

## New Approximation Schemes for Lattice Theories

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### ABSTRACT

We describe a class of approximation procedures which is applicable to a variety of lattice theories including lattice gauge theories. The approach is non-perturbative in the temperature or its inverse. The low order approximants are expected to be most reliable at low temperatures. As examples we approximate the free energy of the classical  $x - y$  model and Abelian gauge fields on a lattice in two ways, one of which gives us monotonously converging bounds on the free energy.



## I. INTRODUCTION

In this paper we will describe a new method for calculating thermodynamic averages in lattice systems. Our approach is non-perturbative in the temperature or coupling constant or their inverse, and should be applicable to a variety of lattice theories describable by an explicit Hamiltonian, including many latticized Lagrangian field theories. The method is based on parameterizing the constraints which naturally appear in the partition function in such a way that the theory can be calculated while approximately incorporating these constraints.

Roughly speaking, the theory is computed as a power series in some quantity (say  $\lambda$ ) which characterizes an approximate parameterization of the constraints, and then extrapolation methods (e. g. , Padé approximants) are used to evaluate the calculated expressions at the value of  $\lambda$  at which the parameterization becomes equal to the original constraint. Since a constraint may have several possible parameterizations, the method is quite flexible, and one has the freedom to choose the most convenient representation for the particular problem at hand. This point will be discussed further in the next section. In addition, one has the freedom to choose an appropriate extrapolation technique. Two such procedures will be discussed here: one based on Padé approximants (section III), and a more powerful one based on generalized Padé approximants (section IV).

To illustrate our methods we will concern ourselves primarily with two related theories: the classical  $x - y$  model and its locally gauge invariant cousin, the lattice gauge theory with  $U(1)$  symmetry.<sup>1</sup> The naive continuum limit of this latter theory describes (free) photons, and so the theory will be called quantum photodynamics (Q. Ph. D.). In particular, we shall limit ourselves to calculations of the free energy for these theories. These calculations illustrate well the general methods, and in addition, some rigorous theorems for these quantities can be proved which place the version of our approximation scheme described in section IV on firm mathematical ground. Specifically, we are able to establish for at least some theories, a monotonously converging sequence of upper bounds to the magnitude of the free energy. It seems to us likely that similar bounds can be established for other quantities of interest, but this has not yet been done.

The paper is organized as follows: In section II we first describe the theories with which we shall deal. We then discuss the kinds of parameterization which will be useful for our calculations, and outline the general approach. We also argue that the low order approximations should be most accurate at low temperatures, an assertion which is supported by calculations performed on soluble models in sections III and IV.

In section III we present the simplest version of our method which consists of straightforward Padé approximants to the free energy in the constraint parameter,  $\lambda$ . We compute low order approximants for the

x - y model and Q.Ph. D. for a range of temperatures and lattice dimensions and present the results. Although this version of the method sometimes gives good approximations to the free energy (notably at low temperatures), we have not yet been able to prove convergence of the approximants. In this section also, a diagrammatic technique for calculating the power series in  $\lambda$  for the free energy is described. The algorithm is similar to the linked cluster expansion of statistical mechanics and simplifies the calculations of this and the next section.

In section IV another, more sophisticated version of our approach based on generalized Padé approximants (GPA) is discussed. This method consists of using GPA's to approximate the free energy for finite systems, and then, using a procedure due to Bessis, Moussa, and Villani,<sup>2</sup> extrapolating to the thermodynamic limit. In certain cases (that is, with certain boundary conditions) one can prove that the approximants so derived form a sequence of monotonously converging bounds to the free energy. We present the results of this method for the x - y model and Q.Ph. D.

In section V we make a few general comments about the method and its possible generalizations, touching on the question of phase transitions, and posing some as yet unsolved, mathematical problems.

The paper ends with two appendices. In the first, we briefly describe constraint parameterizations for the Ising model, and in the second, we present some results from the theory of Padé approximants and generalized Padé approximants which will be useful.

## II. GENERAL METHOD

### A. Definitions of the Models and Notation

This subsection contains a brief description of the models we shall consider. For more detailed discussions of these and related systems, see refs. (1) and (3).

Consider a d-dimensional hypercubic lattice. The classical x - y model is obtained by associating a two dimensional vector of magnitude 1 with each site of the lattice. If we represent this vector by  $U = e^{i\theta}$   $-\pi \leq \theta \leq \pi$ , then the partition function for the classical x - y model can be written

$$\begin{aligned}
 Z_N &= \int \prod_i dU_i dU_i^+ \delta(|U_i|^2 - 1) e^{\beta \sum_{i, \hat{j}} (U_i U_{i+\hat{j}}^+ + U_i^+ U_{i+\hat{j}})} \\
 &= \frac{1}{(2\pi)^N} \int_{-\pi}^{\pi} \prod_i d\theta_i e^{\beta \sum_{i, \hat{j}} \cos(\theta_i - \theta_{i+\hat{j}})}
 \end{aligned} \tag{2.1}$$

where the sum in the exponent runs over all lattice sites,  $i$ , and all positive and negative directions of the lattice,  $\hat{j}$ . The interactions are therefore nearest neighbor, each spin interacting with its 2d neighbors. Unless otherwise specified, the subscript  $N$  in  $Z_N$  will denote an  $N \times N \times \dots \times N$  lattice with  $N^d$  sites in  $d$  dimensions. We will assume periodic boundary conditions unless otherwise stated. (Other boundary conditions will be discussed in section IV.)

From  $Z_N$  we may define a function,  $F_N$

$$F_N = \frac{1}{\tilde{N}} \ln Z_N \quad (2.2)$$

which is an intensive function,  $F$ , in the thermodynamic limit,  $N \rightarrow \infty$ :

$F = \lim_{N \rightarrow \infty} F_N$ .  $\tilde{N}$  is an appropriate function of  $N$  which can be chosen in accordance with the boundary conditions, but for periodic boundary conditions we will take  $\tilde{N} = N^d$ .  $F_N$  is related to the usual free energy per site,  $\mathcal{F}_N$ , by  $F_N = -\beta \mathcal{F}_N$ .

We can make a character expansion of the function  $Z$  by using the expansion

$$e^{\beta \cos \phi} = \sum_{n=-\infty}^{\infty} I_n(\beta) e^{in\phi} \quad (2.3)$$

$I_n(\beta)$  being the modified Bessel function of order  $n$ . Using (2.3) in

(2.1) we have

$$Z_N = \frac{1}{(2\pi)^{\tilde{N}}} \sum_{\{n_\ell\}} \prod_{\ell} I_{n_\ell}(\beta) \int_{-\pi}^{\pi} \prod_{\kappa} d\theta_{\kappa} e^{i \sum_{\kappa} \theta_{\kappa} (\sum_{\hat{j}} n_{\kappa, \hat{j}} - n_{\kappa - \hat{j}, \hat{j}})} \quad (2.4a)$$

$$= \sum_{\{n\}} \prod_{\ell} I_{n_\ell}(\beta) \prod_{\kappa} \delta_{\sigma_{\kappa}, 0} \quad (2.4b)$$

where  $\ell$  runs over all the links, (there is an  $I_n(\beta)$  with an independent index for each link) and  $\kappa$  runs over all the sites. The coefficient of  $\theta_\kappa$  in the exponent of (2.4a) is a sum over positive directions  $\hat{j}$ , and so contains  $2d$  terms which represent all of the links which impinge on a given site. The minus signs can be determined by associating an arrow with each link pointing in the positive  $\hat{j}$  direction. Links pointing into (out of) a site have a  $+(-)$  sign in the sum. This sum is denoted as  $\sigma_\kappa$  in 2.4b, and each term becomes a kronecker  $\delta$ -function of  $\sigma_\kappa$  after integrating over the spins. (We shall sometimes denote  $\delta_{\sigma_\kappa, 0}$  by  $\delta(\sigma_\kappa)$ ). We note that for  $d = 1$  the sum in (2.4b) is trivial, and we have

$$Z_{N,s}(d = 1) = \sum_n I_n^N(\beta) \tag{2.5}$$

$$F_s(d = 1) = \ln I_0(\beta) \tag{2.6}$$

The subscript  $s$  refers to the  $x - y$  (spin) model, and the subscript  $g$  will sometimes be used to denote Q. Ph. D., or the gauge model. The  $\delta$ -functions in (2.4b) are the kinds of constraints we will want to parameterize.

We turn now to Q. Ph. D. Imagine again the  $d$ -dimensional hypercubic lattice. Associate with the link emanating from site  $j$  and pointing in the  $\hat{\mu}$  direction a spin  $U_{j,\hat{\mu}} = e^{i\theta_{j,\hat{\mu}}}$ . The partition function for Q. Ph. D. can then be written

$$\begin{aligned}
 Z_{N, g} &= \int \prod_{\ell} dU_{\ell} dU_{\ell}^{\dagger} \pi \delta(1 - |U_{\ell}|^2) e^{\frac{1}{2} \beta \sum_p U_{j, \hat{\mu}} U_{j+\hat{\nu}, \hat{\nu}}^{\dagger} U_{j+\nu, \hat{\mu}}^{\dagger} U_{j, \hat{\nu}}^{\dagger} + \text{h.c.}} \\
 &= \frac{1}{(2\pi)^{\bar{N}}} \int_{-\pi}^{\pi} \prod_{\ell} d\theta_{\ell} e^{\beta \sum_p \cos(\theta_{j, \hat{\mu}} + \theta_{j+\hat{\nu}, \hat{\nu}} - \theta_{j+\hat{\nu}, \hat{\mu}} - \theta_{j, \hat{\nu}})}
 \end{aligned}
 \tag{2.7}$$

The product over  $\ell$  is a product over all links, and  $\bar{N}$  is the number of links when we use periodic boundary conditions. The sum in the exponent runs over all elementary squares, or plaquettes of the lattice.

Using the identity (2.3), we can write (2.7) as

$$Z_{N, g} = \sum_{\{n\}} \prod_p I_{n_p}(\beta) \prod_{\ell} \delta_{\gamma_{\ell}, 0} \tag{2.8}$$

For each plaquette we have a factor of  $I_{n_p}(\beta)$ , and associated with each link is a kronecker  $\delta$  function of  $\gamma_{\ell}$ , which is defined as follows: In  $d$ -dimensions, there are  $2(d - 1)$  plaquettes which impinge on each link. In this  $(d - 1)$ -dimensional subspace we construct a set of axes by drawing  $(d - 1)$  lines perpendicular to the link under consideration, and which lie in the  $(d - 1)$  lattice planes which include the link. The positive axes can be chosen to point in the same direction as the positive axes of the lattice. Now each plaquette which includes link  $\ell$  as an edge will lie along either a positive or negative axis of our coordinate system. Associated with each plaquette is an index,  $n_i$ .  $\gamma_{\ell}$  is defined as

$$\gamma_{\ell} = \sum_{i=1}^{2(d-1)} q_i n_i \tag{2.9}$$

when the sum runs over all the plaquettes which impinge on link  $\ell$ , and  $q_i = +1(-1)$  if plaquette  $i$  lies along a positive (negative) axis of the coordinate system described above. (This constraint is considerably more complicated verbally, than it is conceptually.)

In one and two dimensions this theory is trivial to solve, and is

$$Z_{N, g}^{(d=1, 2)} = \sum_{n=-\infty}^{\infty} I_n^{N_p}(\beta) \quad (2.9)$$

where  $N_p$ , the number of plaquettes in  $d$ -dimensions is

$$N_p = \begin{cases} N & (d=1) \\ \frac{d(d-1)}{2} N^d & d > 1 \end{cases} \quad (2.10)$$

so,

$$F_g^{(d=1, 2)} = \ln I_0(\beta) \quad . \quad (2.11)$$

Notice that this is the same as (2.6) for the spin system in one dimension.<sup>4</sup>

Finally, we note, from (2.1) that the spin system is invariant under a global  $U(1)$  transformation  $\theta_i \rightarrow \theta_i + \alpha$ , while (2.7) tells us that the gauge theory is invariant under local  $U(1)$  transformations

$$\theta_{i, \hat{\mu}} \rightarrow \theta_{i, \hat{\mu}} + \alpha_i \quad .$$

In this expression  $i$  refers to a lattice site ( $\alpha_i$  can differ from site to site), and  $\hat{\mu}$  runs over all 2d links which terminate on a given site.

### B. Mutilating the $\delta$ -function

From the point of view of the representations (2.4) or (2.8), the feature of the partition function which makes the theory difficult to solve is the presence of the kronecker  $\delta$ -function constraints. Our approach is to parameterize these constraints in some way which makes the theory tractable. Consider for instance

$$\delta(n) = \lim_{\lambda \rightarrow \infty} e^{-\lambda n^2} \quad (2.12)$$

which is a valid representation for a kronecker- $\delta$ . If we insert representations of the form (2.12) into (2.4) or (2.8) we define a new function  $R(\lambda)$  whose limit as  $\lambda \rightarrow \infty$  is the partition function of the theory of interest. While a calculation of the exact limit may not be possible, it is possible to calculate  $R(\lambda)$  for small values of  $\lambda$ , and then use extrapolation techniques to approximate the result as  $\lambda \rightarrow \infty$ .

Consider a simple example:

$$\partial_x \ln I_0(x) = \partial_x \ln \sum_n I_n(x) \delta(n) = \lim_{\lambda \rightarrow \infty} \ln \sum_n I'_n(x) e^{-\lambda n^2} = \lim_{\lambda \rightarrow \infty} R(\lambda). \quad (2.13)$$

To calculate the right hand side for small  $\lambda$ , we can simply expand the exponential. Now, we know that  $R(\infty)$  is finite, and so the simplest way

to extrapolate the power series is to form the diagonal Padé approximants  $[m, m]$  in  $\lambda$  which have a finite limit as  $\lambda \rightarrow \infty$ . (For a description of Padé approximants see appendix B.) If we define  $P_m = [m, m]_{\lambda = \infty}$  we have

$$P_1 = 1 - \frac{2}{4x + 1}$$

$$P_2 = 1 - \frac{576 x^2 + 216 x}{1152 x^3 + 144 x^2 + 156 x - 1} . \quad (2.14)$$

These approximations agree well with the exact answer in the large  $x$  limit. If we expand in  $x^{-1}$ ,

$$\partial_x \ln I_0(x) \approx 1 - \frac{1}{2x} - \frac{1}{8x^2} - \frac{5}{32x^3} + \dots \quad (2.15)$$

we find that for large  $x$ ,  $P_1$  agrees with the first two terms of (2.15), while  $P_2$  gets the first three terms right. Although this example is rather special, it does have many of the properties that appear in more physical problems. Moreover, as we shall agree, the agreement at large  $x$  is probably a fairly general feature of the scheme.

Now, there are many other possible representations for the  $\delta$ -function we could have used in (2.13). For example,

$$\delta(n) = \lim_{\lambda \rightarrow \infty} \frac{1}{1 + \lambda n^2} \quad (2.16a)$$

$$\delta(n) = \lim_{\lambda \rightarrow \pi} \frac{\sin \lambda n}{\lambda n} \quad (2.16b)$$

or

$$\delta(n) = \lim_{\lambda \rightarrow \infty} e^{-\lambda(n^2)^q} ; q > 0 . \quad (2.16c)$$

What dictates which representation we should use? The choice is determined by the exact nature of the problem at hand, the extrapolation procedure, and considerations of calculational ease. For instance, in the sample problem of (2.13), had we used the representation (2.16a) instead of (2.12),  $R(\lambda)$  would have been a series of Stieltjes (see appendix B). Much more is known about the convergence of Padé approximants for Stieltjes series than for most other series, and so from a formal point of view, our extrapolation procedure would have been under better control. On the other hand, had we used generalized Padé approximants to extrapolate our calculations (see appendix B) both parameterizations would have shared the same established convergence properties, and in fact, would have given identical results in limit  $\lambda \rightarrow \infty$ . In the cases of physical interest, e.g. the x - y model or Q. Ph. D., calculational considerations, as well as thermodynamic extensivity of the partition function will place further restrictions on our choice of parameterizations.

Let us consider now the theories defined in (2.4) and (2.8). For each  $\delta$ -function appearing in these expressions we insert the parameterization of (2.12). The partition functions then become

$$Z_{N,s} = \lim_{\lambda \rightarrow \infty} R_{N,s}(\lambda) = \lim_{\lambda \rightarrow \infty} \sum_{\{n\}} \prod_{\ell} I_{n_{\ell}}(\beta) e^{-\lambda \sum_{\kappa} \sigma_{\kappa}^2} \quad (2.17)$$

and

$$Z_{N,g} = \lim_{\lambda \rightarrow \infty} R_{N,g}(\lambda) = \lim_{\lambda \rightarrow \infty} \sum_{\{n\}} \prod_p I_{n_p}(\beta) e^{-\lambda \sum_{\ell} \gamma_{\ell}^2} \quad (2.18)$$

We notice two things about these representations. First, they have the form (for fixed  $\beta$ ) of an ordinary partition function describing a system of spins, each one of which can take on integer values,  $-\infty \leq n \leq \infty$  with a single spin probability weighting of  $I_n(\beta)$ , coupled together in some way with a coupling constant,  $\lambda$ . In particular, the functions  $\ln R(\lambda)$  appear to be extensive functions of  $N$  for all  $\lambda$ , which suggests that we can develop for  $F$  the analogue of the linked cluster expansion<sup>5</sup> in the coupling constant  $\lambda$ . Notice that if we had chosen instead a parameterization like (2.16a) this extensivity would not be a property of the  $R_N$ 's for finite  $\lambda$ ,  $F_N$  would not have a good thermodynamic limit, and a simple linked cluster expansion (LCE) would not exist. These remarks will be elucidated in the next section where we develop the LCE.

The second property to notice is that the  $R_N(\lambda)$ 's satisfy, at least for finite  $N$ , the sufficient conditions (appendix B, theorems 5 and 6) for a function to be monotonically approximated by a convergent sequence of generalized Padé approximants. Indeed, we can write

$$\begin{aligned}
 R_{N,s}(\lambda) &= \int_0^\infty d\xi e^{-\lambda\xi} \sum_{\{n\}} \prod_{\ell} I_{n_\ell}(\beta) \delta(\xi - \sum_{\kappa} \sigma_{\kappa}^2) \\
 &= \int_0^\infty e^{-\lambda\xi} d\phi(\xi)
 \end{aligned}
 \tag{2.19}$$

and a similar expression for  $R_{N,g}(\lambda)$ , which satisfies  $d\phi(\xi) \geq 0$ , and

$$(-\partial_{\xi})^j e^{-\lambda\xi} \geq 0$$

for all real, positive  $\lambda, \xi$ , and  $j = 0, 1, 2, \dots$  (The  $\delta$ -function in 2.19 is understood to have its full weight at the end point,  $\xi = 0$ ). Other representations (e.g. (2.16a)) also satisfy these conditions, but, as we shall see in section IV, this one is preferred for reasons of calculational ease.

The kinds of parameterizations discussed here will not always be limited to simple  $\delta$ -function constraints. For instance, in a theory with a non-abelian symmetry the constraints which appear will not be simple  $\delta$ -functions in the character indices, but one will still be able to parameterize them by similar methods. Another example of a system with a symmetry group different than  $U(1)$ , and therefore with different kinds of constraints is the Ising model (symmetry group  $Z_2$ ) parameterizations for which we briefly describe in appendix A.

Now, in defining the representations (2.17, 18) we have introduced a new coupling constant,  $\lambda$ . We might ask whether we can attach any physical

significance to this coupling. Consider, for instance, the x - y model.

Each  $\delta$ -function constraint comes from integrating over all the configurations of some spin:

$$\lim_{\lambda \rightarrow \infty} e^{-\lambda \sigma_{\kappa}^2} = \delta(\sigma_{\kappa}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta_{\kappa} e^{i\theta_{\kappa} \sigma_{\kappa}} \quad (2.20)$$

Now suppose there is some dynamical reason why the major contribution to the partition function comes from small values of  $\theta_{\kappa}$ . Then we could expand  $e^{i\theta_{\kappa} \sigma_{\kappa}}$  without making too much of a mistake. This expansion in powers of  $\sigma_{\kappa}^2$  could be qualitatively identified with an expansion of  $e^{-\lambda \sigma_{\kappa}^2}$  (other parameterizations could make the identification closer), which might be good for small enough  $\lambda$ . When the lattice temperature is near zero ( $\beta$  very large), we expect that the spins will want to be more or less lined up, and the major contribution to  $Z_N$  will come from values of the  $\theta_{\kappa}$ 's near zero. In this case,  $R_N(\lambda)$  for some small  $\lambda$  should be a good approximation to  $R_N(\infty)$ . So, in general, there should be some  $\lambda_c(\beta)$  such that  $R_N(\lambda \gtrsim \lambda_c) \simeq R_N(\infty)$ , and the larger  $\beta$  is the smaller  $\lambda_c$  should be. Now consider an approximant, like a Padé approximant which is designed to match  $R_N(\lambda)$  for small  $\lambda$ . Suppose we form a low order approximant,  $H(\lambda)$  to  $R(\lambda)$  which is accurate for  $\lambda \lesssim \lambda_1 \ll \lambda_c$ . Since  $R_N(\lambda \lesssim \lambda_1) \neq R_N(\infty)$ ,  $R_N(\lambda)$  will have to vary a lot as we take  $\lambda \rightarrow \infty$ , and there is no a priori reason why the extrapolation  $H(\lambda) \rightarrow H(\infty)$ , which is smooth, should track the extrapolation of  $R_N$ . To put it another way, there is a lot of important

information in the partition function which has not been used in building  $H(\lambda)$ . If, on the other hand,  $\lambda_c$  is small enough so that  $H(\lambda \sim \lambda_c) \approx R_N(\lambda \sim \lambda_c)$  then, since  $\partial_\lambda R_N(\lambda > \lambda_c) \approx 0$ ,  $\partial_\lambda H(\lambda \sim \lambda_c) \approx 0$ , and if the extrapolation procedure  $H(\lambda) \rightarrow H(\infty)$  is smooth enough we might expect that  $H(\infty) \approx H(\lambda \sim \lambda_c) \approx R_N(\lambda \sim \lambda_c) \approx R_N(\infty)$ . In other words, if  $H(\infty)$  has, in principle, anything at all to do with  $R_N(\infty)$  (e.g., if the approximants eventually converge to  $R_N(\infty)$ ), then, an approximant of some given low order should be more accurate the smaller  $\lambda_c$  is, i.e., the larger  $\beta$  is. This is because for large  $\beta$ , most of the important information is contained in the first few terms of an expansion in powers of  $\lambda$ . This heuristic argument accounts for the agreement at large  $x$  of (2.15) and (2.14) (this approximation for small  $x$  is pretty awful) and is also supported by the computational results presented in the next two sections.

### III. EXTRAPOLATION TECHNIQUE I: PADÉ APPROXIMANTS TO F

In this section we discuss the simplest extrapolation procedure based on Padé approximants. It consists of using a parameterization of the type described in the last section, calculating some quantity of interest, and constructing a sequence of Padé approximants which are evaluated at the physically relevant value of the extrapolation parameter,  $\lambda$ . In the case where  $\lambda$  must be extrapolated to  $\infty$ , only the  $[n, n]$  Padé approximants survive as candidates for this technique. But for parameterizations such as (2.16b), other sequences of approximants may work.

From the discussion of appendix B, it is clear that for an arbitrary parameterization we will be unable to make rigorous statements about the convergence of these Padé approximants. One might suppose that the best bet would be to choose the Stieltjes parameterization, (2.16a), and construct Padé approximants to  $R_N(\lambda)$  which we will now be able to write as a series of Stieltjes. That is, as

$$\begin{aligned}
 R_{N,s}(\lambda) &= \int_0^{\infty} d\xi \frac{1}{1+\lambda\xi} \sum_{\{n\}} \prod_{\ell} I_{n_{\ell}}(\beta) \delta(\xi - \sum_{\kappa} \sigma_{\kappa}^2) \\
 &= \int_0^{\infty} \frac{1}{1+\lambda\xi} d\phi(\xi)
 \end{aligned} \tag{3.1}$$

and a similar expression for  $R_{N,g}(\lambda)$ . Unfortunately, this simple procedure fails because the logarithm of the Padé approximants to (3.1) are not really extensive in the thermodynamic limit.

To illustrate this point, consider the 1-dimensional x - y model with the parameterization (2.16a). Expanding in powers of  $\lambda$ , we find

$$\begin{aligned}
 R_{N,S}(\lambda) &= \sum_{\{n\}} \prod_{\ell} I_{n_{\ell}}(\beta) \left[ 1 + \lambda \sum_i (n_i - n_{i+1})^2 \right]^{-1} \\
 &= M_0^N - \lambda 2NM_0^N \rho_2 + \lambda^2 4NM_0^N \left[ \rho_4 + (2N - 3)\rho_2^2 \right] + \dots
 \end{aligned} \tag{3.2}$$

where

$$M_r = \sum_{-\infty}^{\infty} n^r I_n(\beta) = \left. \partial_{\theta}^r e^{\beta \cos \theta} \right|_{\theta=0}, \tag{3.3}$$

$$\rho_r = M_r / M_0$$

and the expansion to order  $\lambda^2$  is valid for  $N \geq 3$ . Note that given  $M_0$ , the rest of the  $M_r$  can be easily generated by the recursion relation

$$M_r(\beta) = \beta \sum_{j=0}^{r-1} \frac{(r-1)!}{j!(r-1-j)!} \sin\left[\frac{\pi}{2}(j+1-r)\right] M_j(\beta). \tag{3.4}$$

Calculating the [1, 1] Padé to  $R_N$  and evaluating it at  $\lambda = \infty$ , we find

$$D_1(\beta) = M_0^N - \frac{NM_0^N \rho_2^2}{\rho_4 + (2N - 3)\rho_2^2}. \tag{3.5}$$

Now, we are really interested in approximations for intensive thermodynamic quantities, so we compute from  $D_1$  an approximation to  $F_N(\beta)$ , namely

$$\frac{1}{N} \ln D_1(\beta) = \ln M_0 + \frac{1}{N} \ln \left[ \frac{\rho_4 + (N-3)\rho_2^2}{\rho_4 + (2N-3)\rho_2^2} \right] \quad (3.6)$$

which in the limit  $N \rightarrow \infty$  becomes just the trivial first term,  $\ln M_0 = \beta$ . This same unhappy situation persists for all Padé approximants,  $D_n$ , to  $Z_N$  where  $n \ll N$ . That is, if we simply take the thermodynamic limit  $N \rightarrow \infty$  we always recover only the trivial zeroth order approximation for the free energy. Moreover, it does not help to take the logarithm of the expansion (3.2) and Padé that. The required cancellation between terms of order  $N^2$  in the coefficient of  $\lambda^2$  will not occur, and when  $N \rightarrow \infty$  no non-trivial corrections will survive. As we stated before, this is because the approximants  $\ln D_n(\beta)$  are not non-trivially extensive.

This same problem crops up in connection with the extrapolation scheme discussed in the next section. There we will treat it using a trick due to Bessis, et al.<sup>2</sup>, in which the thermodynamic limit is taken in a particular way. But we may also circumvent the problem by replacing the parameterization (2.16a) by the form (2.12). In this case  $R(\lambda)$  will have the correct extensivity properties for a partition function with coupling constant  $\lambda$ . The quantity

$$f_s(\lambda) = \frac{1}{N} \ln R_{N,s}(\lambda)$$

will therefore be properly intensive, and the diagonal Padé approximants to this quantity will give non-trivial approximations to  $F$  when  $\lambda \rightarrow \infty$ .

In addition, with this parameterization we can establish a linked cluster expansion which makes the terms in the expansion of  $f_s(\lambda)$  relatively easy to calculate. Unfortunately,  $f_s(\lambda)$  will not generally be a Stieltjes series, and so it is difficult to prove convergence of the approximations.

Let us turn now to the calculation of  $F$  using this approach. The partition functions with the parameterization (2.12) are displayed in (2.17) and (2.18). The powers series in  $\lambda$ , the  $\lambda \rightarrow \infty$  limit of which gives  $F$ , can be generated via a linked cluster expansion. The linked cluster expansion (LCE) is a diagrammatic algorithm for calculating thermodynamic averages in a power series of some parameter. It is an expansion which is formally (i. e., combinatorically) similar to a perturbation expansion of connected Feynman diagrams in field theory in that spurious, disconnected diagrams are automatically removed, and the remaining connected diagrams are properly modified. The linked cluster expansion will now be described (but not derived) in some detail, mainly for the benefit of readers who may be unfamiliar with the technique. A more complete discussion can be found in Refs. (5). Those familiar with such calculations or uninterested in these details may skip to the paragraph preceding equation (3.9).

The expansions for both our theories are quite similar. For definiteness let us first consider the x - y model, (2.17). We may write

$$f_s(\lambda) = d\beta + \sum_{j=1}^{\infty} C_j(\beta)(-\lambda)^j \quad . \quad (3.7)$$

The  $C_j$  are generated as follows: The expansion includes two kinds of interactions represented by an x and a line, as in Fig. 1. Primatively, the x represents the effects of the terms  $\propto n_i^2$  in the  $\sigma_k^1$ 's, and the line represents the effects of the terms  $\propto n_i n_{i+\mu}$ . Define the rank of the x to be two, and the rank of each end of the line to be one. To calculate  $C_j$ , first draw all connected topologically distinct graphs which can be made from a total of j x's and lines such that the total rank of each vertex is even. The graphs for j = 4, for instance, are shown in Fig. 2. In a general linked cluster expansion there are, in principle graphs with vertices of odd rank, such as those of Fig. 3, but in our case these turn out to be identically zero. For the x - y model, each graph is evaluated according to the following rules (subject to the caveat discussed in comment ii):

- 1.) For each x, a factor of 2.
- 2.) For each line, a factor of 2.
- 3.) For each vertex of rank m, a factor  $L_m$  (see below).
- 4.) For each k identical interactions a factor  $1/k!$  .

These rules deserve the following comments:

i.) The factor of 2 for each  $x$  follows from the fact that each link  $n_i$ , appears in two  $\delta$  -functions (a line has two ends).

ii.) The factor of 2 for each line reflects the factor of two that accompanies terms like  $n_{\kappa, \hat{\mu}} n_{\kappa, \hat{\nu}}$  in the square of  $\sigma_{\kappa}$ . One might wonder why the factor accompanying a line is always +2, since it is clear that in  $\sigma_{\kappa}^2$  there are negative as well as positive terms like  $n_{\kappa, \hat{\mu}} n_{\kappa, \hat{\nu}}$ . This can be understood as follows: consider a term coming from the expansion in  $\lambda$  of  $R(\lambda)$  and let us represent it by a graph, which will have the same structure as a LCE graph. Since a non-zero graph has only vertices of even rank, an arbitrary graph will be composed of the intersection of closed two-dimensional manifolds each one of which is circumscribed by a closed chain of lines. For instance, the graph of Fig. 4 can be decomposed as indicated. Now, suppose we religiously inserted the  $\pm$  signs associated with the bilinear terms in the expansion of the exponential in (2.17). We want to show that the overall sign of each closed chain is positive. To do this refer to Fig. 5. An arbitrary closed path can always be decomposed for purposes of this argument into a product of elementary closed paths in the manner indicated. (For graphical simplicity we have stayed in one plane of the lattice, but this is not necessary.) Since the dashed lines are always inserted in pairs the overall sign of the graph is not changed. So the overall sign of the graph is the same as the product of the signs of the elementary graphs. In d-dimensions all of the elementary

graphs apparently consist of from two to four lines. The two and three line graphs refer to one site only, as in Figs. (6a - 6c). For such closed graphs in which there are no sign changes associated with the link indices as the circuit is traversed, it is easy to see that the overall sign is +. The exceptional elementary graph is 6d which is also positive. Since all elementary graphs appear to be positive, all graphs made up of arbitrary closed circuits are positive, and this positivity clearly persists in the linked cluster expansion. We have been unable to find any exceptions to this rule, but we have not rigorously proved that they do not exist. If there are non-positive elementary graphs, the rules will have to be modified, and more care will be necessary when counting configurations of the graphs in the lattice (see the discussion below).

iii.) The factors  $L_m$  are the Mayer semi-invariants of the  $\rho_m$  (3.3). They are defined by inverting the equations:

$$\rho_1 = L_1$$

$$\rho_2 = L_2 + L_1^2$$

$$\rho_3 = L_3 + 3L_2L_1 + L_1^3$$

$$\rho_4 = L_4 + 4L_3L_1 + 3L_2^2 + 6L_2L_1^2 + L_1^4$$

etc.

(3.8)

The coefficients of the terms in the expression for  $\rho_r$  are the number of ways  $r$  objects can be divided into the classes represented by the  $L$ 's. For example, in the expression for  $\rho_4$ , the coefficient of  $L_2 L_1^2$  is 6 because there are 6 distinct ways in which 4 objects can be divided into one group of two and two groups of one. This, incidentally, explains why all the non-zero graphs have only vertices of even rank. Since all the  $\rho_r$  with  $r$  odd are zero, so are all the odd  $L_r$ .<sup>6</sup>

iv.) An identical interaction means either the same  $\times$  at the same point or the same line between the same two vertices. So, for example, the graphs of Figs. 2a and 2e each carry a factor of  $1/4!$ , 2b and 2d both have a factor of  $1/2! \times 1/2!$ , while 2f has no such symmetry factors.

After all the graphs of a given order are computed, they are multiplied by their appropriate geometrical weight and are added together to give the coefficient,  $C_j$ . The geometrical weight is the number of distinct ways in which the graph can be embedded in the lattice per lattice site. Consider for instance the graph of Fig. 2d embedded in a two-dimensional lattice. The kinds of configurations this graph can have are shown in Fig. 7. Note, in particular, that in Figs. 7b and 7d the graph doubles back on itself. These configurations are to be included, but the value of the graph remains the same--it is still graph 2d even though it looks like graph 2e. Calculating these geometrical weights is the only hard part of the linked cluster calculation. Some of the counting problems are particularly fascinating in  $d$ -dimensions.

If not all graphs of a given topology have the same value (e. g. if we have missed some elementary graphs, the signs may vary), then the prescription given here for calculating  $F$  must be modified. The nature of the modifications can be understood by remembering that, in any case,  $F$  is just the sum over connected graphs of the type we have described where the vertices can freely wander over the entire lattice. For more details see the article by Wortis in the first work of reference 5.

The expansion we have discussed is for the  $x - y$  model. The computation of  $f_g(\lambda)$  for Q. Ph. D. is much the same. The constant ( $\lambda$  independent) term is  $\frac{d(d-1)}{2} \beta$  instead of  $\beta d$  in (3.7). The linked cluster graphs for Q. Ph. D. are quite similar. The graphs to be computed look like the graphs for the  $x - y$  model, only now a vertex represents a plaquette (rather than a link) of the original lattice, and a line segment subtends a link (rather than a site) of the lattice. Furthermore, the vertex factors are similar. Rules 3 and 4 are the same, and rule 1 is replaced by the rule that an  $x$  carries a factor of 4. In this theory we are again faced with the problem of varying signs in front of terms  $n_i n_j$ . Unfortunately, not all of the elementary graphs for this model are positive, and so we are not able to construct an argument similar to the one associated with Fig. 5 for the  $x - y$  model. It may therefore be necessary to revert to more or less explicit counting of the linked cluster graphs on the lattice. Some simplifications are possible but they are too technical and inconclusive to describe here.

This completes the discussion of the linked cluster expansion, and we are now ready to present the results of some low order calculations. We have computed the first order approximation to  $F$ ,  $P_1$  for the  $d$ -dimensional classical  $x - y$  model. Since  $F$  is exactly calculable for  $d = 1$ , we have computed  $P_2$  for  $d = 1$  to see the improvement. For  $d$ -dimensional Q. Ph. D., we have computed  $P_1$ . Here we are also able to compare with the exact result for  $d = 2$ .

Consider first the  $x - y$  model. The expansion to order  $\lambda^2$  for  $f$  is

$$f_s(\lambda) = d\beta - \lambda 2d\beta + \lambda^2 \beta d [\beta(4d + 2) + 2] \quad (3.9)$$

and

$$P_{1, s} = [1, 1] \Big|_{\lambda = \infty} = \beta d \frac{\beta(2d + 1) - 1}{\beta(2d + 1) + 1} \quad (3.10)$$

The second approximant,  $P_2$ , for  $d = 1$  is fairly straightforward to compute, and can be written in the following, unilluminating form:

$$P_2(d = 1) = \beta + \frac{2t_1 t_2 t_3 - t_2^3 - t_4 t_1^2}{t_4 t_2 - t_3^2} \quad (3.11a)$$

where

$$\begin{aligned}
 t_1 &= 2\beta \\
 t_2 &= 6\beta^2 + 2\beta \\
 t_3 &= \frac{80}{3}\beta^3 + 24\beta^2 + \frac{4}{3}\beta \\
 t_4 &= \frac{608}{3}\beta^4 + \frac{716}{3}\beta^3 + 54\beta^2 + \frac{2}{3}\beta
 \end{aligned} \tag{3.11b}$$

In Fig. 8 we plot for  $d = 1$   $P_1/\beta$ ,  $P_2/\beta$ , and compare it to the exact result  $\frac{1}{\beta} \ln I_0(\beta)$  (see 2.6). We see that the larger  $\beta$  is the better the approximation is. Moreover, for larger  $\beta$ ,  $P_2$  is a better approximation than  $P_1$ . On the basis of our heuristic arguments and the mathematical example of (2.13 - 15), we expect that higher order approximants will show convergence (although perhaps not uniformly) over wider and wider ranges of  $\beta$ .

In Fig. 9, we present  $P_1/\beta d$  for integer values of  $d$ ,  $2 \leq d \leq 6$ . Note from (3.10) that in the limit  $d \rightarrow \infty$ ,  $P_1/\beta d \rightarrow 1$ , independent of  $\beta$ , for  $\beta > 0$ , a result we expect from saddle point methods.

Turning now to Q.Ph. D., we find for the expansion of  $f_g(\lambda)$

$$f_g(\lambda) = \frac{d(d-1)}{2}\beta - \lambda 2d(d-1)\beta + \lambda^2 2d(d-1)\beta [2 + \beta(2d+1)] \tag{3.12}$$

and

$$P_{1,g} = [1, 1] \Big|_{\lambda = \infty} = \frac{d(d-1)}{2}\beta \left[ \frac{\beta(2d+1) - 2}{\beta(2d+1) + 2} \right]. \tag{3.13}$$

In Fig. 10, we have plotted  $\frac{2P_{1,g}}{d(d-1)\beta}$  for  $2 \leq d \leq 6$ , as well as the exact result for  $d = 2$ ,  $F(d = 2)/\beta$ . Not surprisingly, these curves are qualitatively similar to those in Fig. 9 for the  $x - y$  model, but lie somewhat lower for the same dimension. Migdal (Ref. 4) has argued that one might expect the critical behavior of a locally invariant theory in  $d_g$  dimensions to be the same as a theory invariant under a global transformation of the same symmetry group in  $d_s$  dimensions when  $d_g = 2d_s$ , at least when the critical temperature is fairly small. Let us take our approximations  $P_{1,g}$  and  $P_{1,s}$  which should be most accurate for large  $\beta$  (small  $T$ ), and ask what the relation between  $d_g$  and  $d_s$  must be in order to get the same free energy per degree of freedom. Equating  $\frac{2P_g(d_g)}{d_g(d_g-1)}$  and  $\frac{P_s(d_s)}{d_s}$ , we find

$$d_g = 2d_s + \frac{1}{2} \quad (3.14)$$

quite close to Migdal's conjecture. The extra term  $\frac{1}{2}$  is likely to be an artifact of the low order of our approximation.

#### IV. EXTRAPOLATION TECHNIQUE II: GENERALIZED PADÉ APPROXIMANTS

In the last section we described a straightforward, plausible method for extrapolation to the value  $\lambda = \infty$ , the point of physical interest for us. In this section we discuss a somewhat more complex, but more powerful method, for which rigorous convergence properties can be proved. The extrapolation procedure has been described by Bessis, Moussa and Villani<sup>2</sup> in the context of usual perturbation theory in statistical mechanics, but can also be used with our representations.

The method consists of first calculating generalized Padé approximants to the partition function  $Z_N$  of a system with a finite number of sites. Under certain conditions these approximants form a sequence of converging bounds to  $Z_N$ , and their logarithms, therefore, form a converging sequence of bounds to  $F_N$  defined in (2.2). Suppose that  $F_N$  is a monotonic (say, monotonically decreasing) function of  $N$ , at least for  $N > N_0$ , and suppose that for finite  $N$  we have a sequence of converging upper bounds to  $F_N$ . Then, we can use the following theorem<sup>7</sup> to establish a sequence of converging upper bounds to  $F \equiv \lim_{N \rightarrow \infty} F_N$ :

##### Theorem A:

Let

$$F_N^{(1)} > F_N^{(2)} > \dots > F_N^{(j)} > \dots > F_N \quad (4.1)$$

be a monotonous sequence of converging upper bounds for  $N > N_1$ . Suppose that for  $N > N_0$  ( $N_0 \geq N_1$ )  $F_N$  reaches its inf for  $N = \infty$  ( $F_\infty \equiv F$ ). Then for  $N > N_0$   $F_N^{(j)}$  has an inf,  $\bar{F}^{(j)}$  which satisfies

$$\bar{F}^{(1)} > \bar{F}^{(2)} > \dots > \bar{F}^{(j)} > \dots > F \quad (4.2)$$

and

$$\lim_{j \rightarrow \infty} \bar{F}^{(j)} = F \quad (4.3)$$

This rather circuitous procedure for approaching the thermodynamic limit is necessitated by the fact that the approximants,  $F_N^{(j)}$  do not have a good thermodynamic limit. That is,  $F$  can be written as

$$F = \lim_{N \rightarrow \infty} F_N = \lim_{N \rightarrow \infty} \lim_{j \rightarrow \infty} F_N^{(j)} \quad (4.4)$$

but the limits cannot be freely interchanged. The use of theorem A defines a sequence of points in the  $N - j$  plane along which we may proceed to the correct answer.

Two general ingredients are required to use this method. First, we must define approximants which bound and converge to the finite  $N$  partition function. For our problems GPA's will accomplish this, but in principle other approximation schemes could be used. Second we must determine that  $F_N$  is a monotonic function of  $N$ . Since we are dealing with finite  $N$ , this property may be sensitive to the choice of boundary conditions. This will be discussed further below.

As a first example, consider the  $x - y$  model with periodic boundary conditions. We may write the function  $R_{N,s}(\lambda)$  as

$$R_{N,s}(\lambda) = \int_0^\infty d\xi K(\lambda, \xi) d\phi(\xi) \quad (4.5)$$

where  $d\phi(\xi)$  is the same as that appearing in (3.1) and the form of  $K_s(\lambda, \xi)$  depends on how we choose to parameterize the  $\delta$ -function constraints in character space. Since  $d\phi(\xi) \geq 0$ , we may apply theorem 6 of appendix B if we choose a kernel satisfying (B.17). The Stieltjes kernel of (3.1) is one choice, but for us, a computationally more convenient choice is the exponential

$$K(\lambda, \xi) = e^{-\lambda\xi} \quad (4.6)$$

corresponding to the parameterization (2.12). (Both choices, in fact, give identical GPA's for  $R_{N,s}(\lambda)$  when  $\lambda \rightarrow \infty$ , the value of interest.)

Using the prescription of appendix B, section b, we can form the GPA's,  $B_{n,0}(\lambda)$  and  $B_{n,-1}(\lambda)$  to (4.5). By theorems 5 and 6, these will provide the best converging bounds for finite, real positive  $\lambda$ :

$$B_{n,-1}(\lambda) \leq R_N(\lambda) \leq B_{n,0}(\lambda)$$

and

$$\lim_{n \rightarrow \infty} B_{n,j}(\lambda) = R_N(\lambda) \quad .$$

Now, with parameterization (4.6) we are interested in the limit  $\lambda \rightarrow \infty$ . In particular, we want to compute  $B_{n,j}^{(\infty)}$  as approximations to  $R_N^{(\infty)} = Z_N$ . We clearly have

$$\lim_{\lambda \rightarrow \infty} \lim_{n \rightarrow \infty} B_{n,j}(\lambda) = R_N^{(\infty)} = Z_N, \quad ,$$

but it is not clear that the order of the limits on the left-hand side can be interchanged. In fact, for  $j = -1$  the interchange is certainly not justified since  $B_{n,-1}^{(\infty)} = 0$  for all finite  $n$ . However,  $R_N^{(\infty)}$  is finite, and  $R_N(\lambda)$  is sufficiently well behaved so that we can prove that the limits can be interchanged for  $j = 0$ .<sup>8</sup> The argument is given at the end of Appendix B, and rigorously establishes that these approximants provide a set of monotonically converging upper bounds.

To compute the  $B_{n,0}$  we first need the power series expansion in  $\lambda$  of  $R_N(\lambda)$ . Since we work at finite  $N$ , the coefficients will depend on our boundary conditions. It is simplest to choose periodic boundary conditions, because then we can use the results of the linked cluster expansion, which considerably simplifies the combinatorics. The reasoning is as follows: define

$$R_N(\lambda) = C_N \bar{R}_N(\lambda)$$

where

$$\bar{R}_N(\lambda) = 1 + \sum_{j=1}^{\infty} \bar{r}_j \lambda^j \quad . \quad (4.7)$$

The coefficients  $\bar{F}_j$  of  $\lambda^j$  will in general contain terms of order  $\tilde{N}^j$ ,  $\tilde{N}^{j-1}$ , ...  $\tilde{N}$ . With periodic boundary conditions there will be no terms of order  $\tilde{N}^0$ . Because we used kernel (4.6), taking the logarithm of  $\bar{R}$  removes the terms proportional to  $\tilde{N}^q$ ,  $q > 1$  from all the coefficients. Dividing by  $\tilde{N}$  we have an intensive quantity. But this is exactly what is calculated in the linked cluster expansion. That is, we lose no information in the limit  $N \rightarrow \infty$  if we use periodic boundary conditions. (Note that  $\frac{1}{\tilde{N}} \ln C_N$  is also independent of  $\tilde{N}$ .) The only caveat is that we must remember to stick to lattices which are large enough to accommodate the largest diagram in the expansion. So, for instance, calculating to order  $\lambda^\ell$  require a lattice of at least  $\ell$  sites on a side.

With this in mind, we can write

$$R_N(\lambda) = e^{\tilde{N}f(\lambda)} \quad (4.8)$$

where  $f(\lambda)$  is the power series in  $\lambda$  calculated according to the linked cluster expansion.  $R_N(\lambda)$  can now be expanded in a power series in  $\lambda$ . Essentially this amounts to reinverting the cumulant formulae (3.8). Remember that (4.8) is not valid if we have boundary conditions which are not periodic. In that case there will be terms which disappear in  $f(\lambda)$  in the limit  $N \rightarrow \infty$ , and which are not recovered in (4.8).

From the power series expansion of  $R_N(\lambda)$ , we can compute the  $B_{n,0}(\lambda)$  as described in appendix B. In the limit  $\lambda \rightarrow \infty$  the  $B_{n,0}(\lambda)$  will provide

converging upper bounds to  $Z_N$ , so their logarithms will give converging upper bounds to  $F_N$ . For the one dimensional x - y model, with periodic boundary conditions, we have

$$F_N = \frac{1}{N} \ln Z_N = \ln I_0(\beta) + \frac{1}{N} \ln \left( 1 + \sum_{j=1}^{\infty} E_j^N(\beta) \right) \quad (4.9)$$

where

$$E_j(\beta) = \frac{I_j(\beta)}{I_0(\beta)} .$$

Since  $0 \leq E_j(\beta) < 1$ , it is clear that  $F_N$  in (4.9) is a monotonically decreasing function of  $N$ , and we may use theorem A of this section to establish a monotonically converging sequence of upper bounds to  $F$ .

We have computed  $B_{1,0}(\lambda = \infty)$  and  $B_{2,0}(\lambda = \infty)$  for this model for a range of values of  $N$ . In Fig. 11 we plot

$$\frac{1}{N\beta} \ln B_{n,0}(\lambda = \infty) \quad (4.10)$$

for  $n = 1, 2$  as a function of  $N$  for several values of  $\beta$ . (For  $\beta = 100$   $B_{2,0} < B_{1,0}$  also, but the difference is not visible on this graph.) In Fig. 12 we plot the inf. of these curves as a function of  $\beta$  and compare it with the exact result,  $\frac{1}{\beta} \ln I_0(\beta)$ . Notice that even the first order bound is quite good at large  $\beta$ . When  $\beta = 100$  the ratio of inf of (4.10) with  $n = 1$

to the exact result is  $\sim 1.03089$  while the corresponding ratio with  $n = 2$  is  $\sim 1.03010$ . For smaller  $\beta$  the bounds are less good, but the improvement is more dramatic. These observations are consistent with our arguments that the approximation scheme should be best at low temperatures.

Now suppose  $F_N$  with periodic boundary conditions is monotonically decreasing also for higher dimensions. We have assumed this to be true and have computed the lowest order bounds ( $n = 1$ ) to  $F$  for both the  $x - y$  model and Q. Ph. D. in  $d$ -dimensions. In Fig. 13 we present these bounds normalized by  $(d\beta)^{-1}$  as a function of  $\beta$  for the  $x - y$  model for integer dimensions,  $2 \leq d \leq 6$ . Fig. 14 is the corresponding graph for Q. Ph. D. (with normalization  $2[d(d - 1)\beta]^{-1}$ ). On this graph, we have also drawn the exact Q. Ph. D. result for  $d = 2$ . (Note that monotonicity in  $N$  of  $F_N$  for Q. Ph. D. in two dimensions can be easily demonstrated.)

Since it is relatively simple to compute the  $B_{n,0}$  for a theory with periodic boundary conditions, these will generally be the favored choice, assuming that the corresponding  $F_N$  are monotonic. But it is interesting to compute bounds with other boundary conditions to see how they compare with those computed for the periodic lattice. To this end, let us examine the two dimensional  $x - y$  model with fixed edge boundary conditions. First we will prove that the  $F_N$  are monotonic for this theory, and then we will discuss the bounds.

Consider a square  $(N + 2) \times (N + 2)$  lattice. The boundary conditions are defined as follows: The spins along the edge are fixed at  $\theta_i = 0$  and

the coupling constant between two adjacent edge spins is half the usual coupling constant. The partition function can then be written

$$Z_N = e^{-2(N+1)\beta} \int_{-\pi}^{\pi} \prod_s d\theta_s \prod_{\ell} e^{\beta \cos(\theta_i - \theta_{i+\hat{x}})} \prod_b \delta(\theta_b) \quad (4.11)$$

where  $\prod_b$  runs over all spins on the boundary. We may now define  $F_N$  as in (2.2) where  $\tilde{N}$  is the sum of the spins times their weight factor,  $\omega$ .

The weight factor is determined as follows: each link impinging on a spin has coupling constant of  $\beta$  or  $\frac{1}{2}\beta$ .  $\omega$  is  $1/4\beta$  times the sum of the coupling constants of the links impinging on a spin. For an internal spin,  $\omega = 1$ , for an edge spin,  $\omega = \frac{1}{2}$ , and for a spin on the corner of the lattice  $\omega = \frac{1}{4}$ .

Now, consider the function

$$G(\lambda) = \sum_{\{n\}} \prod_{\ell_1, \ell_2} I_{n_{\ell_i}}(\beta) \prod_{s_1, s_2} \delta(\sigma_{s_i}) \prod_{b_1, b_2} I_{n_{b_i}}(\beta/2) \prod_{b_I, s_I} I_{n_{b_I}}(\beta) \prod_{s_I} e^{-\lambda \sigma_{s_I}^2} \quad (4.12)$$

Look at Fig. 15. Let  $\ell_1, s_1$ , and  $b_1$  ( $\ell_2, s_2$  and  $b_2$ ) refer to the internal links and spins and external boundary links in the left (right) half of the  $(N+2) \times (2N+3)$  lattice, respectively. The  $b_I$  and  $s_I$  refer to the internal boundary joining the two  $(N+2) \times (N+2)$  lattices which make up the lattice of Fig. 15. It is easy to see that  $G(0) = Z_N^2$  while  $G(\infty) = \bar{Z}_N$ , the partition function of the doubled lattice. Since  $\partial_{\lambda} G(\lambda) < 0$ , we have

$$\bar{Z}_N < Z_N^2 \quad . \quad (4.13)$$

Using the definition of  $\tilde{N}$  given above we easily see that (4.13) implies

$$\bar{F}_N < F_N \quad . \quad (4.14)$$

We can repeat the same procedure doubling the lattice in the other direction and we conclude that

$$F_{2N+1} < F_N \quad . \quad (4.15)$$

So  $F_N$  for a sequence of  $N$ 's is monotonically decreasing. It is clear that the argument can be applied more generally, and so  $F_N$  will be a decreasing function for all  $N$ . It is also clear that the argument can be applied in higher dimensions, and also for many other systems including Q. Ph. D.

We discuss now the bounds obtained with these boundary conditions. We have calculated the lowest order bound to  $F$  for the square lattice. The calculation of the  $B_{1,0}$  for various  $N$  and  $\beta$  is straightforward. The bounds derived from these calculations are summarized in Table I. In all cases the calculation with periodic boundary conditions gives a better bound. It is interesting to note, in the case of the fixed edge boundary conditions the value of  $N$  for which  $F_N$  attains its minimum. This is  $N_{\min}$  in the last column of the table, and corresponds to a  $(N_{\min} + 2)$  by  $(N_{\min} + 2)$  lattice. With periodic boundary conditions the minimum is always obtained for a  $3 \times 3$  lattice. It seems, then, that for low orders the choice of boundary

conditions can have a significant effect on the size of the bound, particularly for smaller values of  $\beta$ . For large  $\beta$  the bound is less sensitive to the choice of boundary conditions. This is not surprising, since the only essential difference between fixed edge and periodic boundaries is that the spins on the boundary are frozen in the former case. At low temperatures the major contribution to  $F_N$  comes from configurations where the spins are almost lined up anyway, and so the difference between the two types of boundaries becomes less significant.

## V. COMMENTS

We would like to make a number of comments about the work presented in this paper.

i) The convergence of the approximations of section III and the bounds of section IV might be accelerated by the following device: Denote the  $j^{\text{th}}$  approximation to a function,  $F$ , by  $A_j$ , and suppose that  $A_\infty = F$ . Form

$$S(\tau) = \sum_{j=0}^{\infty} (A_j - A_{j-1})\tau^j \quad (5.1)$$

where  $A_{-1} \equiv 0$ .  $S(1) = F$ , and the expansion of  $S(1)$  to  $k^{\text{th}}$  order is  $A_k$ . We can now form the  $[n, n]$  Padé approximants to  $S(\tau)$ , evaluated at  $\tau = 1$ , which, if the coefficients in (5.1) are reasonably smooth, should provide a better approximation to  $F$  than  $A_{2n}$ . Of course, in the case where the  $A_k$  are bounds to  $F$ , these Padé approximants are not in general guaranteed

to be bounds. We have carried out these calculations for the one-dimensional  $x - y$  model using both the approximants of section III and the bounds of section IV. Except for the approximants of section III when  $\beta \ll 1$ , the  $[1, 1]$  Padé of (5.4) gives a better approximation than the corresponding  $A_2$ .

ii) With the exponential parameterization of the  $\delta$ -function there is a very close relation between the logarithm of the  $B_{n,0}$ 's of section IV, and the straight Padé approximants for the free energy. The coefficients of the power series for the Padé of the free energy (section III), are just the cumulants of the coefficients in the expansions of section IV. We can now ask, if the  $B_{n,0}$ 's at  $\lambda = \infty$  converge to  $Z_N$ , under what conditions will the  $P_n$  of section III converge to  $F$ ?

iii) It is worth pointing out that for the lattice gauge theories, our approximations are "not gauge invariant" in the following sense: Before making the character expansion, one may make a gauge choice in configuration space which fixes some of the link variables. Only the remaining, dynamical links will then be parameterized as  $\delta$ -functions, and so the coefficients in the expansion in powers of  $\lambda$  will be different. Of course, there will still be convergence to the correct answer even with a gauge choice, but the rate of convergence may differ. We have not examined this dependence closely.

iv) Our procedure was formulated in character space and, as we argued, is in some sense a low temperature approximation. A similar technique suggests itself in which the usual configuration space expression

of  $Z$  is used (Eq. 2.1). A sufficiently large set of a priori independent spins is introduced at each site with, for example, one member of the set coupled to the neighboring site in each direction of the lattice. All the spins at a site are coupled together through the use of  $\delta$ -functions. The theory can now be approximated by parameterizing and expanding the  $\delta$ -functions. One might expect such an approximation to be best at high temperatures, since the starting point is a collection of independent interactions which might naively be expected to dominate at high temperatures.

v) One important question which we have not been able to address very well is the question of whether the system undergoes a phase transition. The quantity we have been dealing with,  $F$ , is expected in most cases to exhibit only a soft singularity near a phase transition, to which numerical approximations are rather insensitive. What is needed is either a mathematically firm scheme for approximating quantities with strong singularities, or a method of integrating our approximation scheme and the renormalization group.<sup>9</sup>

The approach we have outlined in this paper is clearly rather open ended. There seems to be a lot of room for massaging the techniques to try to obtain better results. It is also clear that there are many possible applications for these schemes, some of which will be discussed elsewhere. It is hoped that one will be able to apply the general method fruitfully to a variety of theories in which a systematic non-perturbative approximation procedure is desired.

## ACKNOWLEDGMENTS

I am grateful to many people for stimulating and informative conversations, particularly W. Bardeen, J.-L. Basdevant, D. Bessis, J. L. Gammel, J. Lieberman, and R. Pearson.

## APPENDIX A

The Ising model is defined by the partition function

$$Z = \sum_{s_i = \pm 1} e^{\beta \sum_{i, \hat{\mu}} s_i s_{i+\hat{\mu}}} \quad (\text{A. 1})$$

$$= \sum_{s_i = \pm 1} \prod_{\ell} e^{\beta s_i s_{i+\hat{\mu}}}$$

where  $\ell$  runs over all nearest neighbor links of the lattice. The character expansion of the exponential takes the form

$$e^{\beta s_i s_j} = \cosh \beta + s_i s_j \sinh \beta$$

$$= \sum_{n=0}^1 C_n (s_i s_j)^n \quad (\text{A. 2})$$

Inserting (A. 2) in (A. 1) and doing the spin sums, we have

$$Z = \sum_{\{n\} = 0}^1 \prod_{\ell} C_{n_{\ell}} \prod_{\kappa} (1 + (-1)^{\sigma_{\kappa}}) \quad (\text{A. 3})$$

where  $\sigma_{\kappa}$  is the sum of all the  $n_i$  associated with links that impinge on site  $\kappa$ . We parameterize the last factor in (A. 3). Notice that this is not a simple  $\delta$ -function. One can invent a large number of parameterizations for this object, but two of the most useful are the following:

$$1 + (-1)^{\sigma} = \lim_{\lambda \rightarrow \infty} 2e^{-\lambda [1 - (-1)^{\sigma}]} \quad (\text{A. 4})$$

and

$$1 + (-1)^{\sigma} = \lim_{\lambda \rightarrow \infty} 2e^{-\lambda \prod_{j=0}^d (\sigma - 2j)^2} \quad (\text{A. 5})$$

These expressions will both yield functions,  $F(\lambda)$  which are properly intensive in the thermodynamic limit. Furthermore, these kernels satisfy the conditions of Theorem 6 (appendix B) and so we will be able to derive converging upper bounds to  $F$  from these expressions.

## APPENDIX B

In this pedagogical appendix we discuss a number of results (well-known in certain circles) concerning Padé approximants and generalized Padé approximants (GPA), which we have found useful. More extensive discussions of these and other related ideas may be found in any of a number of books and review articles.<sup>10</sup>

## a. Ordinary Padé Approximants

Consider a power series

$$F(z) = \sum_{j=0}^{\infty} a_j z^j \quad . \quad (B.1)$$

The  $[n, m]$  Padé approximant can be written

$$[n, m](z) = \frac{P_m(z)}{Q_n(z)} = \frac{\sum_{j=0}^m b_j z^j}{\sum_{j=0}^n c_j z^j} \quad . \quad (B.2)$$

The b's and c's are determined by solving the equation

$$F(z)Q_n(z) - P_m(z) = 0 \quad (B.3)$$

after dropping terms of order  $z^{n+m+1}$  and higher. By convention,

$c_0$  is usually taken to be one.

Except for the special case of Stieltjes series (see below) it is difficult to establish general convergence theorems for sequences of Padé approximants. For rational functions of course, the  $[n, m]$  Padé will be identical to the function for large enough  $n, m$ , and so there is no convergence problem. Typical of the theorems on convergence for a general series is the following:

THEOREM 1: Let  $P_k(z)$  be any infinite sequence of  $[n, m]$  Padé approximants to a formal power series where  $n + m$  tend to infinity with  $k$ . If  $|P_k(z)|$  is uniformly bounded in any closed, simply-connected domain  $D_1$  containing the origin as an interior point and  $|P_k(z)|^{-1}$  is uniformly bounded in any closed simply-connected domain  $D_2$  containing the origin as an interior point, then the  $P_k$  converge to a meromorphic function  $f(z)$  in the interior of the union of  $D_1$  and  $D_2$ .

Even where no formal proof of convergence exists, some subsequence of the Padé approximants with  $n, m \rightarrow \infty$  often seem to give good (convergent?) approximations to the original function, even far outside the domain of convergence of the power series.<sup>11</sup> On the other hand, this is not always true and one must generally exercise some care. In the words of Chief Dan George, "Sometimes the magic works, and sometimes it doesn't."<sup>12</sup>

For Stieltjes series the situation is considerably better. A series of Stieltjes is a series

$$G(z) = \sum_{j=0}^{\infty} g_j (-z)^j \quad (\text{B.4})$$

with

$$g_j = \int_0^{\infty} u^j d\phi(u)$$

where  $\phi(u)$  is a bounded, non-decreasing function taking on infinitely many values in  $0 \leq u < \infty$ . Roughly, this means  $d\phi(u) \geq 0$ . (B.4) need not converge. Note that this is equivalent to the representation

$$G(z) = \int_0^{\infty} \frac{d\phi(u)}{1+zu} \quad . \quad (\text{B.5})$$

For these series we have the following theorems:

THEOREM 2: If  $\sum g_j (-z)^j$  is a series of Stieltjes, then the poles of the  $[n, n+j]$ ,  $j \geq -1$ , Padé approximants are on the negative real axis. Furthermore, the poles of successive approximants interlace and all the residues are positive. The roots of the numerator also interlace those of the denominator.

THEOREM 3: The Padé approximants for series of Stieltjes obey the following inequalities where  $G(z)$  is the sum of the series  $\sum g_j (-z)^j$ , and  $z$  is real and nonnegative.

$$(-1)^{1+j} \{ [n+1, n+1+j] - [n, n+j] \} \geq 0, \quad (\text{B.6a})$$

$$(-1)^{1+j} \{ [n, n+j] - [n-1, n+j+1] \} \geq 0, \quad (\text{B.6b})$$

$$[n, n] \geq G(z) \geq [n, n - 1] \tag{B.6c}$$

$$[n, n]' \geq G'(z) \geq [n, n - 1]' \tag{B.6d}$$

where  $j \geq -1$ . These inequalities have the consequence that the  $[n, n]$  and  $[n, n - 1]$  sequences form the best upper and lower bounds obtainable from the  $[n, n + j]$  approximants with a given number of coefficients and that the use of additional coefficients (higher  $n$ ) improves the bounds.

THEOREM 4: Any sequence in  $n$  of  $[n, n + j]$  Padé approximants for a series of Stieltjes converges to an analytic function in the cut complex plane ( $-\infty \leq z \leq 0$ ). If, in addition  $\sum_{p=1}^{\infty} (g_p)^{-1/(2p+1)}$  diverges, then all the sequences tend to a common limit (this condition is roughly equivalent to  $|g_p| \leq (2p)!$ ). If the  $g_p$  are a convergent series with a radius of convergence  $R$ , then any  $[n, n + j]$  sequence converges in the cut plane ( $-\infty \leq z \leq -R$ ) to the analytic function defined by the power series.

b. Generalized Padé Approximants

Consider a function with a representation of the form

$$F(z) = \int_0^{\infty} b(z, u) d\phi(u) \tag{B.7}$$

with  $d\phi(u) \geq 0$ . The method of generalized Padé approximants we shall discuss consists, in essence, of approximating  $d\phi(u)$  by a sum of  $\delta$ -functions whose weights and positions will be determined by comparing the approximations with moments of the original function.

We introduce (in Baker's notation<sup>10</sup>) a set of approximants:

$$B_{n,j}(z) = \sum_{m=1}^n \alpha_m b(z, u_m) + \sum_{k=0}^j \frac{\beta_k}{k!} \left[ \partial_u^k b(z, u) \Big|_{u=0} \right] \quad (B.8)$$

where  $n = 1, 2, \dots$  and  $j = -1, 0, 1, 2, \dots$ . When  $j = -1$  the second sum in (B.8) is absent. We restrict ourselves in (B.7) to kernels  $b(z, u)$  which can be formally expanded as

$$b(z, u) = \sum_{m=0}^{\infty} b_m(z) (-u)^m \quad (B.9)$$

Denote

$$c_\ell = \int_0^{\infty} u^\ell d\phi(u) \quad (B.10)$$

Inserting (B.9) into (B.7) and (B.8) and equating the two we have

$$\sum_{m=0}^{\infty} b_m(z) \left[ \sum_{\ell=1}^n \alpha_\ell (-u_\ell)^m - (-1)^m c_m \right] + \sum_{m=0}^j b_m(z) \beta_m (-1)^m = 0 \quad (B.11)$$

The  $\alpha_\ell$ ,  $\beta_\ell$ , and  $u_\ell$  are determined by setting the coefficients of the first  $2n + j + 1$   $b_m$ 's equal to zero. Thus we have

$$\sum_{\ell=1}^n \alpha_{\ell} (u_{\ell})^k + \beta_k = c_k \quad 0 \leq k \leq j \tag{B.12}$$

$$\sum_{\ell=1}^n \alpha_{\ell} (u_{\ell})^k = c_k \quad j < k \leq 2n + j .$$

If the kernel  $b(z, u)$  is the Stieltjes kernel:

$$b(z, u) = \frac{1}{1 + zu} \tag{B.13}$$

then the approximants  $B_{n,j}(z)$  are exactly the ordinary  $[n, n + j]$  Padé approximants to the function  $F(z)$  defined in (B.7). Moreover,  $(-u_{\ell})^{-1}$  are the location of the poles and their respective residues are  $(\alpha_{\ell} / u_{\ell})$ .

The approximants  $B_{n,j}(z)$  can be proved to converge for a rather large class of kernels as is shown by the following theorem:

THEOREM 5: Suppose  $b(z, u)$  is regular in a uniform neighborhood of the positive, real  $u$  axis and  $(\ln u)^{1 + \eta} \times b(z, u)$  is bounded as  $u \rightarrow +\infty$ , for some  $\eta > 0$ ; then the approximants  $B_{n,j}(z)$  converge as  $n$  goes to infinity for functions  $F(z)$  of the form (B.7).

Another very important property of these approximants can be established if the kernel  $b(z, u)$  has the property that

$$(-\partial_u)^j b(z, u) \geq 0$$

for all real, positive  $z$  and  $u$ , for  $j = 0, 1, 2, \dots$ . The Stieltjes kernel has this property as does the kernel

$$b(z, u) = e^{-zu} \quad (\text{B. 15})$$

which is the form used in section IV to parameterize the  $\delta$ -functions. For kernels of this type, the following theorem can be proved:

THEOREM 6: The approximants  $B_{n,j}(z)$  to a function of the form (B. 7) obey the following inequalities where  $z$  is real and nonnegative:

$$(-1)^{1+j} \left\{ B_{n+1,j}(z) - B_{n,j}(z) \right\} \geq 0, \quad (\text{B. 16a})$$

$$(-1)^{1+j} \left\{ B_{n,j}(z) - B_{n-1,j+2}(z) \right\} \geq 0, \quad (\text{B. 16b})$$

$$B_{n,0}(z) \geq F(z) \geq B_{n,-1}(z), \quad (\text{B. 16c})$$

where  $j \geq -1$ , if and only if

$$(-\partial_u)^j b(z, u) \geq 0 \quad (\text{B. 17})$$

for all real, nonnegative  $z$  and  $u$ , and  $j = 0, 1, 2, \dots$ . These inequalities have the consequence that the  $B_{n,0}(z)$  and  $B_{n,-1}(z)$  sequences form the best upper and lower bounds obtainable from the  $B_{n,j}(z)$  approximants with a given number of coefficients and that the use of additional coefficients (higher  $n$ ) improves the bounds.

We now demonstrate the following equality for functions with which we are concerned:

$$\lim_{n \rightarrow \infty} \lim_{z \rightarrow \infty} B_{n,0}(z) = \lim_{z \rightarrow \infty} \lim_{n \rightarrow \infty} B_{n,0}(z) = \lim_{z \rightarrow \infty} F(z) \quad (\text{B. 18})$$

where  $z \rightarrow \infty$  along the positive real axis.

Suppose  $b(z, u)$  is of the form  $e^{-zu}$ . For such a kernel (in fact, it is true much more generally) it is easy to show that  $B_{n,0}(z)$  is a monotonically decreasing function for real positive  $z$ . This follows from the fact that the  $u_m$  and  $\alpha_m$  in (B. 8) are positive, which can be deduced by first noticing that the equations (B. 12) are the same whether we use kernel (B. 13) or (B. 15). Then, from the remarks following (B. 13) and the well-known properties of  $[n, n]$  Padé's to Stieltjes series the monotonicity of the  $B_{n,0}(z)$  follows. Now suppose that  $F(\infty)$  is finite and that  $|F(z) - F(\infty)|$  can be made arbitrarily small by choosing  $z$  large enough. By theorem 5 we know that for any small positive  $\delta(z)$ , we can find an  $N_0$  such that for  $N > N_0$ ,

$$B_{N,0}(z) - F(z) < \delta(z) \quad (\text{B. 19})$$

for real positive  $z$ . Since  $B_{n,0}(z)$  is smooth, and monotonically decreasing,  $B_{n,0}(\infty) < B_{n,0}(z)$ . Hence, using (B. 19) we can write

$$B_{N,0}(\infty) - F(\infty) < \delta(z) + F(z) - F(\infty) \quad (\text{B. 20})$$

Now, we can always find a  $z$  such that  $|F(z) - F(\infty)|$  is arbitrarily small. Furthermore, for large enough  $N_0$   $\delta(z)$  can be made arbitrarily small, and so for large enough  $N$  the right-hand side of (B. 20) can be arbitrarily small in magnitude. Thus we have convergence at  $z = \infty$  and the interchange of limits in (B. 18) is allowed.

$\beta$	Periodic Boundary Conditions	Fixed Edge Boundary Conditions	$N_{\min}$ , Fixed Edge
.01	.1209	.4044	4
.1	.5620	.7162	2
1	.9230	.9486	2
10	.9916	.9944	2
100	.9992	.9995	2

TABLE I  
GPA bounds to  $F/2\beta$  for the two dimensional x - y model

## FOOTNOTES AND REFERENCES

- <sup>1</sup>For extensive descriptions of lattice gauge theories see, for example, K. Wilson, Phys. Rev. D10, 2445 (1974); R. Balian, J. Drouffe, and C. Itzykson, Phys. Rev. D10, 3376 (1974) and Phys. Rev. D11, 2098 and 2104 (1975); T. Banks, et al., Cornell University Preprint CLNS-339 (1976).
- <sup>2</sup>D. Bessis, P. Moussa, and M. Villani, Saclay preprint D. Ph-T/75-6 (1975).
- <sup>3</sup>The x - y and related models are discussed by H. E. Stanley in Phase Transitions a Critical Phenomena Vol. 3, p. 485 (Academic Press, London, 1974), and references therein. See also D. D. Betts, p. 569 in the same volume.
- <sup>4</sup>A. A. Migdal, Zh ETF 69, 810 and 1457 (1975) has suggested the possibility that there is a simple connection between the critical behavior of a locally invariant theory in  $d_g$  dimensions and a related globally invariant theory in  $d_s$  dimensions when  $d_g = 2d_s$ . We will comment on this later.
- <sup>5</sup>The linked cluster and related expansions are extensively discussed in Phase Transitions and Critical Phenomena Vol. 3, Domb and Green, ed. (Academic Press, London 1974). See especially the article by M. Wortis, p. 113. See also F. Englert, Phys. Rev. 129, 567 (1963).

- <sup>6</sup>Another method of setting up the calculation would have been to include the single link interactions in the single link weighting. In that case the  $M$ 's would be defined as  $M_r = \sum_n^r I_n(\beta) e^{-\lambda n^2}$ , and there would have been no  $x$  interaction. Keeping  $\lambda$  to all orders in the single link terms while expanding in the terms which couple links seems to mutilate the  $\delta$ -function beyond recognition, and so we have not done it. But in high orders it may be computationally advantageous to use the  $M_r$  described here, omitting the  $x$  interactions, and later expanding the  $M_r$  keeping the appropriate powers of  $\lambda$ .
- <sup>7</sup>This theorem is a slightly rephrased version of Theorem 5 of reference 2.
- <sup>8</sup>I am grateful to J. L. Gammel for a useful communication on this point.
- <sup>9</sup>See also the remarks at the end of reference 2.
- <sup>10</sup>Theorems 1 - 6 are quoted from the article by G. A. Baker in The Padé Approximant in Theoretical Physics, G. A. Baker and J. L. Gammel, ed. pp. 1 - 39 (Academic Press, New York, 1970). See also, J. Zinn-Justin, Physics Reports 1c, 55 (1971), and references therein.
- <sup>11</sup>There exists a statement known as the Padé conjecture which concerns the convergence of Padé approximants for a certain class of meromorphic functions. This conjecture has not been proven, but there are no known counterexamples to it. For a statement of the conjecture, see the first citation in reference 10, p. 20.

<sup>12</sup>Chief Dan George in Little Big Man, produced by National General Studios, 1970.

#### FIGURE CAPTIONS

- Fig. 1: Elements in the linked cluster expansion for the  $x - y$  model and Q. Ph. D.
- Fig. 2: Graphs of fourth order in the LCE.
- Fig. 3: Some linked cluster graphs which are zero.
- Fig. 4: An example of a linked cluster graph and its decomposition into two-dimensional manifolds.
- Fig. 5: An example of a graph and its decomposition into elementary closed paths.
- Fig. 6: The elementary graphs formed from closed paths for the  $x - y$  model.
- Fig. 7: Possible configurations for the graph of Fig. 2d for the two-dimensional  $x - y$  model.
- Fig. 8: The approximants  $P_1/\beta$  (curve a) and  $P_2/\beta$  (curve b), to  $F/\beta$  (curve c) for the one-dimensional  $x - y$  model.
- Fig. 9: The approximants  $P_1/\beta d$  for the  $x - y$  model for integer  $2 \leq d \leq 6$ .
- Fig. 10: The approximants  $2P_1/d(d-1)\beta$  for Q. Ph. D. for  $2 \leq d \leq 6$ . The exact result,  $F/\beta$  for  $d = 2$  is the dashed line.

- Fig. 11: The bounds  $\frac{1}{N\beta} \ln B_{n,0}(\lambda = \infty)$ ,  $n = 1, 2$  for the one-dimensional  $x - y$  model as a function of  $N$ . For each value of  $\beta$  the lower curve is  $n = 2$ , the upper curve  $n = 1$ .
- Fig. 12: The bounds derived in section IV to  $F/\beta$  for the one-dimensional  $x - y$  model. Curve a is the bound derived from  $B_{1,0}$ , curve b from  $B_{2,0}$ , and curve c is the exact result.
- Fig. 13: The bounds  $\frac{\ln B_{1,0}(\lambda = \infty)}{\beta d}$  to  $F/\beta d$  for the  $x - y$  model for  $2 \leq d \leq 6$ .
- Fig. 14: The bounds  $\frac{2 \ln B_{1,0}(\lambda = \infty)}{d(d-1)\beta}$  to  $\frac{2F}{d(d-1)\beta}$  for Q. Ph. D. for  $2 \leq d \leq 6$ . The dashed line is the exact curve  $F/\beta$  for  $d = 2$ .
- Fig. 15: Pictorial representation of the function  $G(\lambda)$  defined in (4.11).

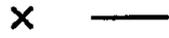


Fig. 1

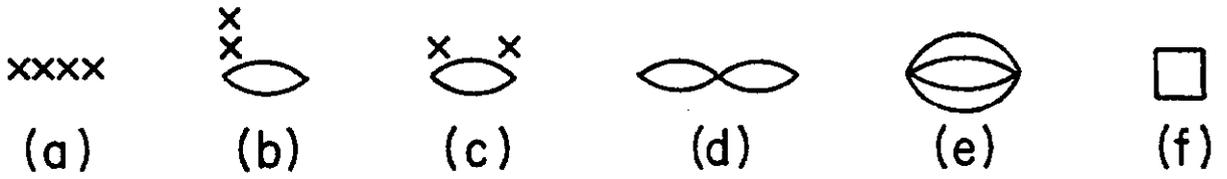
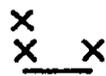


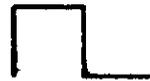
Fig. 2



(a)



(b)



(c)

Fig. 3

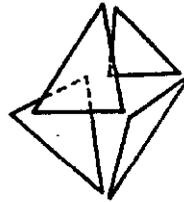
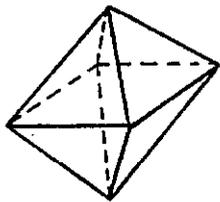


Fig. 4

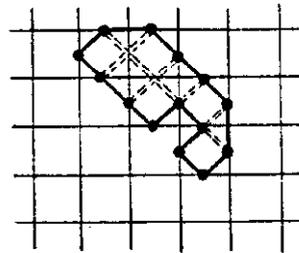
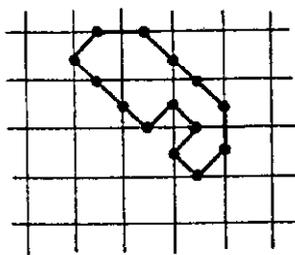


Fig. 5

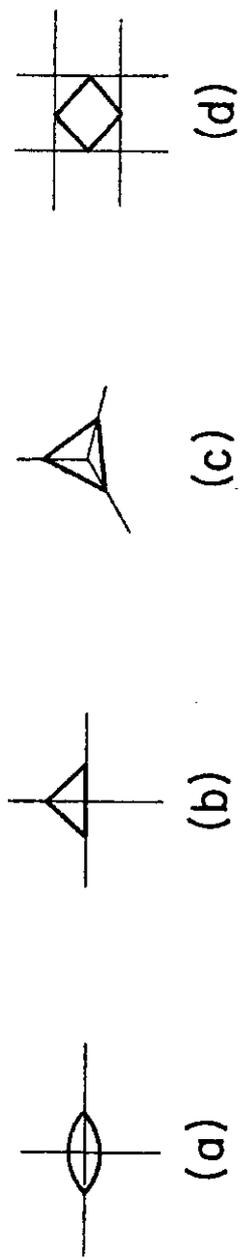


Fig. 6

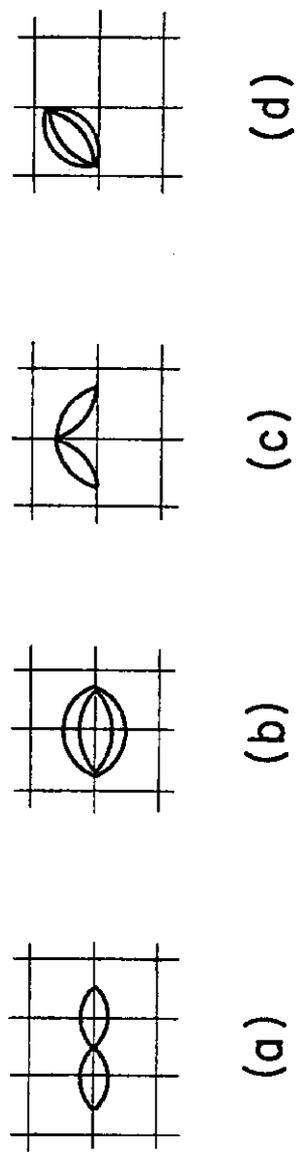


Fig. 7

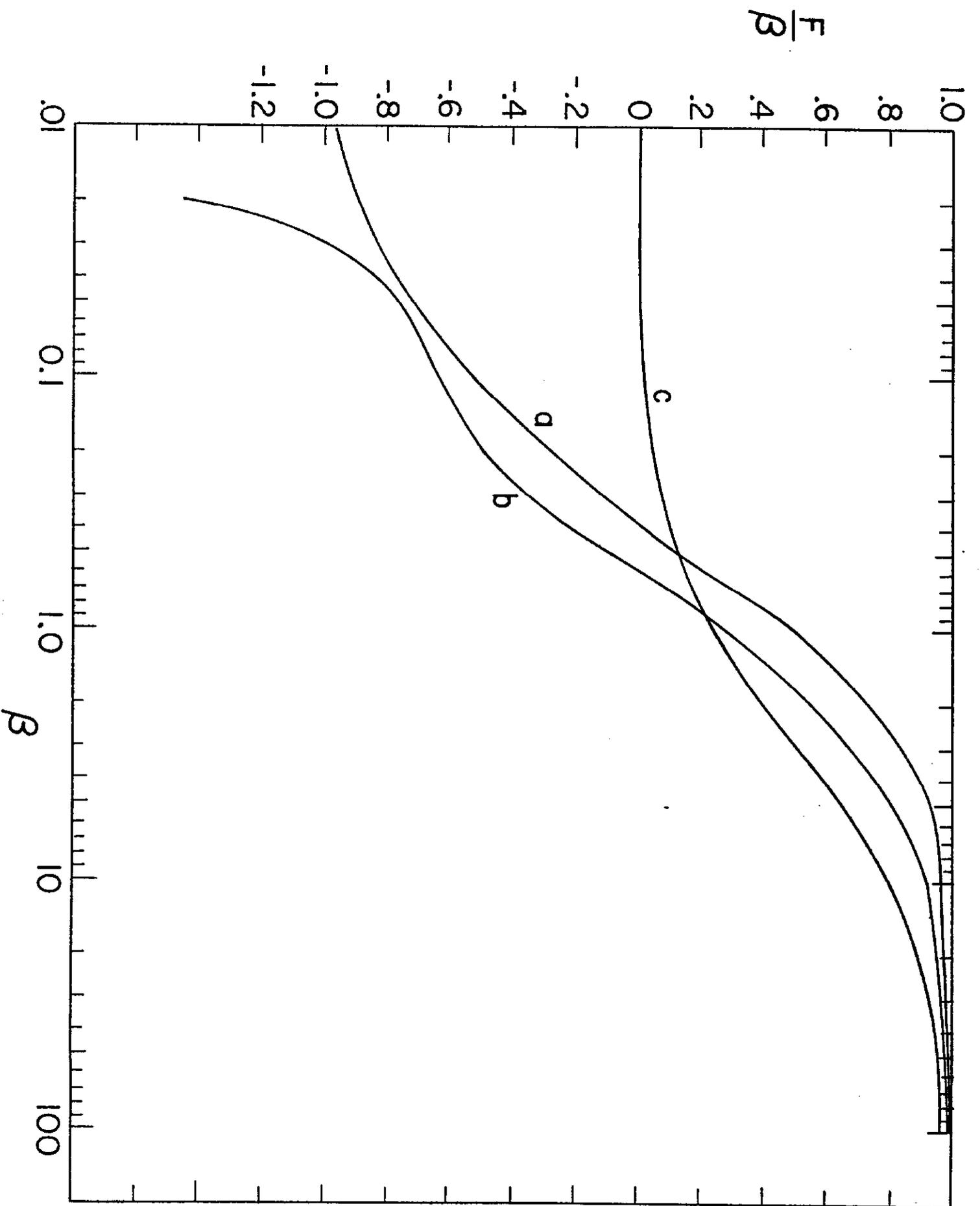


Fig. 8

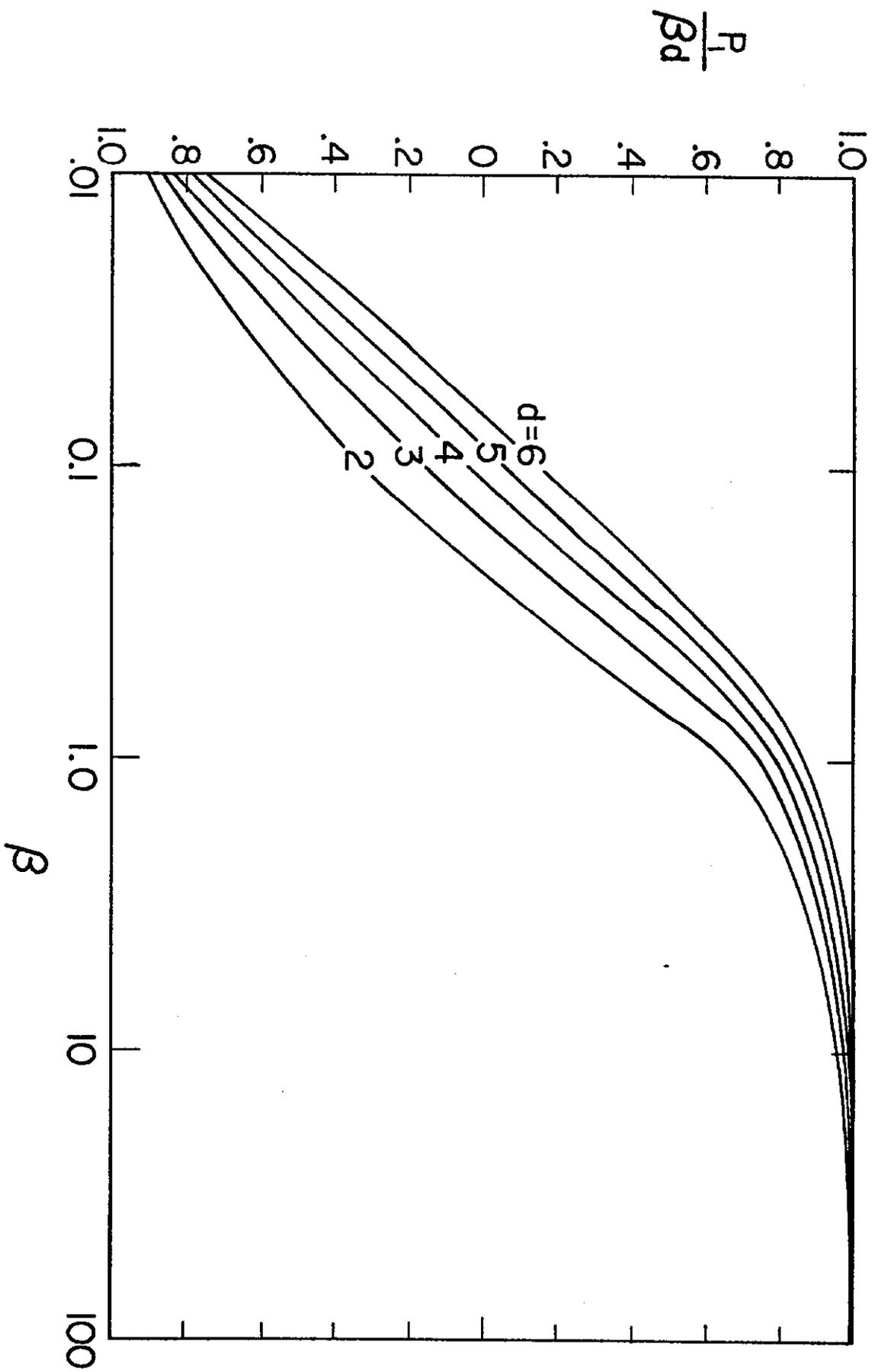


Fig. 9

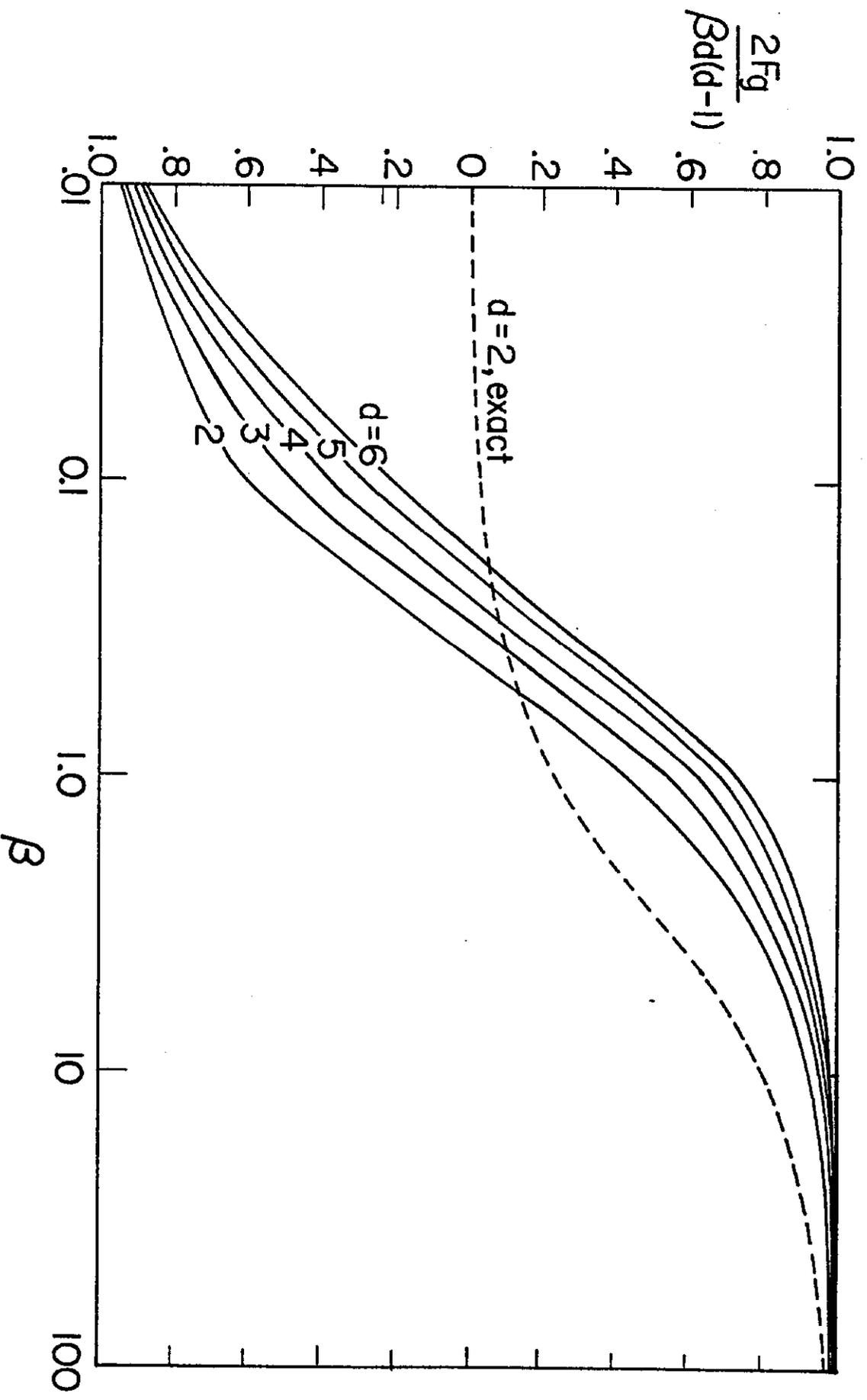


Fig. 10

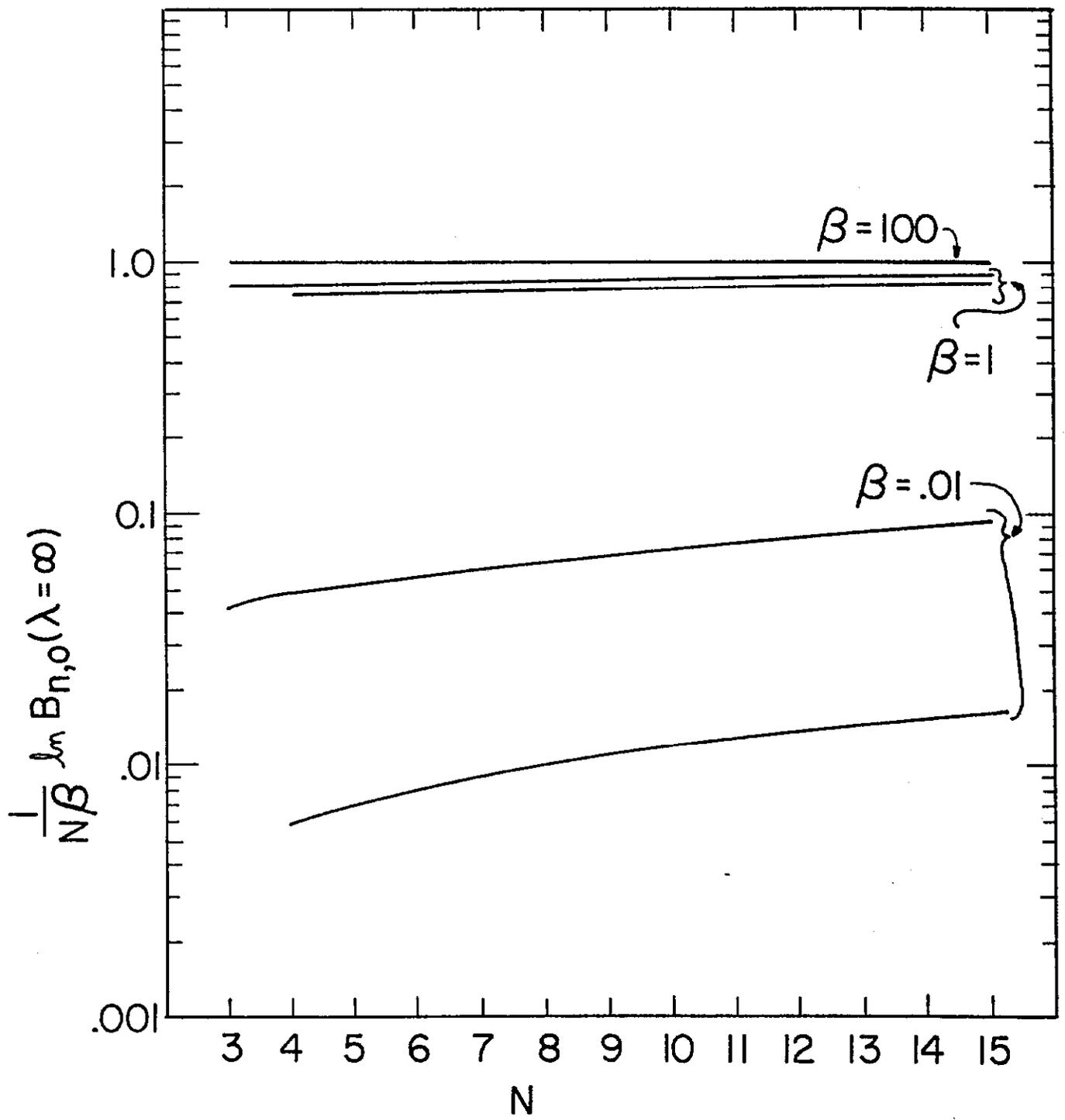


Fig. 11

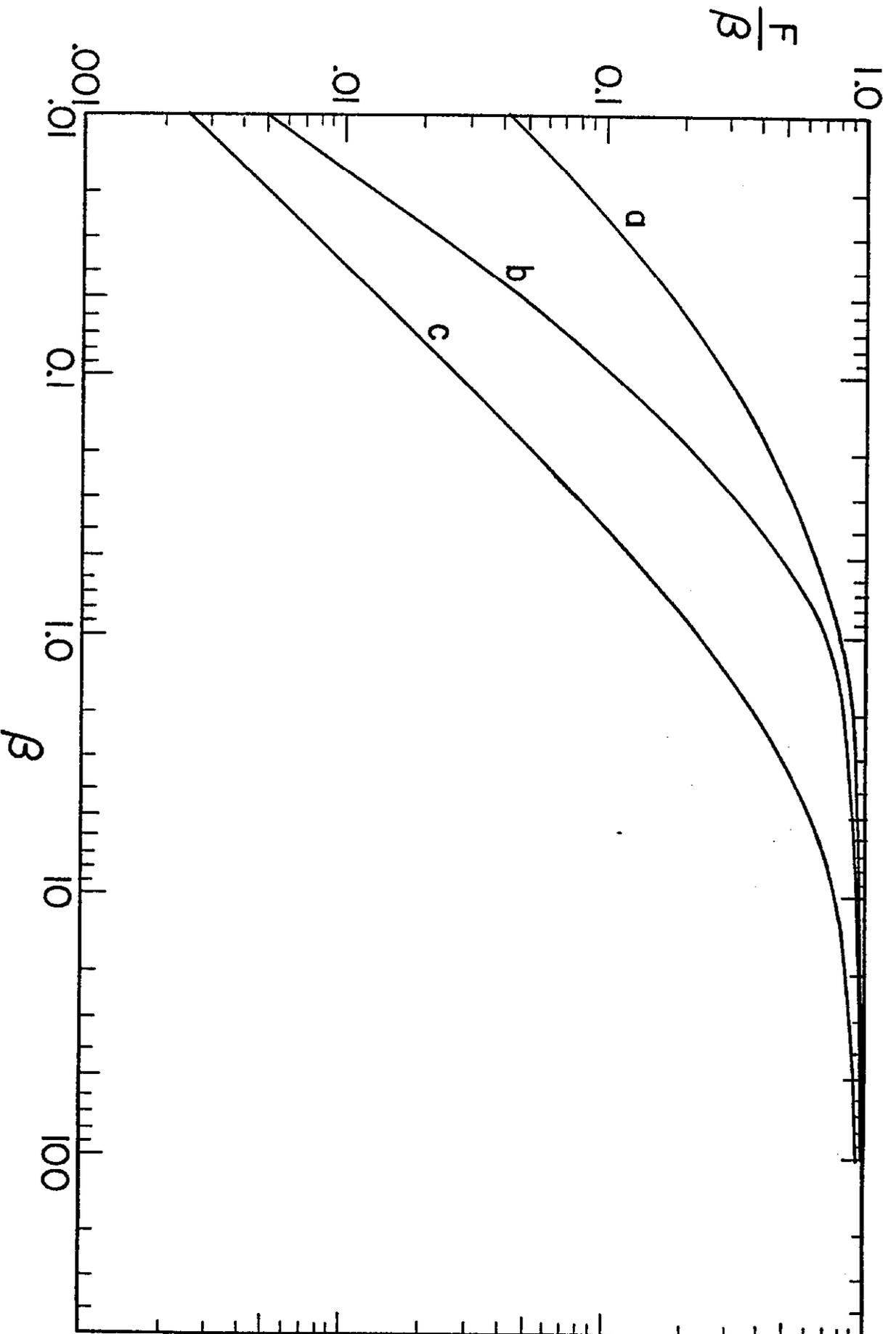


Fig. 12

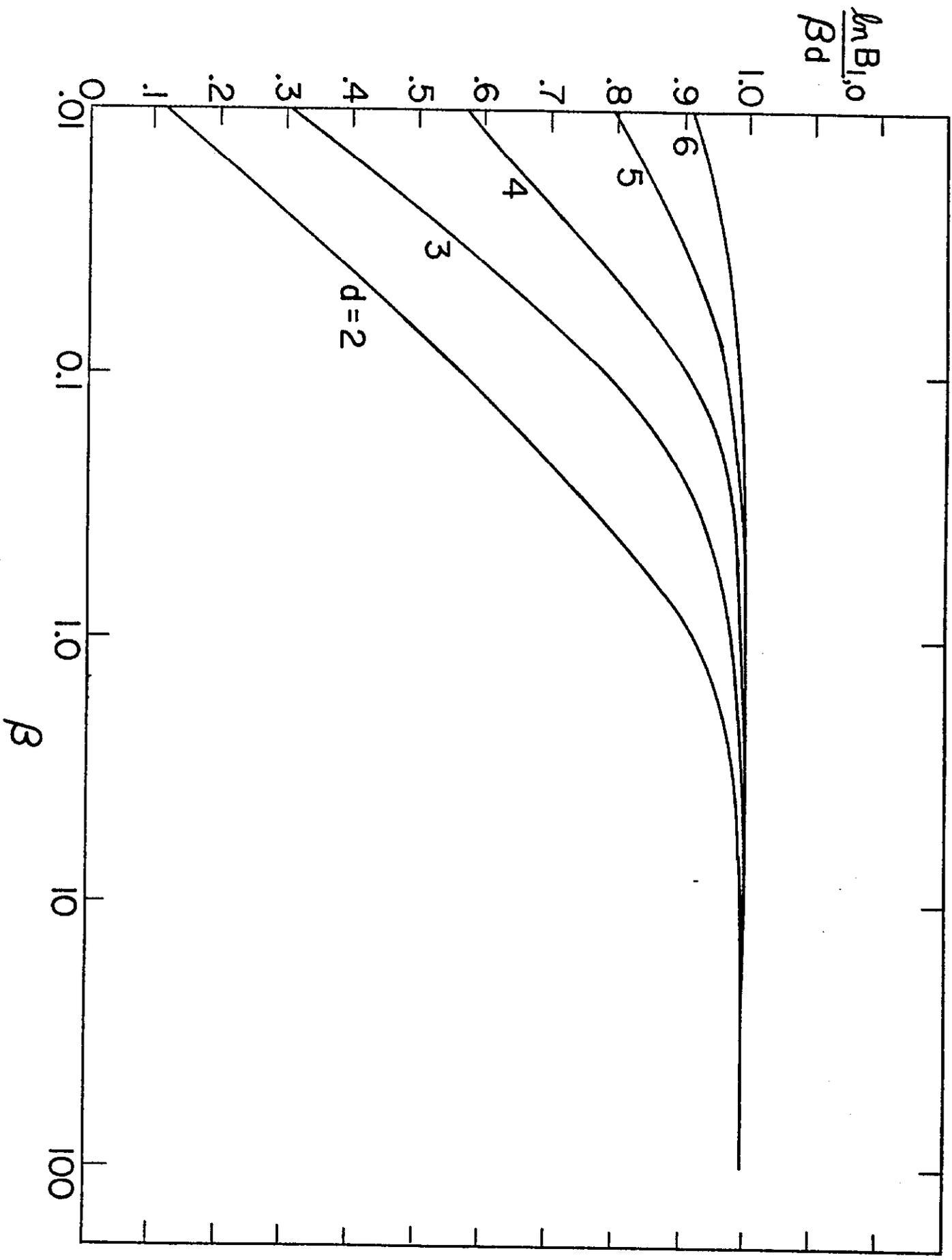


Fig. 13

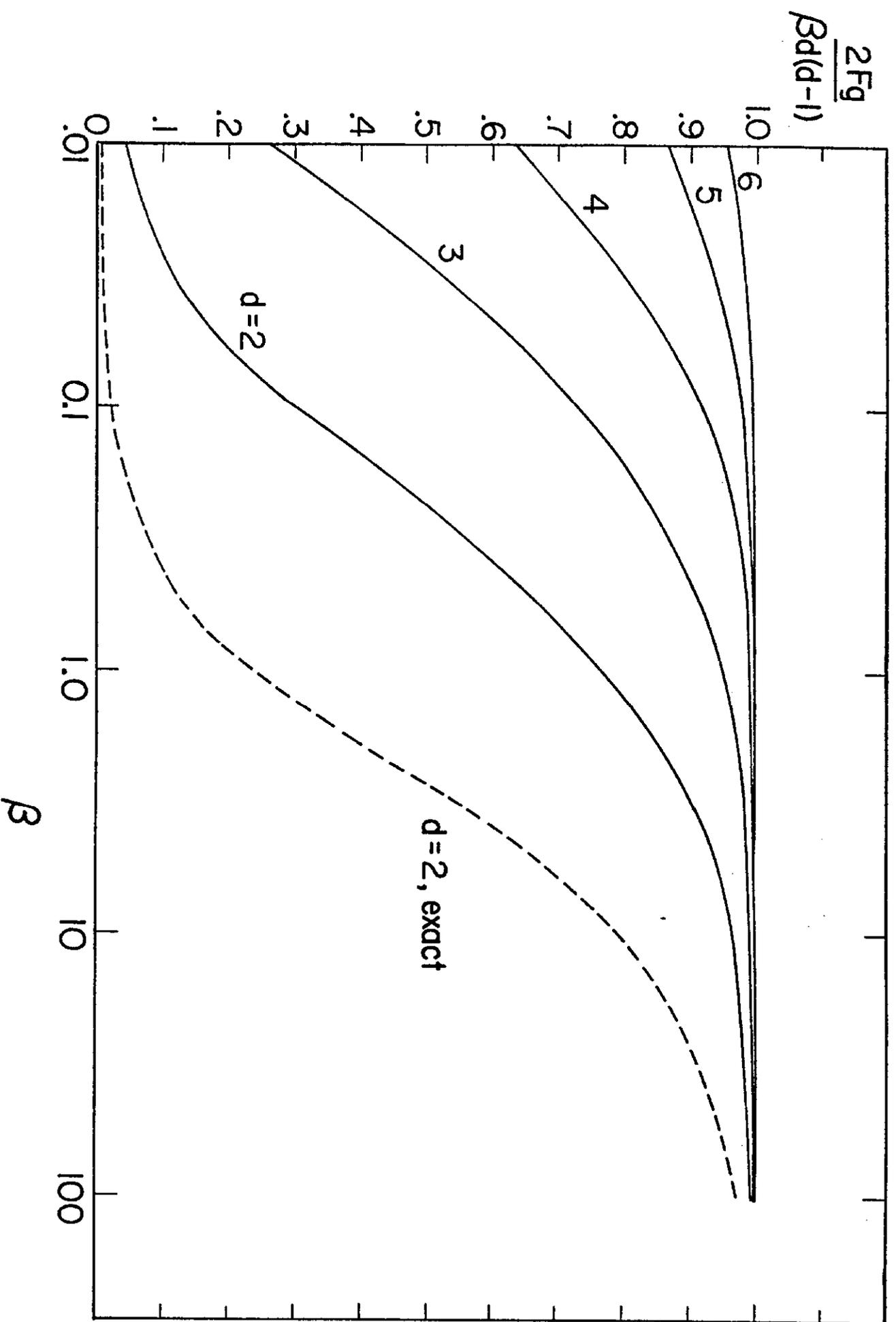
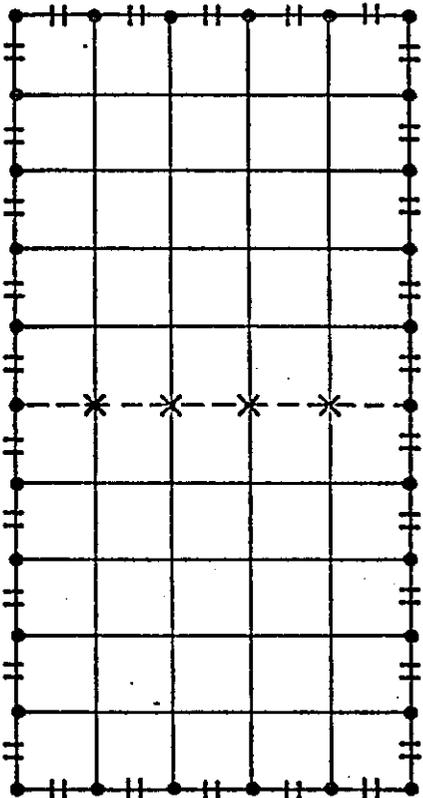


Fig. 14



- =  $\lambda_1, \lambda_2$
- #— =  $b_1, b_2$
- =  $b_I$
- x =  $s_I$
- =  $s_1, s_2$

Fig. 15