EXTRAPOLATED RENORMALIZATION GROUP CALCULATION OF THE SURFACE TENSION IN SQUARE-LATTICE ISING MODEL

by

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ABSTRACT

By using self-dual clusters (whose sizes are characterized by the numbers b=2,3,4,5) we calculate within a real space renormalization group framework, the *longitudinal* surface tension of the square-lattice first-neighbour $\frac{1}{2}$-spin ferromagnetic Ising model. The exact critical temperature T_c is recovered for any value of b; the exact assymptotic behaviour of the surface tension in the limit of low temperatures is *analytically* recovered; the approximate correlation length critical exponents monotonically tend towards the exact value $\nu=1$ (which, at two dimensions, coincides with the surface tension critical exponent μ) for increasingly large cells; the same behaviour is remarked in what concerns the approximate values for the surface tension amplitude in the limit $T \to T_c$. We develop four different numerical procedures for extrapolating to $b \to \infty$ the renormalization group results for the surface tension, and quite satisfactory agreement is obtained with Onsager's exact expression (error varying from zero to a few percent on the *whole* temperature domain).

Furthermore we compare the set of RG surface tensions with a set of *biased* surface tensions (associated to appropriate misfit seams), and find only fortuitous coincidence among them.

I INTRODUCTION

Since Onsager's exact calculation[1] in 1944 of the longitudinal surface tension in the square-lattice Ising model, a certain amount of work has been dedicated to related topics, which no doubt enlighten the important phenomena concerning the interface separating two equilibrium phases. It is clear that if we consider let us say a ferromagnetic d-dimensional Ising model, the surface tension γ (for a convenient definition of d-dimensional surface tension see Ref. (2) and references therein; also Ref. (3)) will in general depend on the orientation of the *misfit seam* (with antiferromagnetic bonds). This dependence has been discussed in various cases[3,5], either directly on $\gamma(T)$ or on the surface entropy $(-d\gamma/dT)$. However, essentially because of the divergence of the correlation length ξ, isotropy should emerge in the neighbourhood of the critical temperature T_c, i.e. if we define $\gamma(T) \sim A(T_c-T)^{\mu}$, in the limit $(T_c-T)/T_c \to 0$, we expect[3,6-8] that A and μ are the same for all orientations of the seam. These facts are exhibited by exact results[8,9] for the *diagonal* surface tension in square lattice and similar systems. Furthermore, scaling arguments applied on the surface tension (first subextensive assymptotic correction of the thermodynamical free energy of the bulk system) lead[10-16] to *constant* $\xi^{d-1}\gamma$ in the neighbourhood of T_c, hence (by using the definition $\xi \sim |T-T_c|^{-\nu}$) $\mu=(d-1)\nu$ (therefore we expect, for two-dimensional Ising systems, $\mu=\nu=1$).

The renormalization group (RG) techniques[17,18] were initially devised for the calculation of the critical temperature (fixed point) and exponents (eigenvalues); however, if appropriately used, they lead to satisfactory results for the *whole* domain of temperatures (a pedagogical example is presented in Ref. (19)). Within this context they have been used[15,20,21] for the calculation of the surface tension. In the present work we calculate, within a real space framework similar to that of the Oliveira et al[15], the longitudinal surface tension

of the square-lattice first-neighbour $\frac{1}{2}$ - spin ferromagnetic Ising model. However we use, in contrast with that work, *self-dual* clusters (whose sizes are characterized by the numbers b=2,3,4,5), which are particularly well adapted[22-27] to RG discussion of critical phenomena (phase transition as well as bond percolation) in the square lattice, as they lead to the *exact* critical temperature T_c (or critical bond percolation probability p_c), *whatever be the cluster size*. The tendency towards Onsager's exact result for the surface tension is clearly exhibited for increasingly large clusters.

In Section II we develop the RG framework and present the numerical results. In Section III we present four different procedures (the *multiple extrapolation procedure* (MEP), the *single extrapolation procedure* (SEP), the *single multiple extrapolation procedure* (SMEP), and finally the *multiple single extrapolation procedure* (MSEP)) for extrapolating the RG results to $b \to \infty$.

Finally in Section IV, and within the purpose of testing an hypothesis concerning our RG results for the surface entropy (or thermal slope of the surface tension) at vanishing temperature, we are led to propose a family of *biased* misfit seams whose main consequences on the surface tension are analysed.

II REAL SPACE RENORMALIZATION GROUP TREATMENT

II.1 Self-dual clusters

Let us first of all present the family of self-dual clusters (see Fig. 1) we shall adopt for the square lattice. To each (internal and terminal) node of the clusters we associate a $\frac{1}{2}$ - spin, and to each of their bonds a *thermal transmissivity**,

$$t \equiv \text{th}\ \beta J \quad , \tag{1}$$

where $\beta \equiv 1/k_B T$ and $J > 0$ is the first-neighbour Ising exchange integral. Next we associate to each cluster an *equivalent* transmissivity $t_b \equiv R_b(t)$, which is obtained through the partial trace on the *internal* nodes. This trace can be performed, with considerable operational advantages, by using the recently introduced[29] "break-collapse" method. The results are listed below**:

$$t_1 \equiv R_1(t) = t$$

$$t_2 \equiv R_2(t) = \frac{2t^2 + 2t^3}{1 + 2t^3 + t^4}$$

$$\sim 2t^2 + 2t^3 \qquad \text{if } t \to 0$$

$$\sim 1 - (1-t)^2 - \frac{3}{2}(1-t)^3 \qquad \text{if } t \to 1$$

$$t_3 \equiv R_3(t) = \frac{3t^3+8t^4+10t^5+8t^6+12t^7+16t^8+6t^9+t^{11}}{1+4t^3+4t^4+4t^5+14t^6+20t^7+11t^8+4t^9+2t^{10}}$$

$$\sim 3t^3 + 8t^4 \qquad \text{if } t \to 0$$

$$\sim 1 - \frac{3}{4}(1-t)^3 - \frac{17}{8}(1-t)^4 \qquad \text{if } t \to 1$$

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* Though these words have been introduced recently by two of us[26,27], this variable has been used since long before[24,28].

** $R_2(t)$ has previously been calculated in Refs. (23,24,26,27).

$$t_4 \equiv R_4(t) = \{ 4t^4+18t^5+42t^6+70t^7+120t^8+232t^9+362t^{10}+462t^{11} +600t^{12}+716t^{13}+638t^{14}+418t^{15}+232t^{16}+120t^{17}+46t^{18} +10t^{19}+4t^{20}+2t^{21}\} / \{ 1+6t^3+10t^4+8t^5+30t^6+68t^7 +102t^8+214t^9+390t^{10}+544t^{11}+ 616t^{12}+622t^{13}+618t^{14} +460t^{15}+225t^{16}+114t^{17}+50t^{18}+10t^{19}+6t^{20}+2t^{21}\}$$

$$\sim 4t^4 + 18t^5 \qquad \text{if} \quad t \to 0$$

$$\sim 1 - \frac{1}{2}(1-t)^4 - \frac{17}{8}(1-t)^5 \qquad \text{if} \quad t \to 1$$

$$t_5 \equiv R_5(t) = \{ 5t^5+32t^6+108t^7+256t^8+582t^9+1300t^{10}+2829t^{11} +5396t^{12}+9756t^{13}+17116t^{14}+28678t^{15}+44716t^{16} +65514t^{17}+90840t^{18}+114171t^{19}+129800t^{20}+133338t^{21} +123288t^{22}+103312t^{23}+75032t^{24}+ 47834t^{25}+28356t^{26} +14611t^{27}+ 6820t^{28}+ 3012t^{29}+1196t^{30}+478t^{31}+124t^{32} +54t^{33}+16t^{34}+5t^{35}+t^{37}\} / \{ 1+8t^3+18t^4+12t^5+59t^6 +160t^7+284t^8+520t^9+1242t^{10}+2496t^{11}+4880t^{12}+9640t^{13} +17565t^{14}+29396t^{15}+ 45326t^{16}+66636t^{17}+ 90744t^{18} +112284t^{19}+128012t^{20}+133628t^{21}+125285t^{22}+102824t^{23} +74540t^{24}+48704t^{25}+28098t^{26}+14552t^{27}+6864t^{28}+2960t^{29} +1187t^{30}+420t^{31}+169t^{32}+44t^{33}+12t^{34}+4t^{35}+2t^{36}\}$$

$$\sim 5t^5 + 32t^6 \qquad \text{if} \quad t \to 0$$

$$\sim 1 - \frac{5}{16}(1-t)^5 - \frac{57}{32}(1-t)^6 \qquad \text{if} \quad t \to 1$$

The functions $R_b(t)$ have a remarkable property (due to the self-duality of the clusters): $R_b(t_c) = t_c \quad \forall b$ where $t_c \equiv \sqrt{2} - 1$, hence $K_B Tc/J = 2/\text{argsh } 1 \simeq 2.269$, which is the *exact* critical temperature[30] for square lattice. Furthermore if we recall[26] that the equivalent transmissivities for series and parallel arrays of n bonds are respectively given by

$$t_s = t^n \tag{2}$$

$$\frac{1 - t_p}{1 + t_p} = \left(\frac{1 - t}{1 + t} \right)^n \tag{3}$$

it is straightfoward to calculate the assymptotic behaviors of t_b for $t \to 0$ and $t \to 1$. Let us first work out the limit $t \to 0$: such situation our cluster becomes equivalent to b parallel bonds, each of them consisting in b bonds (of transmissivity t) in series, therefore

$$\frac{1 - t_b}{1 + t_b} \sim \left[\frac{1 - t^b}{1 + t^b}\right]^b \sim 1 - 2b\, t^b$$

hence $t_b \equiv R_b(t) \sim b\, t^b$ if $t \to 0$ (4)

In the other limit, i.e. $t \to 1$, the cluster becomes equivalent to b bonds in series, each of them consisting of b parallel bonds of transmissivity t, therefore

$$t_b \equiv R_b(t) \sim \left[\frac{1 - \left[\frac{1 - t}{1 + t}\right]^b}{1 + \left[\frac{1 - t}{1 + t}\right]^b}\right]^b \sim$$

$$\sim 1 - \frac{b}{2^{b-1}}(1-t)^b \qquad \text{if} \quad t \to 1 \qquad (5)$$

Furthermore, by using the techniques indicated in Ref. (29) is nothing but tedious to calculate the next assymptotic corrections, so expressions (4) and (5) are extended as follows:

$$t_b \equiv R_b(t) \sim bt^b + 2(b-1)^2\, t^{b+1} \qquad \text{if} \quad t \to 0 \qquad (4')$$

$$\sim 1 - \frac{b}{2^{b-1}}(1-t)^b - \frac{b^2+2(b-1)^2}{2^b}(1-t)^{b+1} \qquad (5')$$

if $t \to 1$

Let us stress that through the dual transformation[26,27] $t \to t^D \equiv (1-t)/(1+t)$ we can pass from (4') to (5') and viceversa.

Within the RG framework we shall now assume the following recursive relation (which renormalizes the square lattice into itself through an expansion factor b/b'):

$$R_{b'}(t') = R_b(t) \qquad (b=2,3,4,5;\ b'=1,2,\ldots,b-1) \tag{6}$$

This relation admits two trivial fixed points (t*=0 and t*=1) and a physically relevant one: $t^*=t_c$, hence the present RG leads to the *exact* critical temperature for *any* choice of (b,b'). The approximate critical exponent $\nu_{b,b'}$ is given by[24-27]

$$\nu_{b,b'} = \frac{\ln b/b'}{\ln \lambda_{b,b'}} \tag{7}$$

$$\lambda_{b,b'} \equiv \left\{ \frac{d\,R_b(t)}{dt} \Big/ \frac{d\,R_{b'}(t)}{dt} \right\}_{t=t_c}$$

and the results for b'=1 and b=2,3,4,5 are indicated in Table 1. A preliminar analysis of the results for b'=2,3,4 showed that the behaviour of $\nu_{b,b'}$ is less monotonous than it is for b'=1.

II.2 Longitudinal Surface Tension

Let us now turn our attention onto a central problem : what family of clusters are we going to use in order to simulate (within a *finite* cluster) the macroscopic misfit seam (see Fig. 2(a)) which generates the surface tension? Our proposal is indicated in Fig. 2(b): to each of those *misfitting* clusters is associated an equivalent transmissivity $Q_b(t)$, and the RG recursive relations will now be

$$Q_{b'}(t') = Q_b(t) \qquad (b=2,3,4,5;\ b'=1,2,\ldots,b-1) \tag{8}$$

However it is straightfoward to verify a peculiar property, namely

$$Q_b(t) = - R_b(t) \qquad \forall\, b \qquad \forall\, t$$

Therefore the relations (8) become, after cancellation of the minus sign on both sides of the equation, the same relations (6) we had before!

We must now write down the RG equation for the surface tension γ : following along the lines of Ref. (15), this will be given by

$$(b')^{d-1} \quad \frac{\gamma'}{T'} = b^{d-1} \quad \frac{\gamma}{T} \qquad (9)$$

hence, in our case (d=2),

$$\gamma' = \frac{b}{b'} \gamma \frac{T'}{T} \qquad (9')$$

Furthermore equation (6) can be rewritten:

$$R_{b'}(\text{th } J/K_B T') = R_b(\text{th } J/K_B T) \qquad (10)$$

where definition (1) was used. Once we make a choice of (b,b'), relations (9') and (10) close the problem, as they provide a RG recursive transformation of the T-γ-space (or equivalently t-γ) onto itself. This set of equations admits two physically important fixed points, namely ($T=T_c$, $\gamma=0$) and ($T=0$, $\gamma=\gamma_o$) where γ_o will be arbitrarily chosen equal to unity (i.e. we shall work with a *reduced* longitudinal surface tension which equals unity at vanishing temperature); the former is an unstable fixed point, the latter is a stable one. The flow diagram (in both T-γ and t-γ spaces) is schematically indicated in Fig. 3. In order to find out the behaviour in the vicinity of the two fixed points, we must consider the Jacobian matrix

$$\begin{pmatrix} \frac{\partial T'}{\partial T} & \frac{\partial T'}{\partial \gamma} \\ \frac{\partial \gamma'}{\partial T} & \frac{\partial \gamma'}{\partial \gamma} \end{pmatrix} \qquad (11)$$

where

$$\frac{\partial T'}{\partial T} = \left(\frac{T'}{T}\right)^2 \frac{ch^2\, J/k_B T'}{ch^2\, J/k_B T} \frac{d\, R_b/dt}{d\, R_{b'}/dt'}$$

$$= \left(\frac{T'}{T}\right)^2 \frac{1 - t^2}{1 - t'^2} \frac{d\, R_b/dt}{d\, R_{b'}/dt'} \qquad (12.a)$$

$$\frac{\partial T'}{\partial \gamma} = 0 \qquad (12.b)$$

$$\frac{\partial \gamma'}{\partial T} = \frac{b}{b'} \frac{\gamma}{T} \left\{\frac{dT'}{dT} - \frac{T'}{T}\right\} \qquad (12.c)$$

$$\frac{\partial \gamma'}{\partial \gamma} = \frac{b}{b'} \frac{T'}{T} \qquad (12.d)$$

In the critical fixed point ($T=T_c$) the Jacobian (11) becomes

$$\begin{pmatrix} \lambda_{b,b'} & 0 \\ 0 & b/b' \end{pmatrix}$$

The fact that both eigenvalues are bigger than unity exhibits the instability of that fixed point; the eigenvectors (1 0) and (0 1) indicate the privileged flow directions (see Fig. 3(a)). Furthermore the relation

$$\frac{1}{\nu} = \frac{\ln \lambda_{b,b'}}{\ln(b/b')}$$

is reobtained, and

$$\frac{\mu}{\nu} = \frac{\ln(b/b')}{\ln(b/b')} = 1 \quad ,$$

the *scaling law* $\mu=(d-1)\nu$ being thus *preserved* by our RG. We remark also the existence of a third fixed point admitted by equation (9'), namely $(T=\infty,\gamma=0)$ or equivalently $(t=0,\gamma=0)$; if we start, for *any* $T>T_c$, the recurrence procedure with $\gamma\neq 0$, we obtain an unphysical divergent surface tension in the limit $T \to \infty$, hence γ must identically vanish for *all* temperatures higher than T_c: the well known exact result is recovered on renormalization group grounds.

Let us now focus the vanishing temperature fixed point: its discussion is somehow delicate because of an indeterminacy that appears in the limit $T \to 0$. Let us first of all rewrite equation (6) as follows:

$$b' e^{-2b' J/k_B T'} \sim b\, e^{-2b\, J/k_B T} \qquad (13)$$

where we have used the assymptotic behavior (5) and also the fact that $\text{th}\, x \sim 1 - e^{-2x}$ if $x \to 0$. From (13) comes*

$$\frac{T'}{T} \sim \frac{b'}{b}\left[1 + \frac{k_B T}{2bJ} \ln(b/b')\right] \qquad (13')$$

and

$$\frac{dT'}{dT} \sim \frac{b'}{b}\left[1 + \frac{k_B T}{bJ} \ln(b/b')\right] \qquad (13'')$$

and the Jacobian is finally given by

$$\begin{pmatrix} b'/b & 0 \\ \dfrac{k_B}{J}\dfrac{\ln(b/b')}{2b} & 1 \end{pmatrix}$$

whose eigenvalues are 1 (marginal case) and b'/b (smaller than unity, exhibiting therefore the stability of this fixed point,

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* On rigorous grounds, the operations (derivatives, substractions, etc) we are performing across the equivalence sign ($\sim$) demand more detailed justification than presented in this derivation.

at least in one particular direction), respectively associated to the eigenvectors (0,1) and (u,v) with

$$\frac{v}{u} = - \frac{k_B}{J} \frac{\ln(b/b')}{2(b-b')} \tag{14}$$

which gives us the initial slope of the approximate surface tension $\gamma_{b,b'}(T)$, i.e.

$$\gamma_{b,b'}(T) \sim 1 - \frac{\ln(b/b')}{2(b-b')} \frac{k_B T}{J} \quad \text{if} \quad k_B T/J \to 0 \tag{15}$$

Let us remark that for $b' < b$ we have that

$$\frac{\ln(b/b')}{b(1-b'/b)} \leq \frac{1}{b}$$

therefore the slope $(d\gamma_{b,b'}/dT)_{T=0}$ vanishes* in the limit $b \to \infty$, as it ought to be for a RG calculation which is expected to converge towards Onsager's exact result[1] (see also Table 1 and Figs. 4, 5 and 6)

$$\gamma_L = 1 - \frac{k_B T}{2J} \ln \coth \frac{J}{k_B T} \tag{16}$$

$$\sim 1 - \frac{k_B T}{J} e^{-2J/k_B T} \quad \text{if} \quad k_B T/J \to 0 \tag{16'}$$

$$\sim 2 \left(1 - \frac{T}{Tc}\right) \quad \text{if} \quad \frac{T_c - T}{T_c} \to 0 \tag{16''}$$

We shall now take advantage of the assymptotic behaviour (5') in order to extend relation (15) up to the next assymptotic correction. Through use of relations (5') and (10) we obtain, in the limit $T \to 0$,

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* If $b'=1$ the slope vanishes as $\ln b/b$ whereas if $b'=b-1$ it vanishes as $1/b$, this is to say more rapidly. We have observed this acceleration of the convergence (if $b'=b-1$ instead of being fixed) in a considerable variety of similar problems.

$$F(T';b') \sim F(T;b) \qquad (5'')$$

where

$$F(T;b) \equiv \frac{k_B T/J}{b\left[1 - \frac{\ln b}{2b}\frac{k_B T}{J} - \left(\frac{b-1}{b}\right)^2 \frac{k_B T}{J} e^{-2J/k_B T}\right]} \qquad \forall T, \forall b$$

Finally if we make use of the recursive relation (9') we obtain

$$\gamma_{b,b'} \sim 1 - \frac{\ln(b/b')}{2(b-b')}\frac{k_B T}{J} - \left(\frac{b-1}{b}\right)^2 \frac{k_B T}{J} e^{-2J/k_B T} \qquad (15')$$

$$\text{if} \quad k_B T/J \to 0$$

We verify that in the limit $b \to \infty$ (with $b' < b$) we recover that *exact* assymptotic behaviour (16') (see also Table 1 and Figs. 4, 5 and 6).

Let us now operationally describe the numerical method we have followed for determining $\gamma_{b,b'}$ for intermediate temperatures. First of all we choose an *arbitrary* temperature T_o lower than T_c, then we use the recursive relation (10), this is to say

$$R_{b'}(\text{th } J/k_B T_{j+1}) = R_b(\text{th } J/k_B T_j) \quad (j=0,1,2,\ldots,n-1) \quad (10')$$

to obtain the sequence of decreasing temperatures $T_1, T_2, \ldots, T_j, \ldots T_n$ where we *arbitrarily* stop at the n-th step with the unique restriction that T_n be *close enough to zero*. Next we calculate the surface tension γ_n associated to T_n by using (15') (or just (15)), and finally we run backwards through relation (9'), i.e.

$$\gamma_j = \frac{b'}{b}\frac{T_j}{T_{j+1}}\gamma_{j+1} \qquad (j=n-1,\ldots,1,0) \qquad (9'')$$

in order to obtain the sequence of decreasing surface tensions $\gamma_{n-1}, \ldots, \gamma_o$ which closes the procedure. An example of such a run is presented in Table 2. The results we have obtained for $b'=1$ and $b=2,3,4,5$ are indicated in Table 1 and also in Figs. 4, 5 and 6. Furthermore if we define $A_{b,b'}$ through the RG result

$$\gamma_{b,b'} \sim A_{b,b'} \left(1 - \frac{T}{Tc}\right)^{\nu_{b,b'}} \quad \text{if} \quad \frac{Tc-T}{Tc} \to 0$$

and denote by $B_{b,b'}$ the positive pure number obtained by multiplying $(k_B T_c/J)$ by the slope of a straight line which starting from the point $(T=Tc,\ \gamma=0)$ tangentially touches the curve $\gamma_{b,b'}(T)$ (see Fig. 4), the present RG procedure enables us to obtain numerical estimates for both coefficients (see Table 1 and Fig. 6), which are expected to tend towards the value 2, according to (16'').

Let us conclude this Section by saying that the results presented in Figs. 4, 5 and 6 and in Table 1 leave no great doubt about the fair convergence of the present RG approximations towards the exact Onsager's expression for the longitudinal surface tension in the square lattice Ising model. In the following section we present four different extrapolation procedures for obtaining an estimate of the $b \to \infty$ limit of the RG results.

III EXTRAPOLATION PROCEDURES

III.1 Multiple extrapolation procedure (MEP)

This procedure is a very simple one: for *any* given temperature, we linearly extrapolate to the origin $\gamma_{b,1}$ vs. b^{-1}. The choice of the b^{-1}-variable essentially comes from the fact that it is quite natural to expect that the temperature scales as $b^{-1/\nu}$, hence the surface tension should scale as $b^{-\mu/\nu}$; but at two dimensions, $\mu/\nu = 1$. As this is basically a finite but *large* size scaling law[31], there is no particular reason for expecting it to hold even for *small* values of b (as in our present case); nevertheless this frequently happens within a reasonable accuracy (see, for example, Refs. (32) and (33)); a measure of the credibility of such extrapolation in every particular case is given by how much the linear correlation factor approaches unity. With the notation $\gamma^M(T)$ for the surface tension obtained through the MEP, we present our results in Fig. 5 (the linear correlation factor grows from about 0.998 at T=0 to unity at $T=T_c$. The high error (with respect to Onsager's exact result γ_L, given in equation (16)) obtained in the immediate neighbourhood of T_c comes from the fact that $\nu_{b,1}$ is — though quite close — not *strictly* equal to ν. We remark that the MEP globally decreases the error by about a factor 2. If we respectively note ν_M, A_M and B_M the critical exponent and amplitudes of $\nu^M(T)$ (defined in total analogy with $\nu_{b,1}$, $A_{b,1}$ and $B_{b,1}$) in the neighbourhood of T_c, our results are $\nu_M \simeq 1.069$, $A_M \simeq 1.83$ and $B_M \simeq 2$.

Let us finally remark that more complex situations might appear in similar problems, in the sense that the critical temperatures $\{T_{b,1}\}$ might be not one and the same for all b. In such cases it can be convenient, before applying the MEP, to reduce the temperature axis in order to force all the critical points to coincide*.

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* Another possibility might be to work on constant γ straight lines instead of constant T straight lines, or even on constant γ/T lines (see Ref. (33)).

III.2 Single extrapolation procedure (SEP)

We present here a quite different extrapolation approach which applies to every *single* function $\gamma_{b,1}(T)$, which can be used for *other* lattices, dimensionalities, models (such as XY or Heisenberg) and equations of state (such as the spontaneous magnetization), and which takes advantage from the fact that, for a large number of cases, exact or almost exact values are available for the critical temperature, the set of critical exponents and the slopes at vanishing temperature. To be more specific, in our present case we shall use the following data: the RG value $T_{b,1}$ for the critical temperature (the present self-dual clusters lead to $T_{b,1}=T_c$ $\forall b$, but for the sake of generality we prefer to maintain here $T_{b,1}$), the RG exponent $\nu_{b,1}$, the RG slope $C_{b,1} \equiv -\frac{J}{k_B}(d\gamma_{b,1}/dT)_{T=0} = \frac{\ln b}{2(b-1)}$, the *exact* values for T_c, ν and the slope $C_L \equiv -\frac{J}{k_B}(d\gamma_L/dT)_{T=0}=0$. We work here with a *reduced* surface tension, otherwise we also ought to assume the knowledge of the exact value $\gamma_L(0)$.

We introduce next the variables

$$x_{b,1}(T) \equiv \left[1 - \frac{T}{T_{b,1}}\right]^{\nu_{b,1}} \qquad (0 \leq T \leq T_{b,1}) \qquad (17)$$

$$x(T) \equiv \left[1 - \frac{T}{T_c}\right]^{\nu} \qquad (0 \leq T \leq T_c) \qquad (18)$$

and the relation

$$\gamma^s_{b,1} = f_{b,1}(x)\,\gamma_{b,1} \qquad (19)$$

among the $b\to\infty$ SEP proposal $\gamma^s_{b,1}$ generated by $\gamma_{b,1}$, and the *correcting function* $f_{b,1}(x)$ which remains to be found. For $T=0$ (hence $x=x_{b,1}=1$) we want $\gamma^s_{b,1}$ to equal unity (because this is

the exact result for γ_L), and as it is so for $\gamma_{b,1}$ it comes that

$$f_{b,1}(1) = 1 \tag{20}$$

Furthermore, relation (19) implies

$$\frac{d\gamma^s_{b,1}}{dT} = \frac{df_{b,1}(x)}{dx}\,\frac{dx}{dT}\,\gamma_{b,1} + f_{b,1}(x)\,\frac{d\gamma_{b,1}}{dT}$$

which becomes, at T=0,

$$\left.\frac{d\gamma^s_{b,1}}{dT}\right|_{T=0} = -\frac{\nu}{T_c}\left.\frac{df_{b,1}(x)}{dx}\right|_{x=1} + \left.\frac{d\gamma_{b,1}}{dT}\right|_{T=0}$$

where we have used the relations (18) and (20). In other words,

$$\left.\frac{df_{b,1}}{dx}\right|_{x=1} = \frac{kT_c/J}{\nu}\,(C_L - C_{b,1}) \tag{21}$$

and, in the present particular case,

$$\left.\frac{df_{b,1}}{dx}\right|_{x=1} = \frac{-1}{\text{argsh } 1}\,\frac{\ln b}{(b-1)} \tag{21'}$$

Moreover, the correcting function $f_{b,1}(x)$ has been introduced mainly to redress the possibly wrong thermal slope of $\gamma_{b,1}$ at T=0, and we want its effects to gradually relax while approaching T_c (hence x=0); it seems therefore reasonable to demand

$$\left.\frac{df_{b,1}(x)}{dx}\right|_{x=0} = 0 \tag{22}$$

This assumption (as well as the forthcoming ones) is strongly supported *a posteriori* by the results it leads to. The simplest

function which simultaneously satisfies restrictions (20), (21) and (22) is the parabola

$$f_{b,l}(x) = \left[1 + \frac{k_B T_c/J}{2\nu}(C_{b,l}-C_L)\right] - \frac{k_B T_c/J}{2\nu}(C_{b-l}-C_L)\, x^2 \qquad (23)$$

and in the present particular case

$$f_{b,l}(x) = \left[1 + \frac{1}{2\ \mathrm{argsh}\ 1}\,\frac{\ln b}{b-1}\right] - \frac{1}{2\ \mathrm{argsh}\ 1}\,\frac{\ln b}{b-1}\, x^2 \qquad (23')$$

Now that the correcting function is uniquely determined the problem might seem closed, but it is not, because we have not yet precised the *arguments* of $\gamma^s_{b,l}$ and $\gamma_{b,l}$ in relation (19). We will postulate that this relation connects $\gamma^s_{b,l}(T)$ with $\gamma_{b,l}(T')$ where

$$x_{b,l}(T') = x(T) \qquad (24)$$

in other words, relation (19) must be understood as follows:

$$\gamma^s_{b,l}(T) = f_{b,l}\left[\left(1 - \frac{T}{T_c}\right)^{\nu}\right]\gamma_{b,l}\left[T_{b,l}\left[1 - \left(1 - \frac{T}{T_c}\right)^{\nu/\nu_{b,l}}\right]\right] \qquad (19')$$

This is clearly the central assumption of the SEP and it states that a kind of *law of corresponding states* holds for the RG approximate functions $\{\gamma_{b,l}(T)\}$ associated to different cluster sizes. We remark that relation (19') becomes identically satisfied in the limit $b\to\infty$, assuming that $T_{b,l}\to T_c$, $\nu_{b,l}\to\nu$ and $C_{b,l}\to C_L$ (to be more precise, if $\gamma_{b,l}(T)$ regularly tends towards $\gamma_L(T)$). Furthermore, we can say that the definitions (17) and (18) (together with assumption (24)) somehow cover up the criticality of the problem, and the simple parabolic - in the x-variable - form (23) we have adopted for the correcting function becomes more natural.

The whole SEP is quite satisfactorily supported by the results to which it leads. We have represented in Fig. 7 the error $(\gamma^s_{b,1}-\gamma_L)/\gamma_L$ associated to the set $\{\gamma_{b,1}\}$ for b=2,3,4,5: discrepancies remain inferior to 3% over the *whole* domain of temperatures for all values of b (error inferior to 1% for b=5). In order to illustrate the validity (within a few percent) of the proposal (23) for the correcting function $f_{b,1}(x)$, we have represented, in Fig. 8, the *worst* of them (namely $f_{2,1}(x)$) together with the *exact* correcting function $\gamma_L(T)/\gamma_{2,1}(T')$.

From our standpoint the main interest of the SEP comes from the fact that, by using only commonly available information (T_c,ν, etc) and one RG approximate result, it is possible to obtain a curve which is satisfactory over the whole domain of temperatures.

III.3 Mixed extrapolation procedures (SMEP and MSEP)

Let us combine here the SEP and the MEP by applying both of them, one after the other, onto the set of RG functions $\{\gamma_{b,1}(T)\}$. The *single multiple extrapolation procedure* (SMEP) consists in the application of the SEP onto the result $\gamma^M(T)$ by using its own values for the critical temperature T_M (in our case $T_M=T_c$) and exponent ν_M and the thermal slope C_M for vanishing temperature. The error of $\gamma^{SM}(T)$ (result obtained through the SMEP) is represented in Fig. 7, and remains, as for the $\{\gamma^s_{b,1}(T)\}$, inferior to a few percent over the whole domain of temperatures (it is smaller than 0.4% for temperatures smaller than let us say $\frac{3}{4}T_c$).

The *multiple single extrapolation procedure* (MSEP) consists in the application of the MEP to the functions $\{\gamma^s_{b,1}(T)\}$, i.e. to linearly extrapolate to the origin $\gamma^s_{b,1}(T)$ vs. b^{-1} for fixed temperatures. Oncemore the result, which will be noted $\gamma^{MS}(T)$ and whose error is represented in Fig. 7,

is quite satisfactory (particularly for temperatures below let us say $\frac{3}{4}T_c$, where it is smaller than 0.4%); the linear correlation factor approaches 1 in the vicinity of $k_B T/J \simeq 1$ but quickly decreases (down to let us say 0.95) when $T=0$ or $T=T_c$ are approached.

IV BIASED SURFACE TENSION

The center of our discussion has been until now the *longitudinal* surface tension; let us now focuse the surface tension $\gamma_\theta(T)$ associated to an arbitrary biased misfit seam which makes an angle θ with let us say the x-axis of the lattice. Clearly

$$\gamma_o(T) = \gamma_L(T) \qquad (25)$$

and

$$\gamma_{\pi/4}(T) = \gamma_D(T) \qquad (26)$$

where γ_L is given by (16) and $\gamma_D(T)$ is the exact *diagonal* surface tension given[8] by

$$\gamma_D = \frac{k_B T}{J\sqrt{2}} \ln \operatorname{sh} \frac{2J}{k_B T} \qquad (27)$$

$$\sim \sqrt{2} \left\{ 1 - \frac{\ln 2}{2} \frac{k_B T}{J} \right\} \quad \text{if} \quad k_B T/J \to 0 \qquad (27')$$

$$\sim 2 \frac{T_c - T}{T_c} \quad \text{if} \quad \frac{T_c - T}{T_c} \to 0 \qquad (27'')$$

We notice that the initial slope of the reduced diagonal tension $\gamma_D/\sqrt{2}$ is *precisely the same* as that of the RG tension $\gamma_{2,1}$ (see the assymptotic behaviour (15)). This fact seemed to us curious enough to try to find out if, for some reason, the family $\{\gamma_{b,b'}\}$ was assymptotically equivalent (at least in the limit of low temperatures) to a family of *biased* surface tensions associated to lower and lower values of θ, until final arrival (in the limit $b \to \infty$) to the *longitudinal* surface tension. The main scope of the present section is to answer this question.

The family of biased misfit seams we are going to consider is indicated in Fig. 9 . This family might seem at first look a quite arbitrary one, but it is not. We have not been able to construct *any* other family of narrow, macroscopically straight, misfit seams which contains the longitudinal and diagonal cases as particular ones, which introduces *no bulk effects* (in the sense that through *any path* across the seam, the effect, in what the surface internal energy concerns, is to reverse the spins) and whose value at vanishing temperature (given by the number of *antiferromagnetic* bonds per unit length along the seam, and normalised by the value of the longitudinal surface tension at that temperature) is *shared* by *all* the misfit seams with the same slope, and is given by:

$$\gamma_\theta(0) = |\cos\theta| + |\sin\theta| \qquad (28)$$

If we consider, for example, $\mathrm{tg}\theta = 1/4$ we obtain $\gamma_\theta(0) = 5/\sqrt{17} \simeq 1.21$ which is perfectly compatible with Fig. 11 of Ref. (3). Furthermore equation (10) of the same reference leads to

$$\left.\frac{d\gamma_\theta(T)}{dT}\right|_{T=0} = -\frac{k_B}{2J}\left\{|\cos\theta|\ln(1+|\mathrm{tg}\theta|)+|\sin\theta|\ln(1+|\mathrm{ctg}\theta|)\right\} \qquad (29)$$

Let us incidentally point out that the reduced quantity

$$\frac{2J}{k_B T}\quad\frac{\gamma_\theta(T)}{\gamma_\theta(0)}$$

$$\sim \frac{2J}{k_B T} - \frac{\ln(1+|\mathrm{tg}\theta|) + |\mathrm{tg}\theta|\ln(1+|\mathrm{ctg}\theta|)}{1 + |\mathrm{tg}\theta|} \qquad (29')$$

in the limit $k_B T/J \to 0$

$$\sim \frac{4J}{k_B T_c} \frac{1}{|\cos\theta| + |\sin\theta|} \left(1 - \frac{T}{T_c} \right) \qquad (29'')$$

$$\text{in the limit } \frac{T_c - T}{T_c} \to 0$$

might well be, in spite of having been constructed for *different* families of misfits, identical to the quantity $\tau(\theta)$ of Ref. (5). Unfortunately the comparison for an arbitrary angle θ is not easy at all because of the complexity of Eqs. (4), (5) and (6) of that reference once they have been decomposed into their real and imaginary parts; however the analysis of a few simple particular situations supports this statement.

Let us now turn back to our initial purpose, i.e. the comparison of $\gamma_{b,b'}(T)$ and $\gamma_\theta(T)$. From Eqs. (15) and (29) we respectively obtain that

$$- \frac{2J}{k_B} \left. \frac{d\gamma_{b,b'}(T)}{dT} \right|_{T=0} = \frac{\ln(b/b')}{b-b'} \qquad (30)$$

and

$$- \frac{2J}{k_B} \frac{1}{\gamma_\theta(0)} \left. \frac{d\gamma_\theta(T)}{dT} \right|_{T=0} = \frac{\ln(1+|\mathrm{tg}\theta|)+|\mathrm{tg}\theta|\ln(1+|\mathrm{ctg}\theta|)}{1+|\mathrm{tg}\theta|} \qquad (31)$$

The comparison of these two pure numbers does not seem to enlighten any relation between our RG surface tension and an exact biased one, therefore the fact that both lead, respectively for $b=2b'=2$ and $\theta=\pi/4$, to ln 2 can be considered as fortuitous.

CONCLUSION

The longitudinal surface tension of a simple square-lattice Ising model has been calculated within a real space renormalization group approach. The self-duality of the clusters that have been used leads to quite good results, in particular the *exact* critical temperature is recovered for all cluster sizes. The two-dimensional scaling law $\mu=\nu$ among the surface tension and correlation length critical exponents is preserved for all cluster sizes as well. The characteristics of the critical fixed point (its instability and others) lead to a natural emergence of the well known fact that the surface tension identically vanishes for all temperatures above the critical one. Analytic results (such as the expression, for *all* cluster sizes, of the first two assymptotic corrections for the thermal behaviour of the surface tension in the limit of low temperatures) as well as numerical results (such as the approximate values for the critical exponent and amplitude in the vicinity of the critical temperature, for the first four non trivial cluster sizes) strongly suggest a fair (maybe monotonic) though not very fast convergence towards Onsager's exact result.

Let us incidentally remark that the coupling constant renormalization equations (or equivalently the thermal transmissivity renormalization equations) that have been explicitely established for the first four non trivial clusters, can be used to discuss a great variety of interesting quantities, such as the susceptibility, spontaneous magnetization, internal energy, specific heat[34], etc.

In order to extrapolate, into the limit of infinite cluster size, the surface tension renormalization group results, two basic lines have been developed. One of them (MEP) is a relatively standard one in the sense that it is related to

finite size scaling ideas; the other one (SEP) is rather peculiar (it makes use of the exact or almost exact values for commonly well known quantities such as critical temperature and exponents as well as thermal slopes at vanishing temperatures; it can independently be used for every *single* finite cluster renormalization group result for the surface tension) and speculates over the validity of a kind of law of corresponding states which relates the temperature-axis of the actual finite size approximate surface tension to the temperature-axis of the extrapolated surface tension. Furthermore both extrapolation lines have been combined in the two possible sequences to give mixed procedures (SMEP and MSEP). In all but the MEP case (where its nature demands the knowledge of the results associated to considerably larger clusters than discussed here) the errors with respect to Onsager's result are encourangingly small (a few percent at most) for the *whole* domain of temperatures, being in the SMEP and MSEP cases lower than 0.4% for all temperatures below let us say $\frac{3}{4}\ T_c$.

Finally the thermal slopes at vanishing temperature of the finite cluster renormalization group surface tensions have been compared to those of the exact surface tensions associated to a certain family of *biased* misfitting seams. There was some suspicion that such relation might exist between these two quantities, in spite of its apparent strangeness. However careful comparison suggests that it is not so.

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CAPTION FOR FIGURES AND TABLES

Fig. 1 - Family of self-dual clusters (each of them is, through $\pi/2$-rotation in its plane, superimposable to itself in such a way that every bond cuts one and only one bond of the other cluster). Each cluster has two terminal nodes, $b(b-1)$ internal nodes and $(2b(b-1)+1)$ bonds.

Fig. 2 - To each full (dashed) bond is associated an exchange integral J $(-J)$, hence a thermal transmissivity t $(-t)$. (a) the misfit seam in the macroscopic system; (b) the family of RG clusters.

Fig. 3 - Schematic RG flow diagram (out of scale) in the T-γ (a) and t-γ (b) spaces for fixed (b,b'). The dots indicate fixed points, the arrows the sense of the flow, and the full line the thermal dependence of the RG approximate reduced surface tension.

Fig. 4 - (Out of scale) Onsager's (dashed line) and RG (full lines; $b'=1$ and $b=2,3,4,5$) results for the reduced surface tension. The slope of the straight line is $(-B_{5,1}J/k_BT_c)$ (see text).

Fig. 5 - Thermal dependence of the relative errors (with respect to the exact Onsager's result $\gamma_L(T)$) of the RG approximate ($\{\gamma_{b,1}(T)\}$; full lines) and the MEP ($\gamma^M(T)$; dashed line) results for the surface tension.

Fig. 6 - Cluster size dependence of the RG coefficients $A_{b,1}$ (open circles), $B_{b,1}$ (full circles), $C_{b,1}$ (full line) and $D_{b,1}$ (dashed line); the arrows point the respective exact values (from Onsager's result).

Fig. 7 - Thermal dependence of the relative errors (with respect to the exact Onsager's result $\gamma_L(T)$) of the SEP ($\{\gamma^S_{b,1}(T)\}$; full lines), the MSEP ($\gamma^{MS}(T)$; dashed line) and the SMEP ($\gamma^{SM}(T)$; dotted line) results for the surface tension. Numerical precision difficulties (chaotic oscillations) forced us to cut the b=4 and b=5 SEP results before arrival to T_c.

Fig. 8 - SEP (full line) and exact (dashed line; defined as $\gamma_L(T)/\gamma_{2,1}(T')$) results for the correcting function $f_{2,1}$ as a function of $x \equiv 1-(T/T_c) = |1-(T'/T_c)|^{\nu_{2,1}}$ (discrepancy inferior to 2.2%).

Fig. 9 - Family of biased misfit seams and their slopes (only the antiferromagnetic bonds are indicated, excepting the top-left case where the ferromagnetic bonds are indicated as well). In the bottom-right case two equivalent misfit seams are indicated.

Table 1 - The RG approximate critical exponents $\nu_{b,1}$ and coefficients $A_{b,1}$, $B_{b,1}$ (see the text), $C_{b,1}$ and $D_{b,1}$ (we recall that $\gamma_{b,b'} \sim 1 - C_{b,b'}\frac{k_BT}{J} - D_{b,b'}\frac{k_BT}{J}e^{-2J/k_BT}$) for various cluster sizes. The associated critical temperature is the *exact* one in all cases.

Table 2 - Illustration (b=2, b'=1) of the RG procedure that has been used to obtain $\gamma_{b,b'}$ vs. T.

b	$\nu_{b,1}$	$A_{b,1}$	$B_{b,1}$	$C_{b,1}$	$D_{b,1}$
2	1.14863	1.41	1.57	$\ln 2/2 \simeq 0.35$	$1/4 = 0.25$
3	1.10936	1.52	1.73	$\ln 3/4 \simeq 0.27$	$4/9 \simeq 0.44$
4	1.09499	1.58	1.83	$\ln 4/6 \simeq 0.23$	$9/16 \simeq 0.56$
5	1.08791	1.63	1.91	$\ln 5/8 \simeq 0.20$	$16/25 \simeq 0.64$
(1) exact	1	2	2	0	1

Table 1

j	$k_B T/J$	$\gamma_{2,1}$
0	1.9	0.1687
1	1.6557	0.2941
2	1.3151	0.4671
3	0.9201	0.6537
4	0.5635	0.8006
5	0.3136	0.8911
6	0.1658	0.9425
7	0.0854	0.9704

Table 2

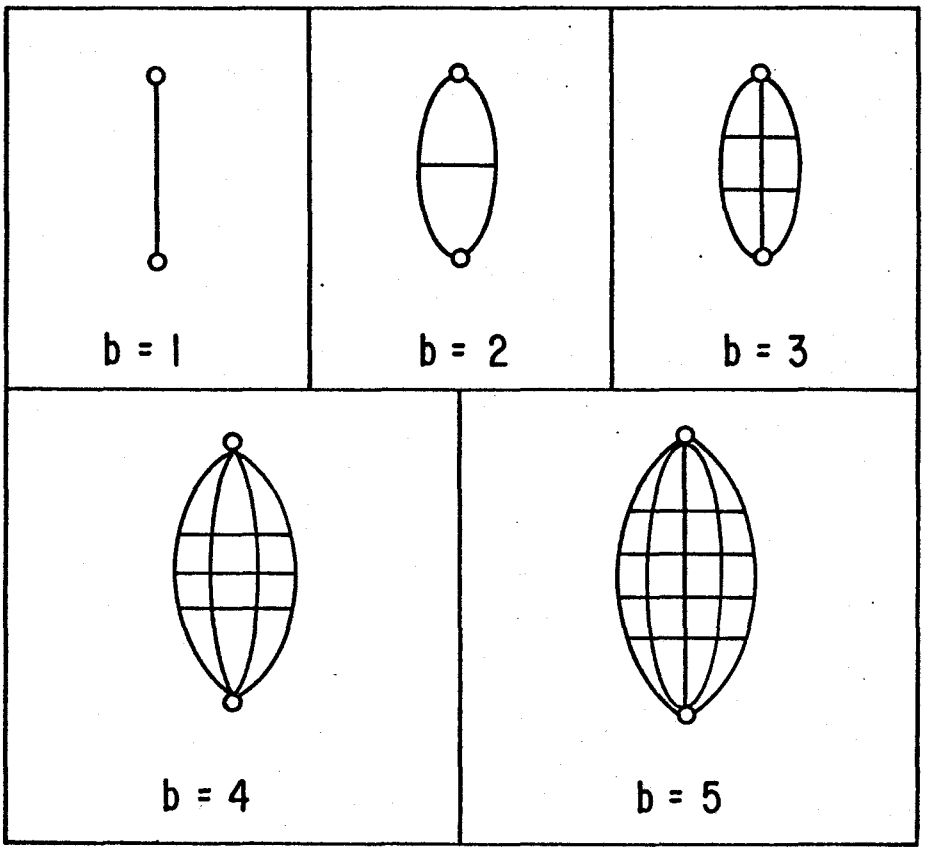

FIG. 1

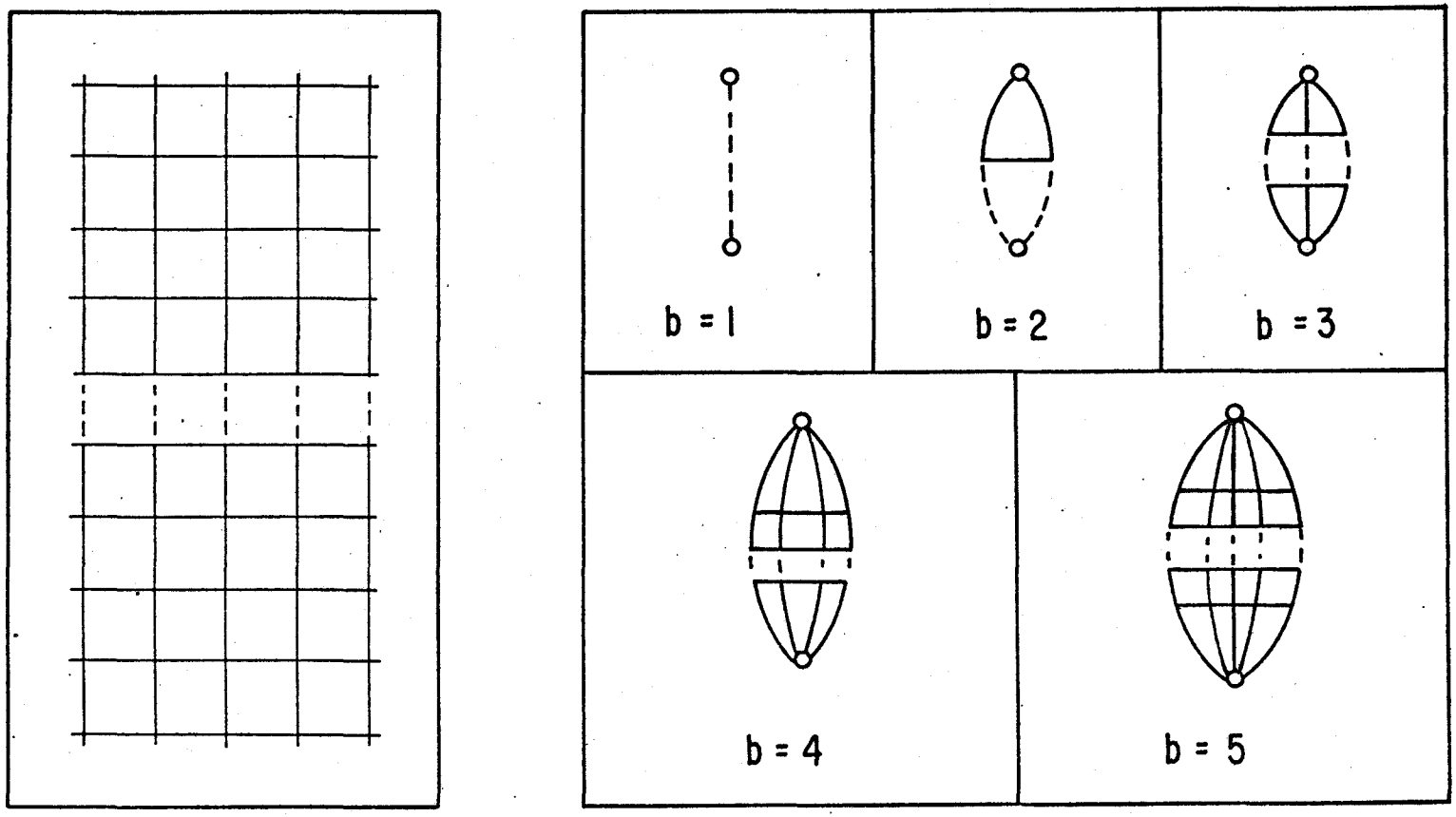

FIG. 2

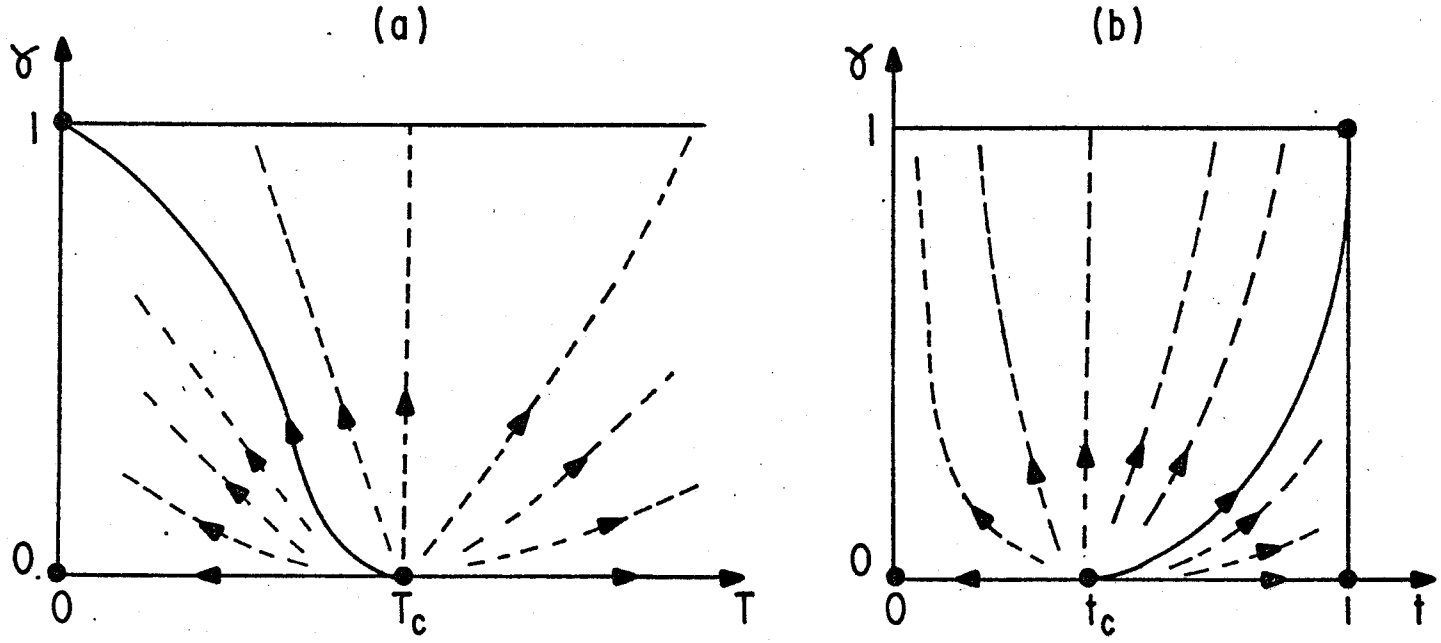

FIG. 3

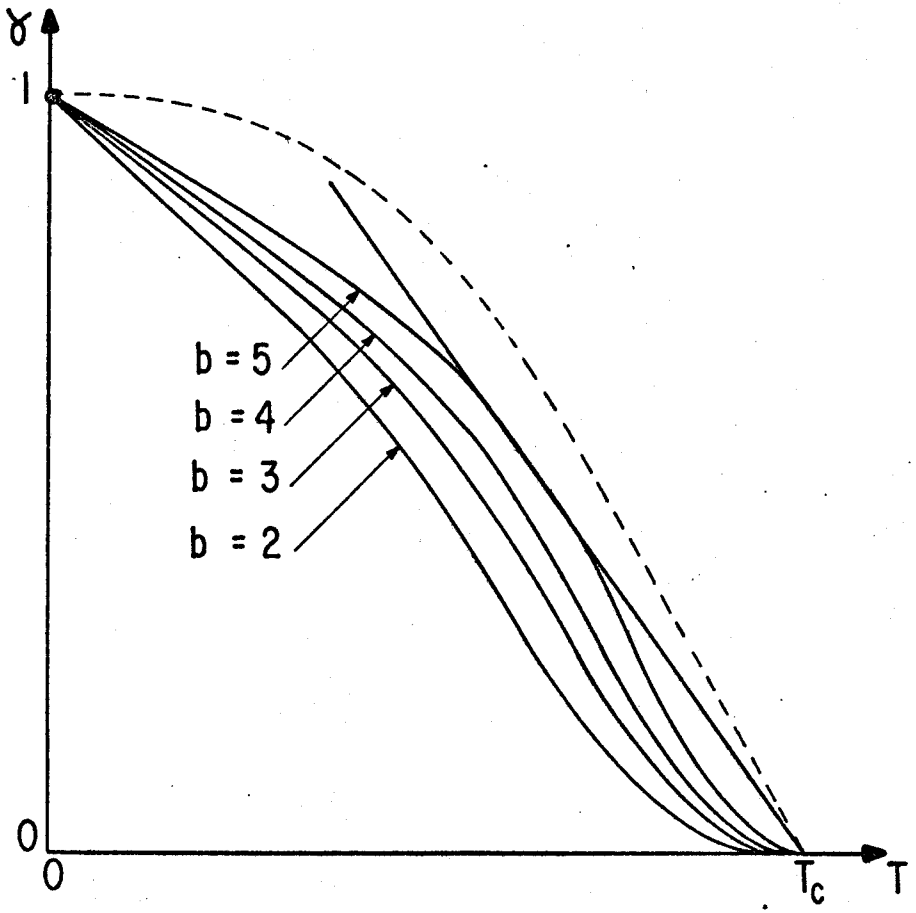

FIG. 4

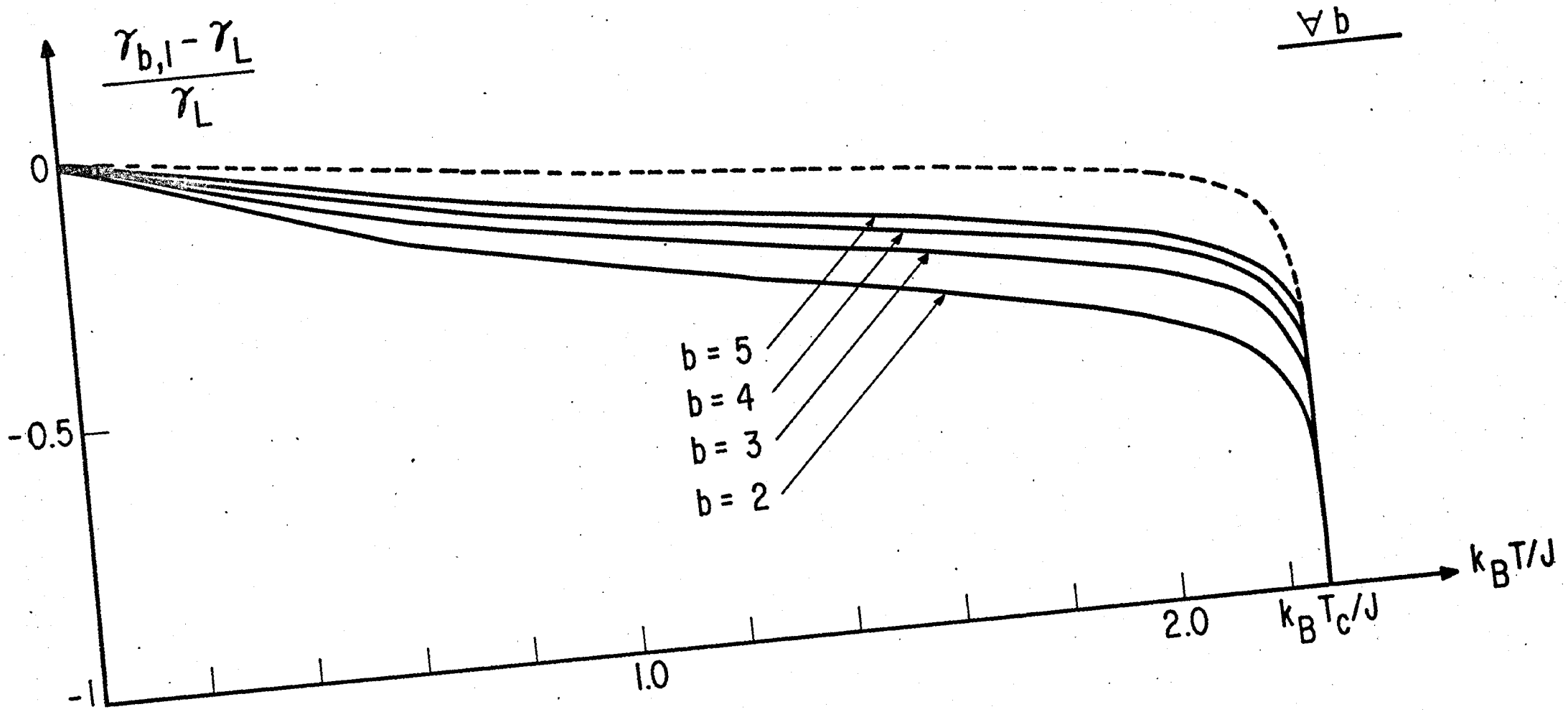
$\frac{\gamma_{b,l} - \gamma_L}{\gamma_L}$
$\forall b$
0
-0.5
-1
b = 5
b = 4
b = 3
b = 2
0
1.0
2.0
$k_B T_c/J$
$k_B T/J$

FIG. 5

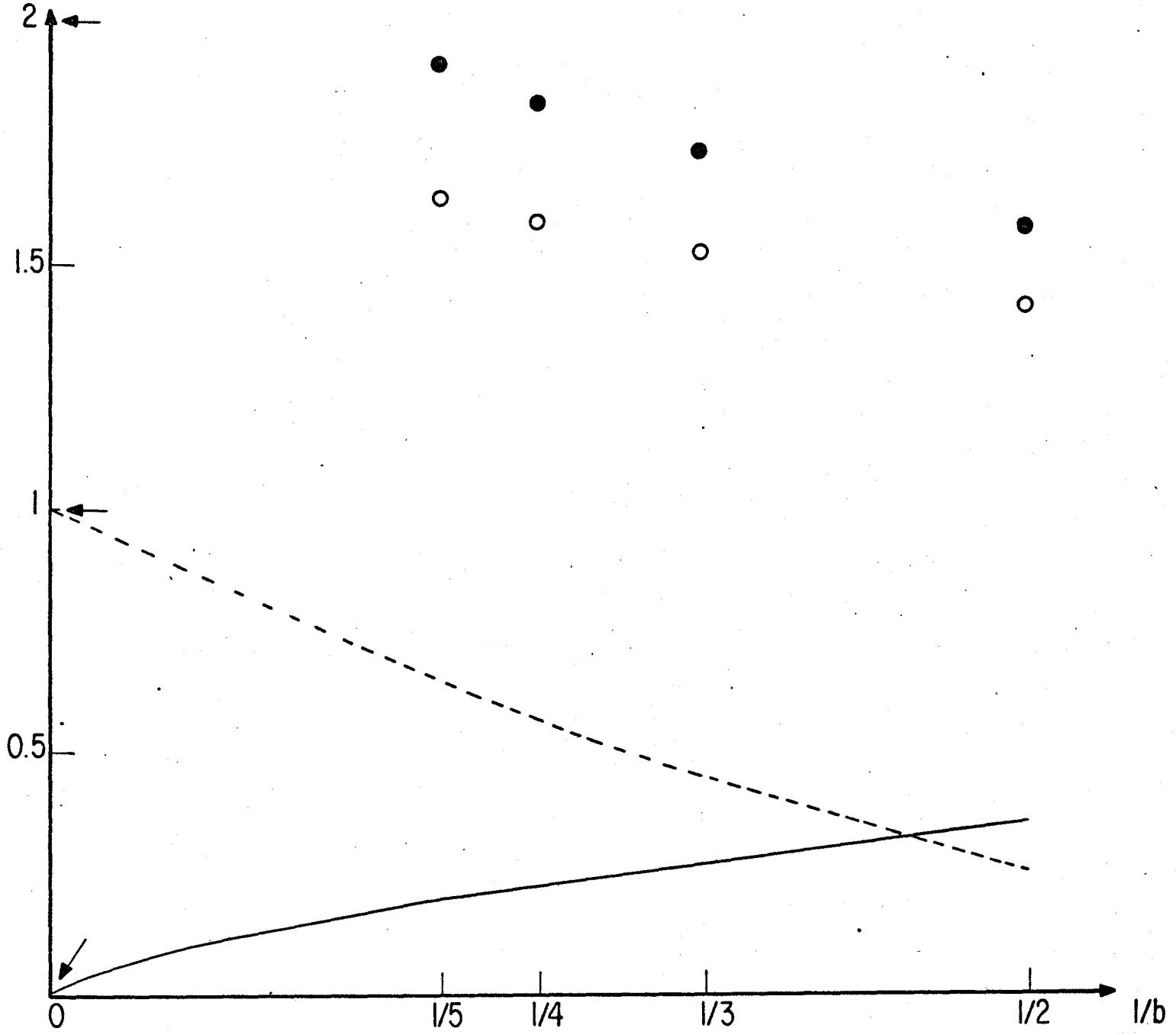

FIG.6

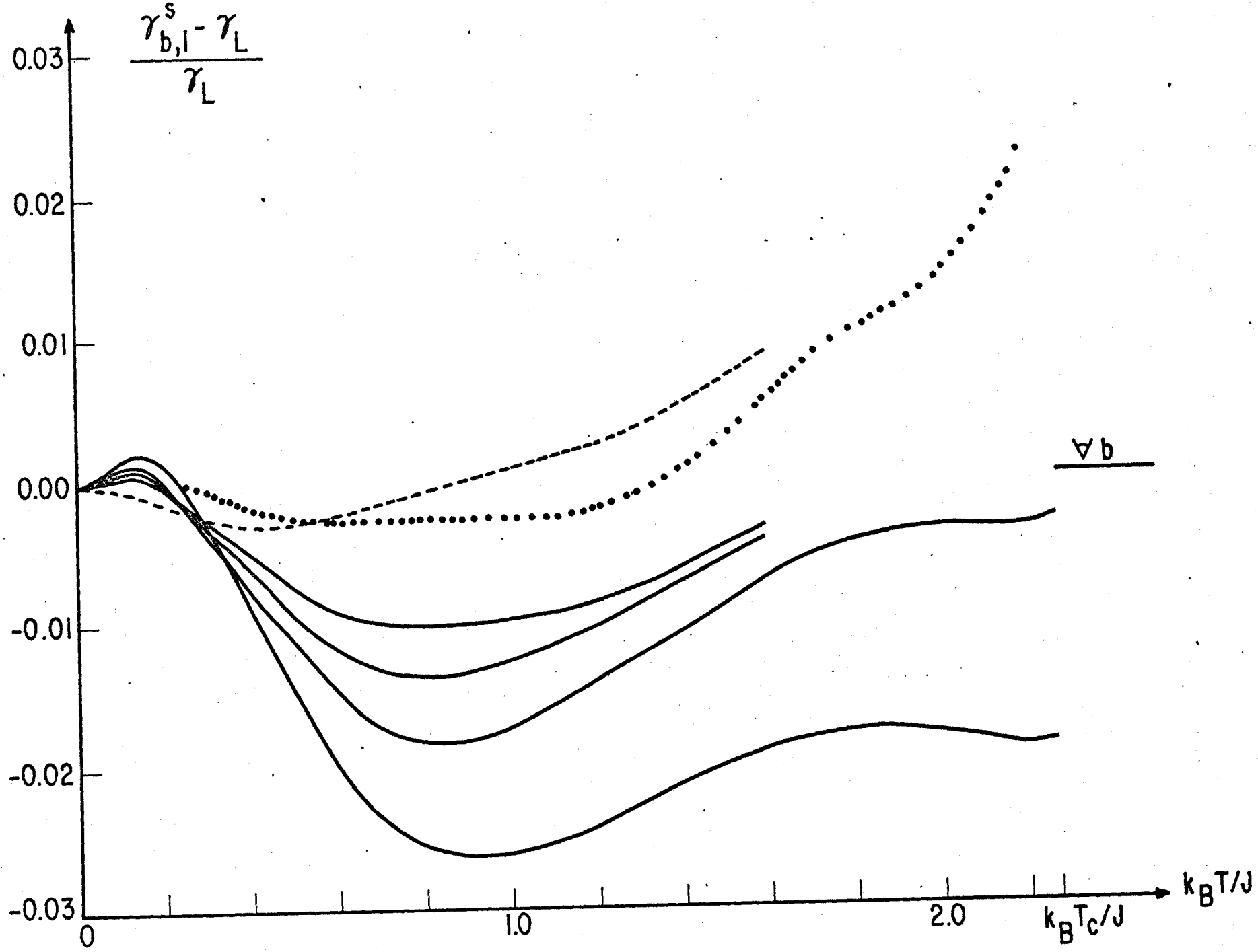
$\frac{\gamma^s_{b,l} - \gamma_L}{\gamma_L}$
0.03
0.02
0.01
0.00
-0.01
-0.02
-0.03
0
1.0
2.0
$k_B T_c/J$
$k_B T/J$
$\forall b$

FIG.7

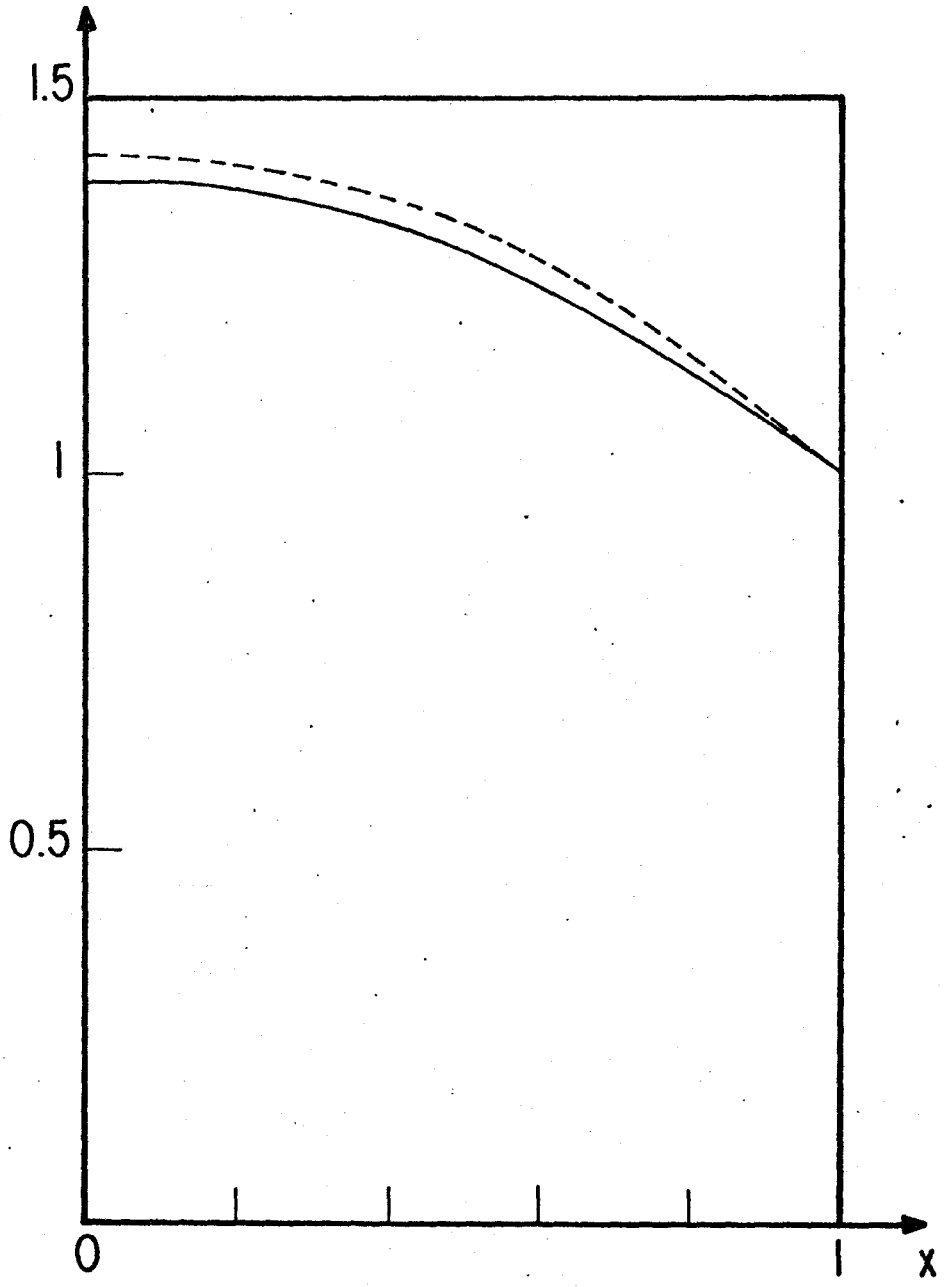

FIG.8

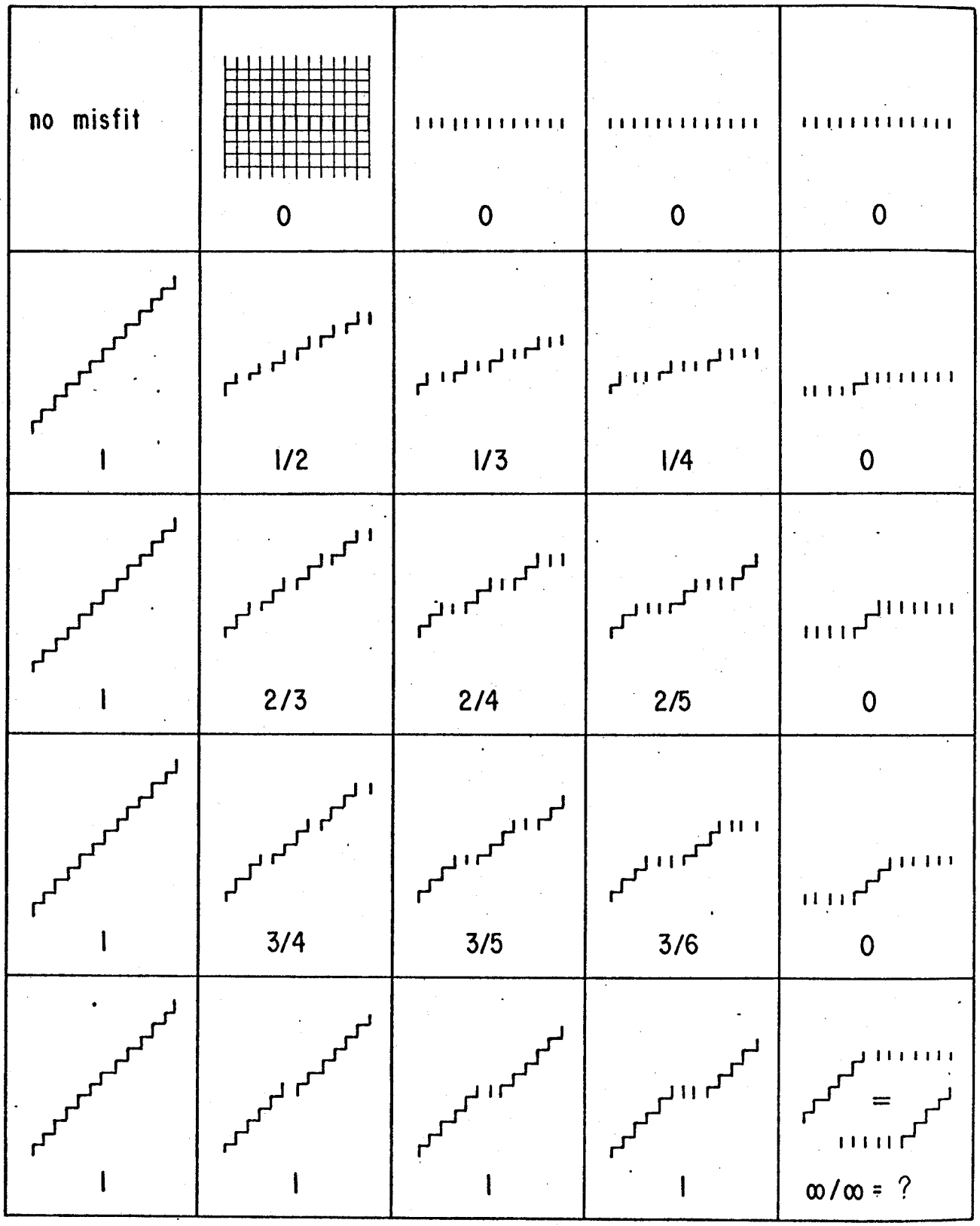

FIG. 9