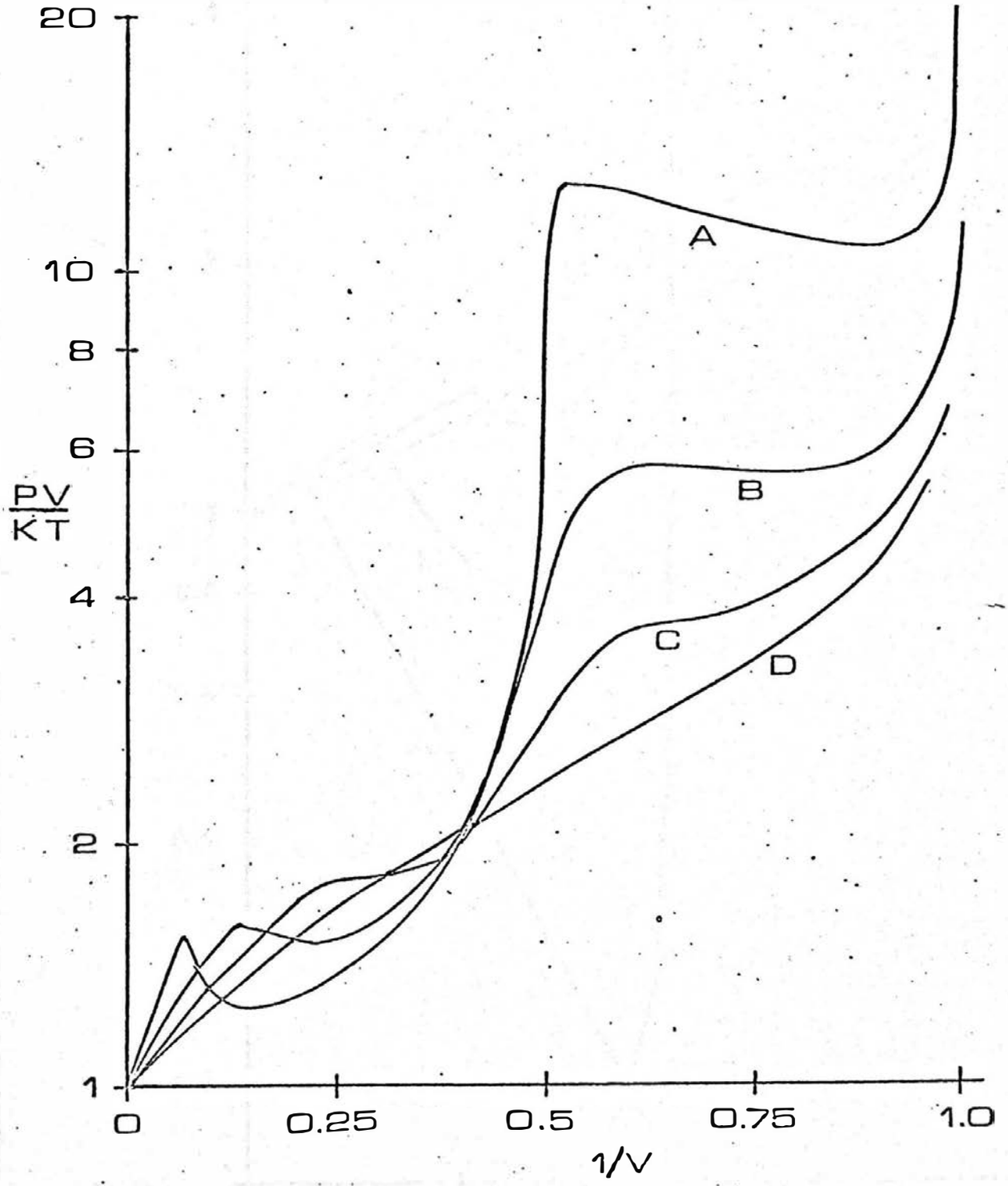

Figure 7a

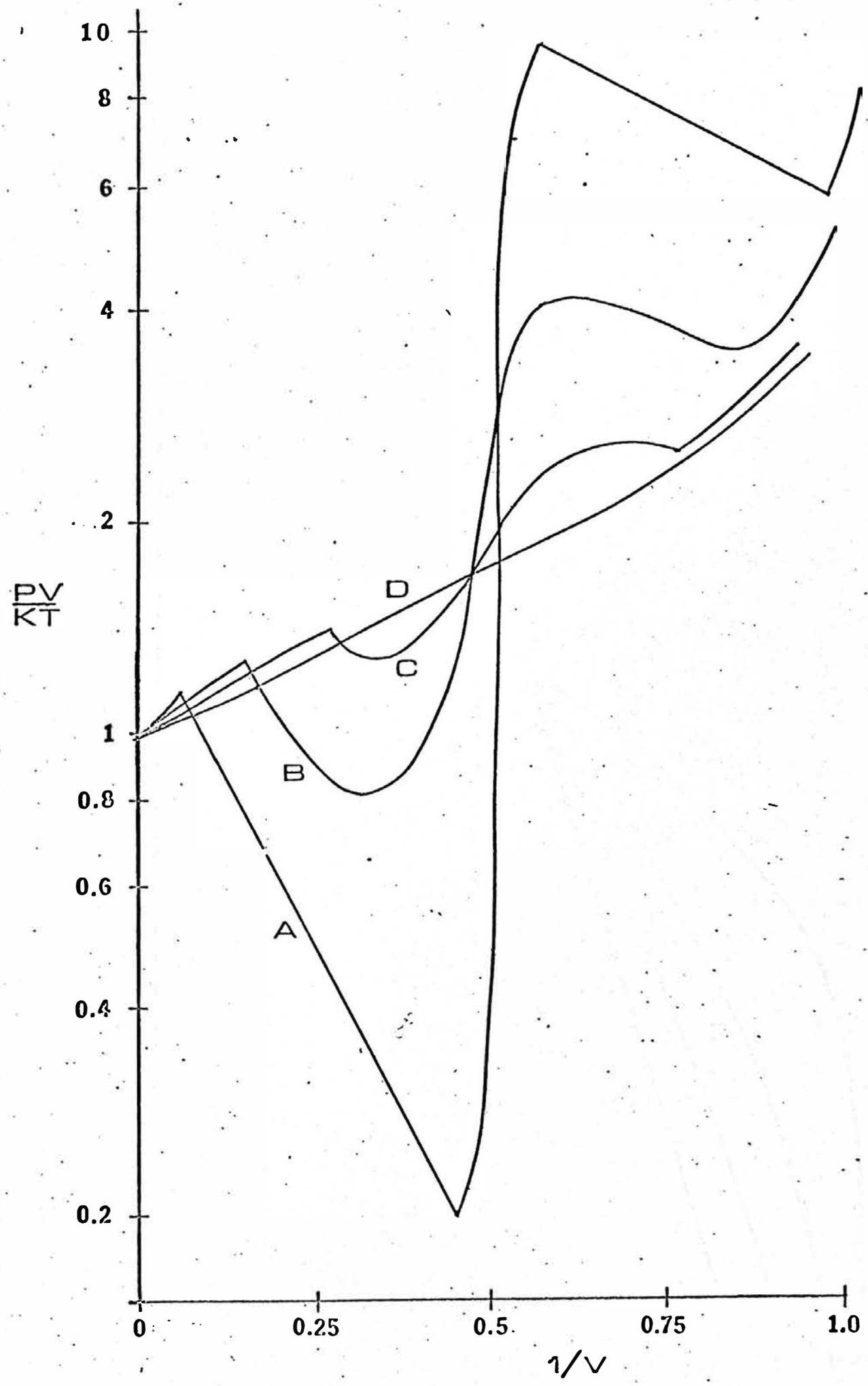

Figure 7b

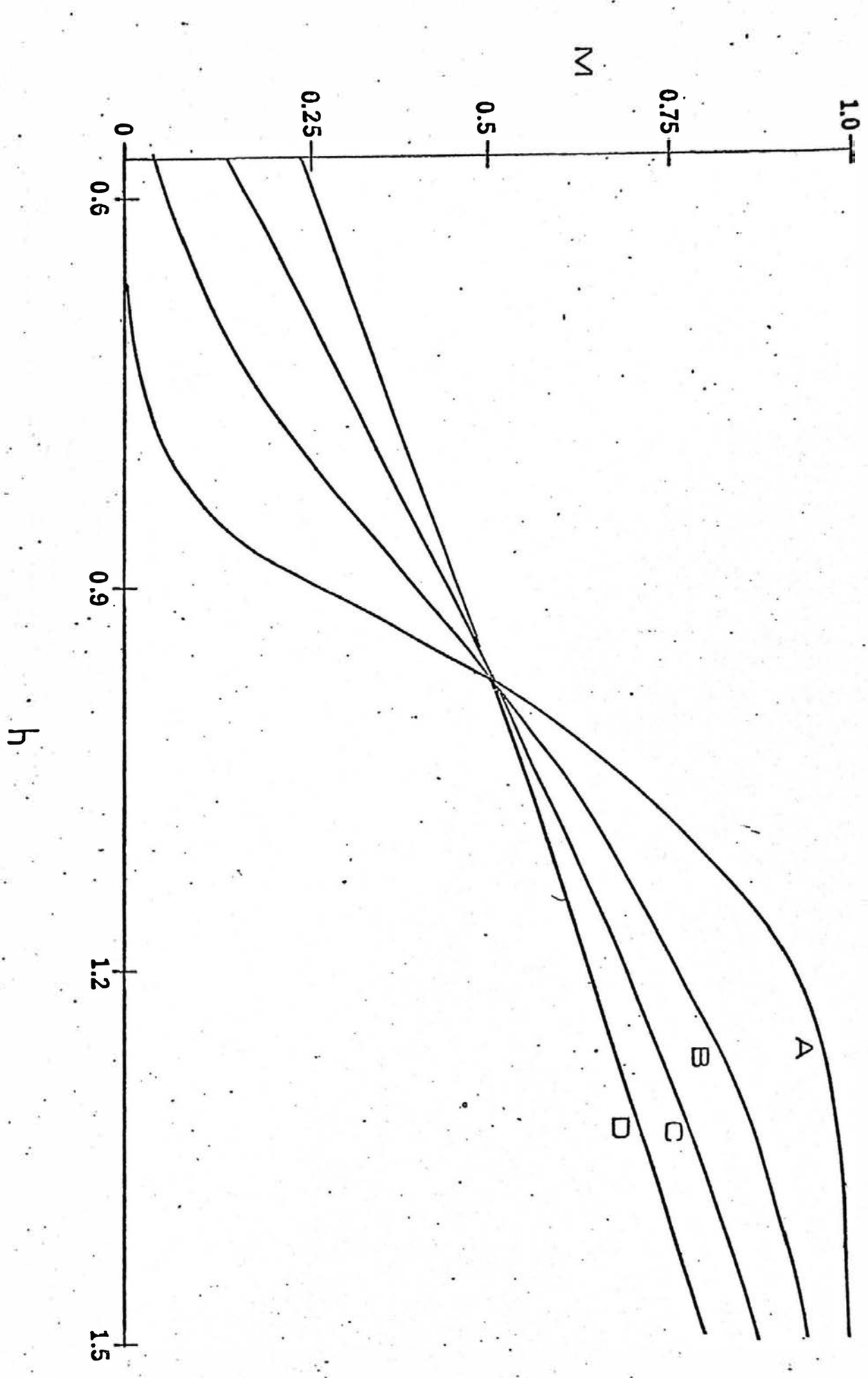

Figure 8a

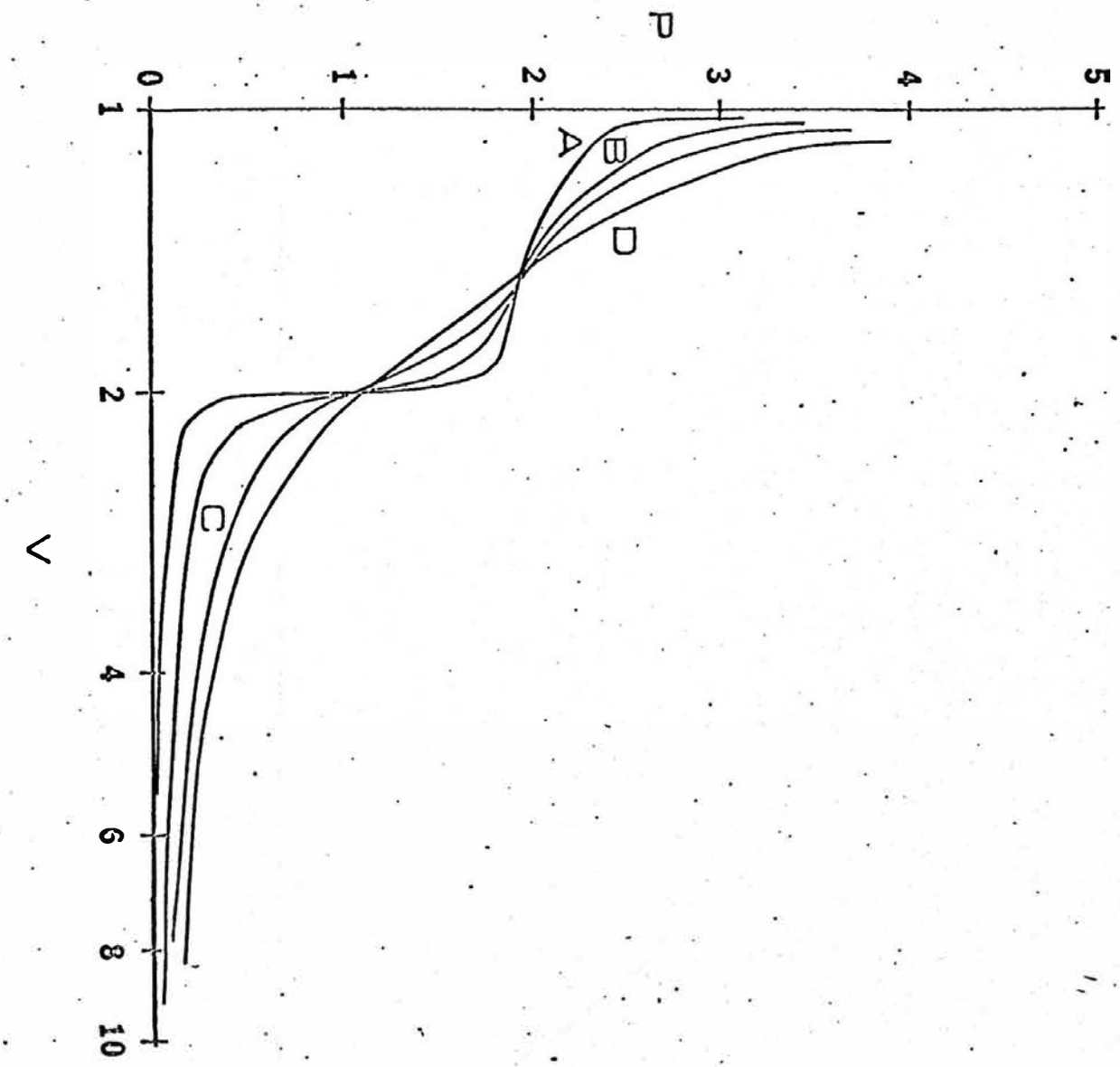

Figure 8b

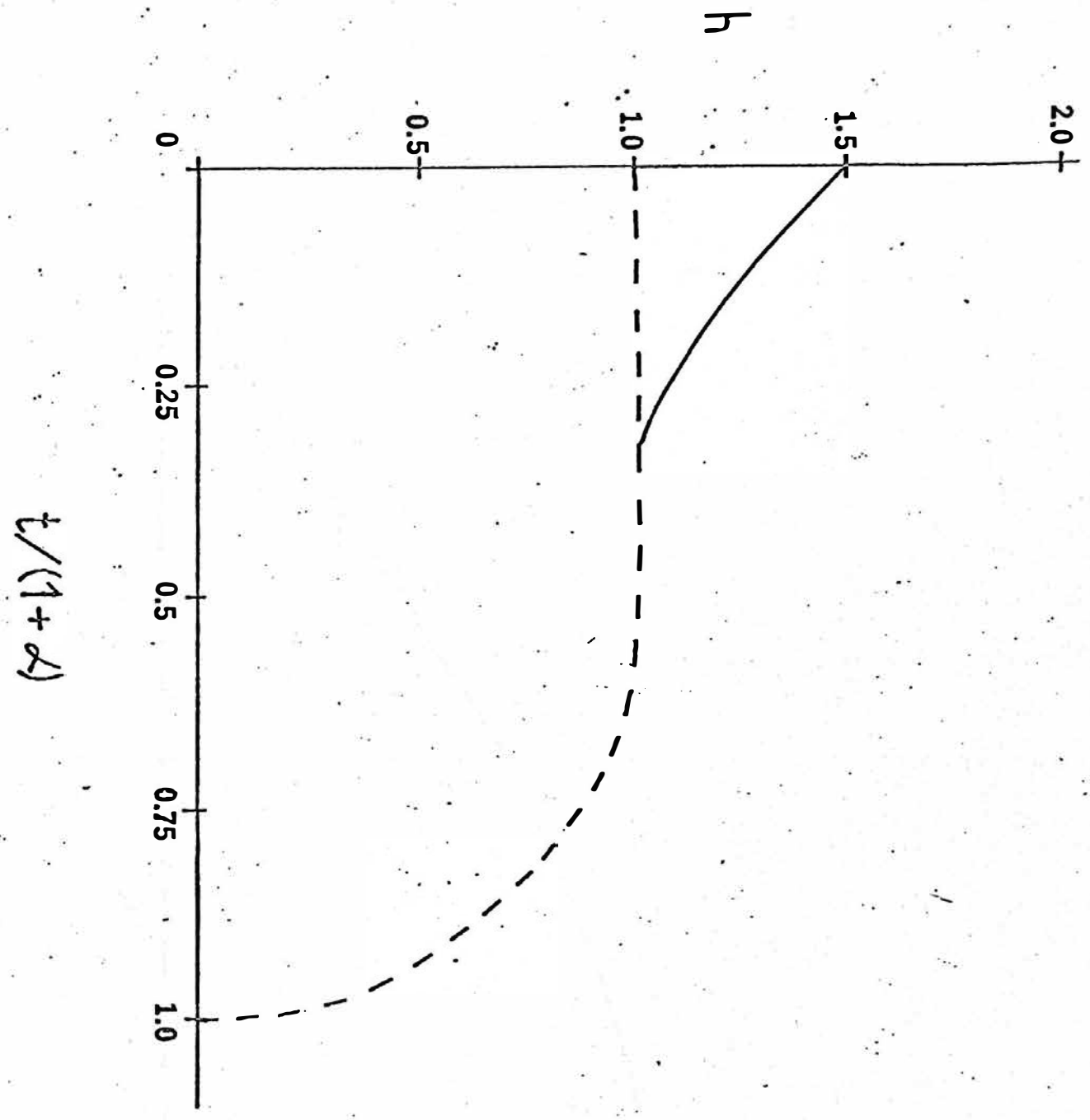

Figure 9a

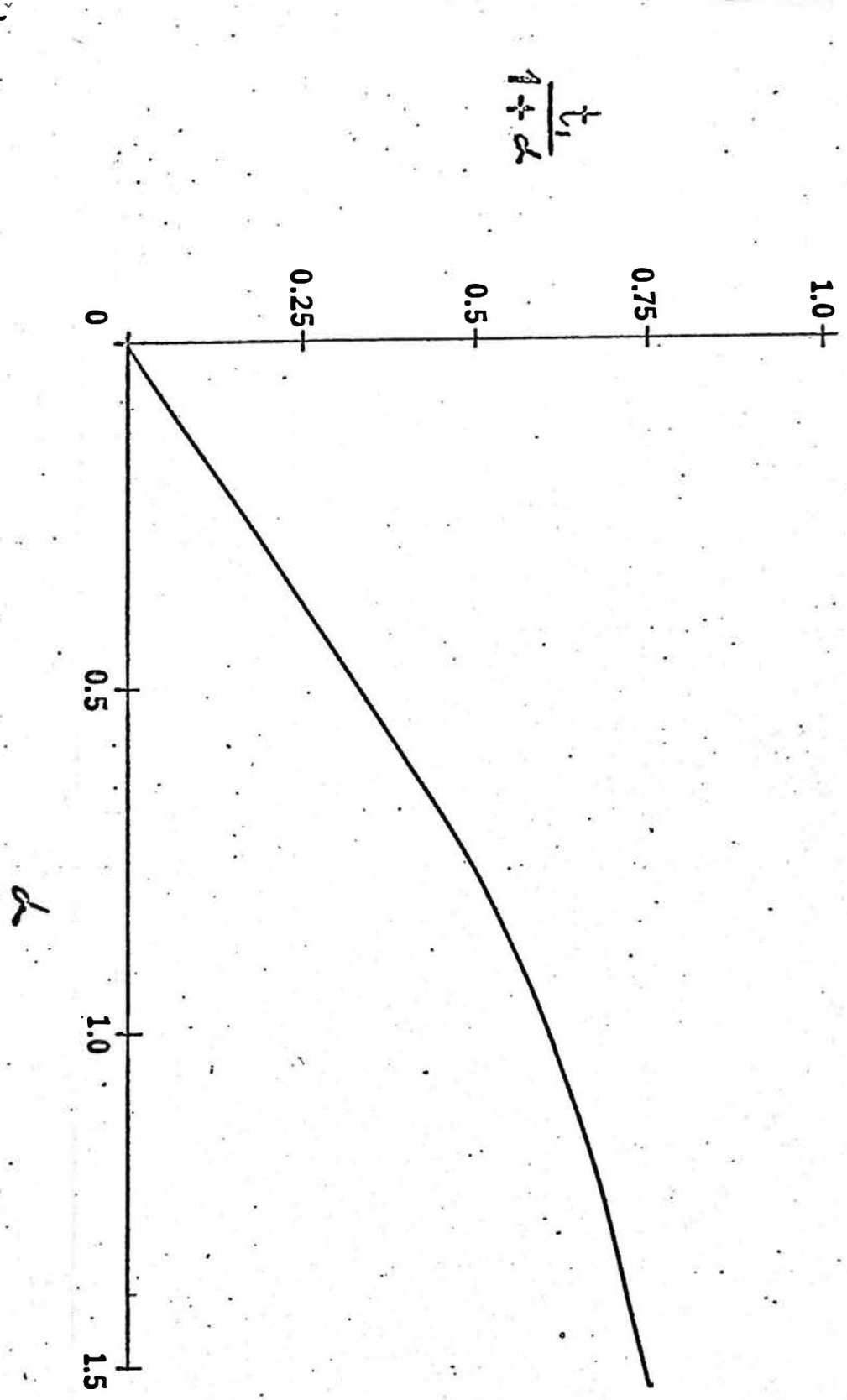

Figure 9b

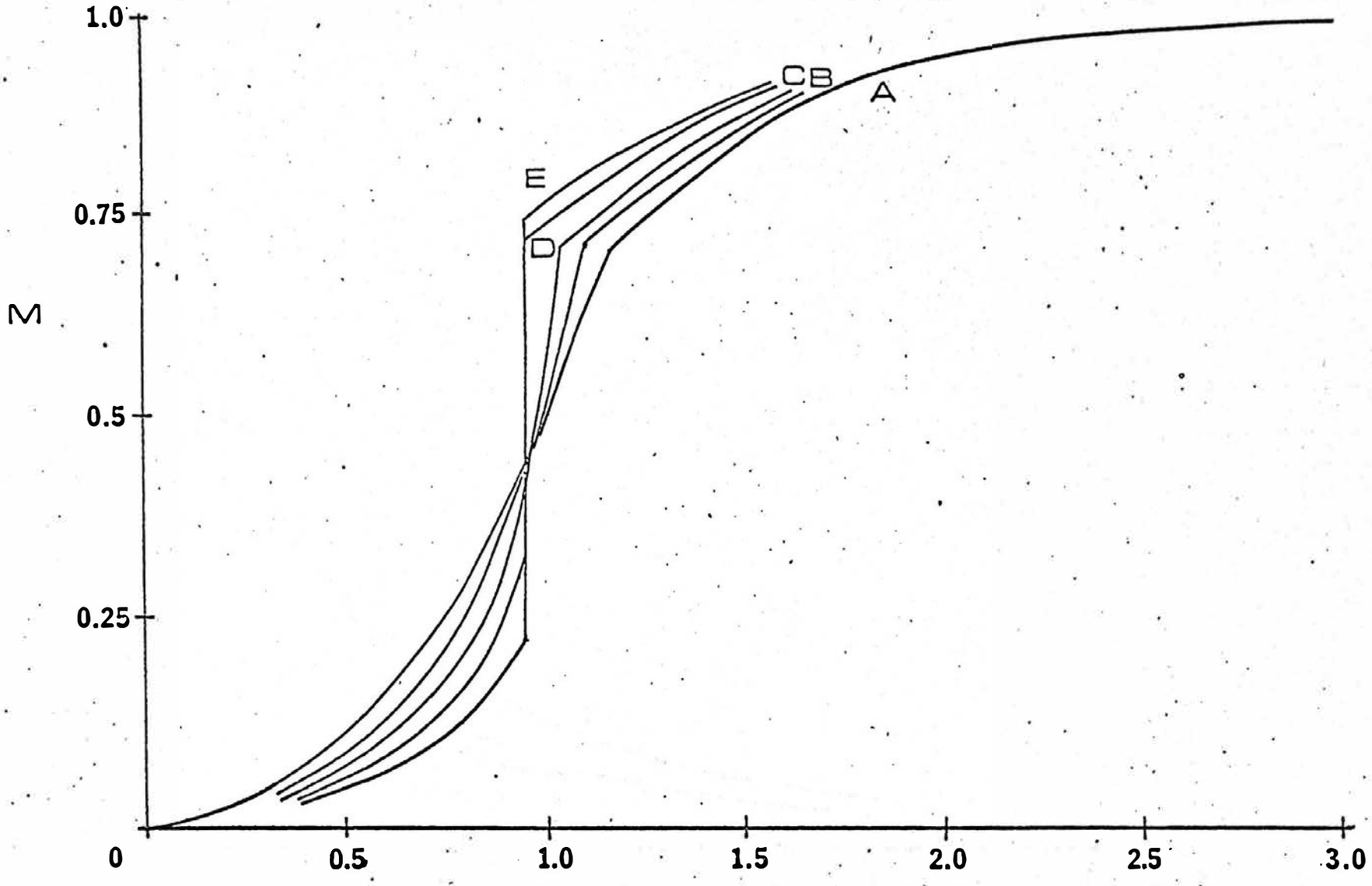

Figure 10

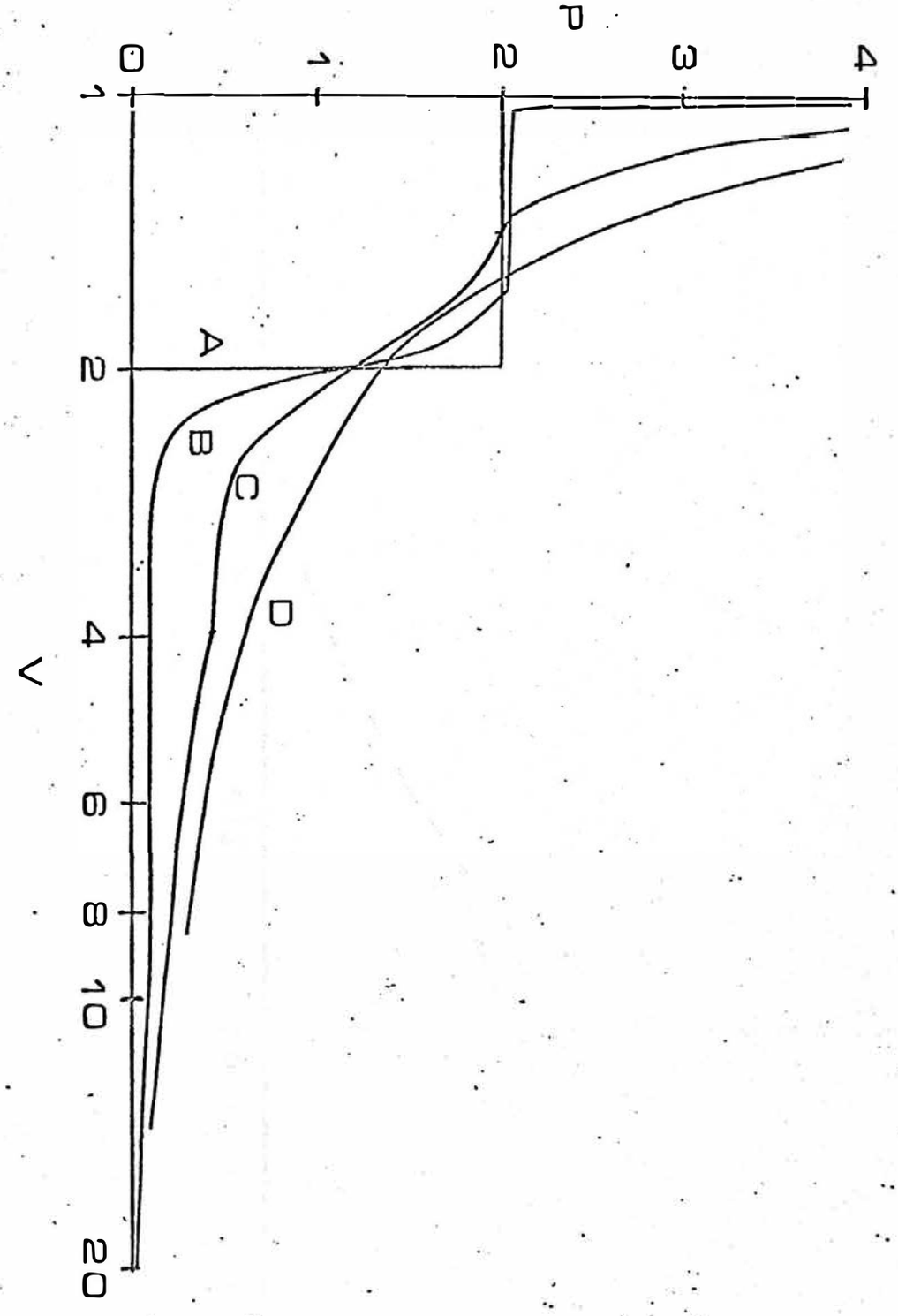

Figure 11a

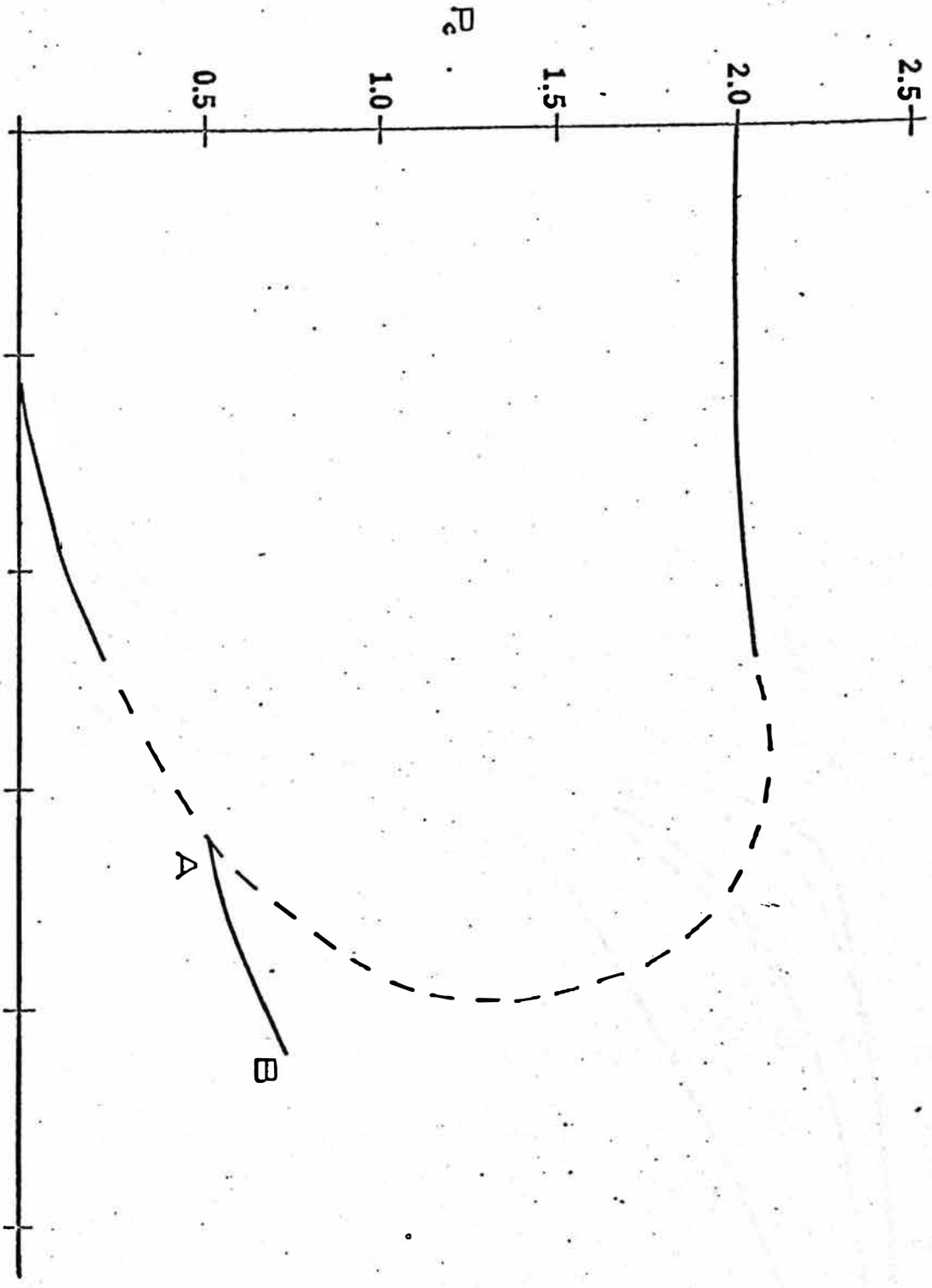

Figure 11b

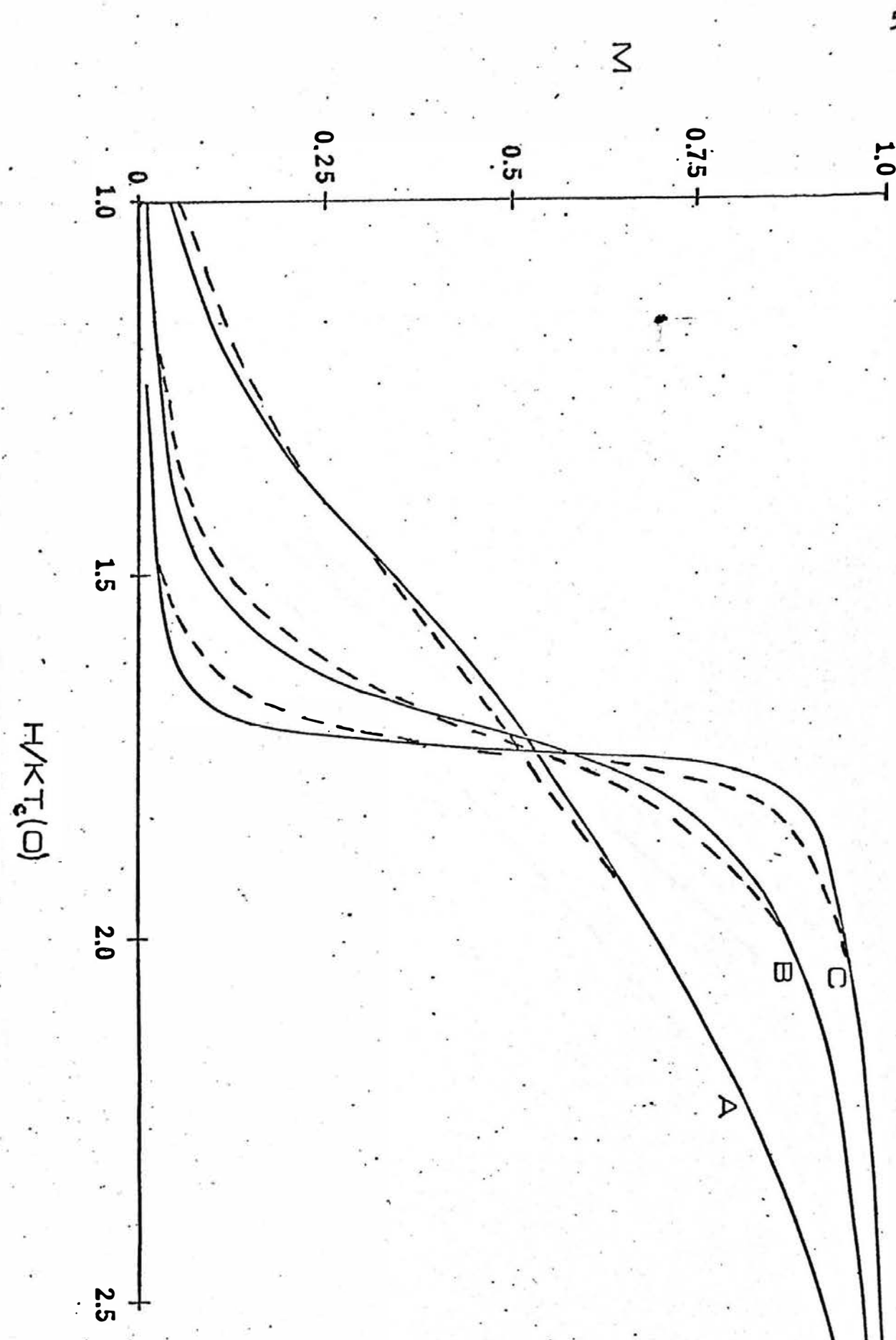

Figure 12

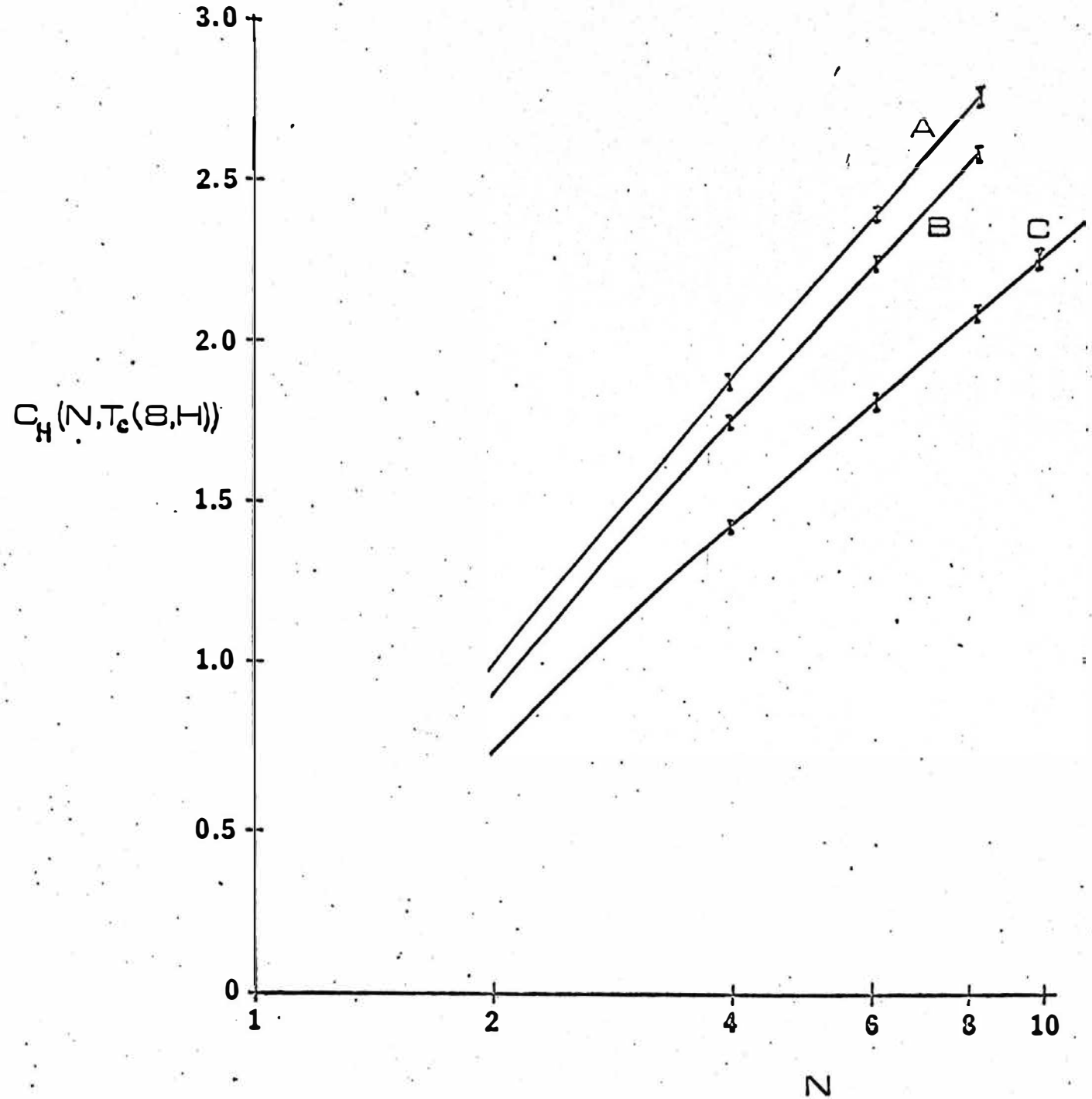

Figure 13