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SURFACE FERRO (OR ANTIFERRO) MAGNETISM IN BULK ANTIFERRO (OR FERRO) MAGNETS: RENORMALIZATION GROUP ANALYSIS

by

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ABSTRACT

The renormalization group techniques are applied, for the first time, to surface magnetism in bulk magnets, *for all signs* of surface and bulk coupling constants. The q-state Potts model is specifically focused, and a interesting q-evolution of the phase diagram is exhibited. In particular the Ising model (q=2) presents a remarkable feature: surface ferro (or antiferro) magnetism can disappear while heating an antiferro (or ferro) magnet, and *reappear again* for higher temperatures, before entering in the paramagnetic phase.

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KEY WORDS: Surface magnetism; Phase diagram; Potts model; Renormalization group.

Ordering in semi-infinite systems (such as bulk materials presenting a free surface) can in principle exhibit interesting conflicts, when the surface favours a type of ordering which competes with that favoured by the bulk. This is typically the case of surface (crystalline or amorphous) structure reconstruction. This can also be the case of magnetic systems where the surface coupling constant J_S differs in sign from the bulk coupling constant J_B (see the recent review by Binder[1] and references therein). This seems to be precisely the case of Cr (*antiferromagnet* with a Neel temperature of 312K). Its (100) free surface has been very recently investigated[2] (using angle-resolved photoelectron spectroscopy), and it presents a *ferromagnetic* ordering up to 780±50K. The experience has been deviced with particular care for avoiding undesirable surface contamination effects[3].

Magnetic competition between surface and bulk has already received theoretical attention through Mean Field Techniques[4] applied to the spin 1/2 Ising model. However the problem presents a theoretical and experimental interest which deserves alternative (and more sophisticated) approaches. In the present letter we discuss theoretically the q-state Potts model (which recovers the Ising model for q=2, and bond percolation for q=1 and ferromagnetic coupling constants) in semi-infinite simple cubic lattice assuming the free surface to be a (1,0,0)one. The framework is a real-space renormalization group (RG) one; although such treatments are already available[5,6] for the ferromagnetic case, this is the first time (as far as we know) they are applied allowing for *all signs* of J_S and J_B. We follow along the lines of Ref. [6] and use Migdal-Kadanoff - like b=3 clusters (b is the RG linear expansion factor) which have been quite satisfactory for the ferromagnetic case ($J_S>0$ and $J_B>0$).

We consider the Hamiltonian $H=-q\sum_{<i,j>} J_{ij}\,\delta_{\sigma_i,\sigma_j}\;(\sigma_i=1,2\ldots,q,\forall i)$

where $<i,j>$ denotes nearest-neighbors, and J_{ij} equals $J_S\,(J_S \lesseqgtr 0)$ when *both* sites i and j belong to the free surface, and equals $J_B\,(J_B \lesseqgtr 0)$ otherwise. It is convenient to introduce the variables (*thermal transmissivity*; see Ref. [7] and references therein) $t_r \equiv \left(1-e^{-qJ_r/k_BT}\right) \Big/ \left[1+(q-1)e^{-qJ_r/k_BT}\right] \in [-1/(q-1),1]$ $(r=S,B)$.

To construct the RG recursive relations in the (t_B,t_S) space, we use the procedures described in Ref. [7]. The bulk (surface) equation is obtained through the renormalization indicated in Fig. 1(a) (Fig. 1(b)), which immediately yields $t_B' = \{1-[x(t_B)]^3\}/\{1+(q-1)[x(t_B)]^3\}$ $(t_S' = \{1-x(t_S)x(t_B)\}/\{1+(q-1)x(t_S)x(t_B)\})$ with $x(t) \equiv \{(1-t^3)/[1+(q-1)t^3]\}^3$. These equations completely close the recurrence problem, and yield the results presented in Fig. 2.

For q=2 we have indicated the RG flow in detail (Fig. 2 (a)): this can be considered as a prototype as, for all q, the RG flow scheme varies smoothly with q. Seven physically different phases are identified through seven *trivial* (fully stable) fixed points (noted ■ in Fig. 2, excepting two of them which are noted because, for q=2, they are superimposed to semi-stable fixed points. These phases are the *paramagnetic* (P), the *bulk ferromagnetic* (BF), the *bulk anti-*

ferromagnetic (BAF), the *surface ferromagnetic* (SF; the bulk is magnetically disordered), the *surface antiferromagnetic* (SAF; the bulk is magnetically disordered), the *simultaneous surface ferromagnetic and bulk antiferromagnetic* (SF/BAF), and the *simultaneous surface antiferromagnetic and bulk ferromagnetic* (SAF/BF) ones. A great amount of physically different *critical* universality classes are exhibited: these correspond to the P-SF, P-BF, P-SAF, P-BAF, SF-BF, SAF-BAF, SF-SF/BAF, SAF-SAF/BF, SF/BAF-BAF and SAF/BF-BF critical lines. Also four physically different *multicritical* universality classes are present (characterized by four fully unstable fixed points noted o in Fig. 2): they correspond to the P-BF-SF, P-BAF-SAF, P-SF-BAF-SF/BAF and P-SAF-BF-SAF/BF multicritical points.

It is worthy to note that the present RG recovers, for q=2, the well known $(J_B, J_S) \to (-J_B, -J_S)$ symmetry (which, among others, determines the isomorphism between ferromagnetic and antiferromagnetic Ising models in square and simple cubic lattices). As a consequence of this fact, several universality classes which are different for $q \neq 2$, coincide two by two for q=2.

Let us now focuse the q-evolution of the (t_B, t_S) phase diagrams (see Fig. 2). When q increases above 2, the $t_S = -1/(q-1)$ axis as well as the $t_B = -1/(q-1)$ one approach the origin $t_B = t_S = 0$, successively forcing several phases to disappear. We adopt the following notation: q_1 is the particular value of q for which the P-SAF-BF-SAF/BF multicritical point touches the $t_S = -1/(q-1)$ axis (and consequently the SAF/BF phase disappears), q_2 is the value for which the P-SAF critical point (at $t_B=0$) touches the same axis (and consequently the SAF phase disappears for the *square* lattice), q_3 is the

value for which the P-SAF-BAF multicritical point touches the same axis (and consequently the SAF disappears), and q_4 is the value for which the P-SF-BAF-SF/BAF multicritical point touches the $t_B = -1/(q-1)$ axis (consequently the BAF phase disappears). The following inequalities are satisfied:
$2 < q_1 < q_2 < q_3 < q_4$. Baxter has proven[7] that $q_2=3$. The present RG approximation yields $q_1 \simeq 2.21$, $q_2 \simeq 2.25$, $q_3 \simeq 2.28$ and $q_4 \simeq 2.64$. One of the most interesting features is the "re-entrances" that are present for the Ising model with competing surface and bulk coupling constants. If we have let us say a ferromagnetic bulk ($J_B > 0$), and an antiferromagnetic surface ($J_S < 0$), within an appropriate range of J_S/J_B, the surface antiferromagnetic order parameter (sublattice magnetization) can vanish and then reappear below the bulk Curie temperature T_C, presumably present a soft singularity at T_C, and finally vanish again at a Néel - like temperature above T_C. In spite of its apparent strangeness, this interesting phenomena can be intuitively understood in some sense if one takes into account that the bulk ferromagnet acts, on the (relatively strong) surface antiferromagnet and as long as non neglectable bulk order exists, quite similarly as an external uniform magnetic field acts on a standard antiferromagnet (we recall that the Néel temperature of the antiferromagnetic surface would be proportional to J_S if the surface was magnetically isolated from the bulk). If we note J_S^C/J_B the value of the ratio J_S/J_B associated with each one of the four multicritical points, the present RG yields the results depicted in Fig. 3; they satisfactorily compare with series[4] and Monte Carlo[9] results available for q=2.

Let us summarize the present work by saying that the renormalization group analysis that has been undertaken suggests qualitatively interesting features in the full phase diagram (both signs for J_B and J_S) of the Potts model. Further experimental and/or theoretical evidence would be very welcome. In particular, it would be interesting to establish, on (nearly) exact grounds, whether the peculiar phase diagram herein obtained for q=2, indeed appears at q=2, or rather is to be associated with q > 2.

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CAPTION FOR FIGURES

Fig. 1 - RG recursive relation for the bulk (a) and the surface (b) transmissivities (O and ● respectively denote terminal and internal sites). The big cluster of (b) contains only six branches as the other three corres pond to the vacuum.

Fig. 2 - q=2 flow diagram (a) and the q-evolution of the phase diagrams (b-f) in the $(\tau, J_S/J_B)$ space where $\tau \equiv \text{sign}\,(J_B)T/T_C$, T_C being the bulk Curie temperature. ■, ● and O respectively denote trivial (fully stable), critical (semi-stable) and multicritical (fully unstable) fixed points. The dashed lines are indicative.

Fig. 3 - q-evolution of J_S^C/J_B (for $|J_S/J_B|$ above $|J_S^C/J_B|$ surface magnetic ordering can occur even in the absence of bulk ordering). At q=2, J_S^C/J_B equals 1.60 (series [4]), 1.50 (Monte Carlo[9]) and 1.74 (present RG) for the P-BF-SF case, and equals -1.9 (series[4]) and -2.28 (present RG). If intended for the simple cubic lattice, the present RG cannot be retained much above q=3 as the bulk transitions will become of the first order; if intended for the hierarchical lattice of Fig. 1, it is exact for all values of q.

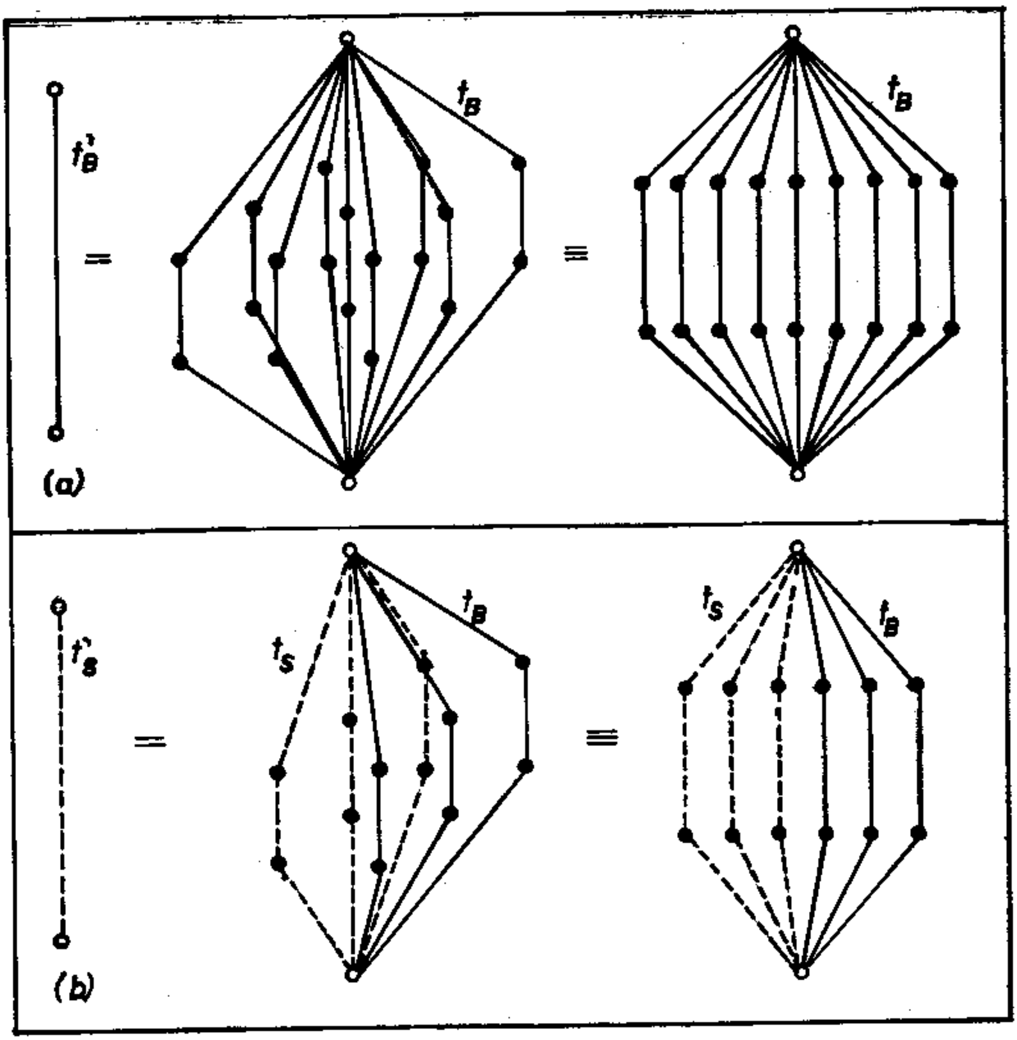

FIG. 1

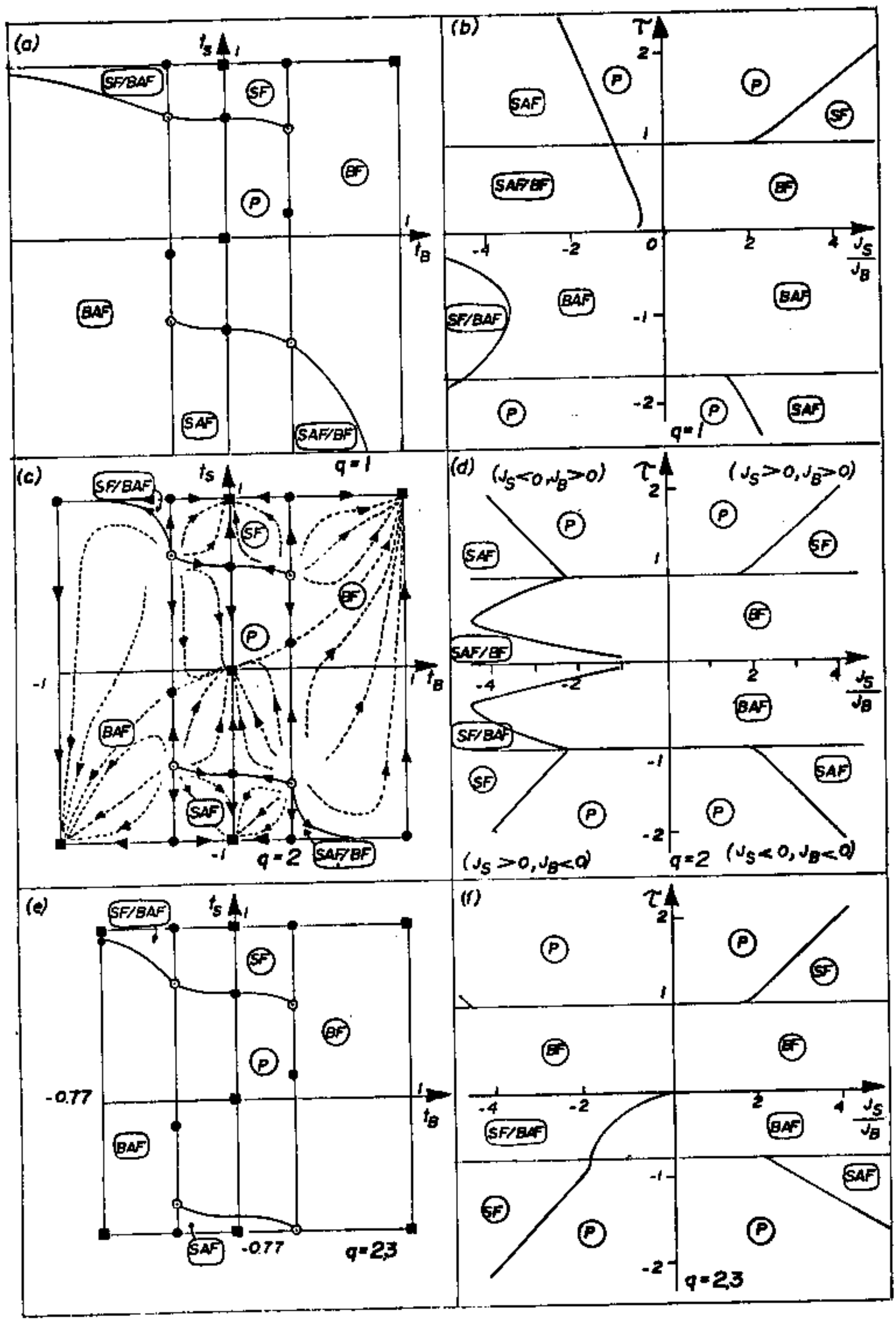
(a)
t_S
SF/BAF
SF
BF
P
t_B
BAF
SAF
SAF/BF
(b)
τ
P
SAF
SF
SAF/BF
BF
J_S/J_B
BAF
SF/BAF
q=1
(c)
SF/BAF
q=1
t_S
SF
BF
P
t_B
BAF
SAF
q=2
SAF/BF
(d)
$(J_S<0, J_B>0)$
$(J_S>0, J_B>0)$
SAF/BF
SF/BAF
$(J_S>0, J_B<0)$
q=2
$(J_S<0, J_B<0)$
(e)
SF/BAF
-0.77
q=2,3
(f)
q=2,3

FIG. 2

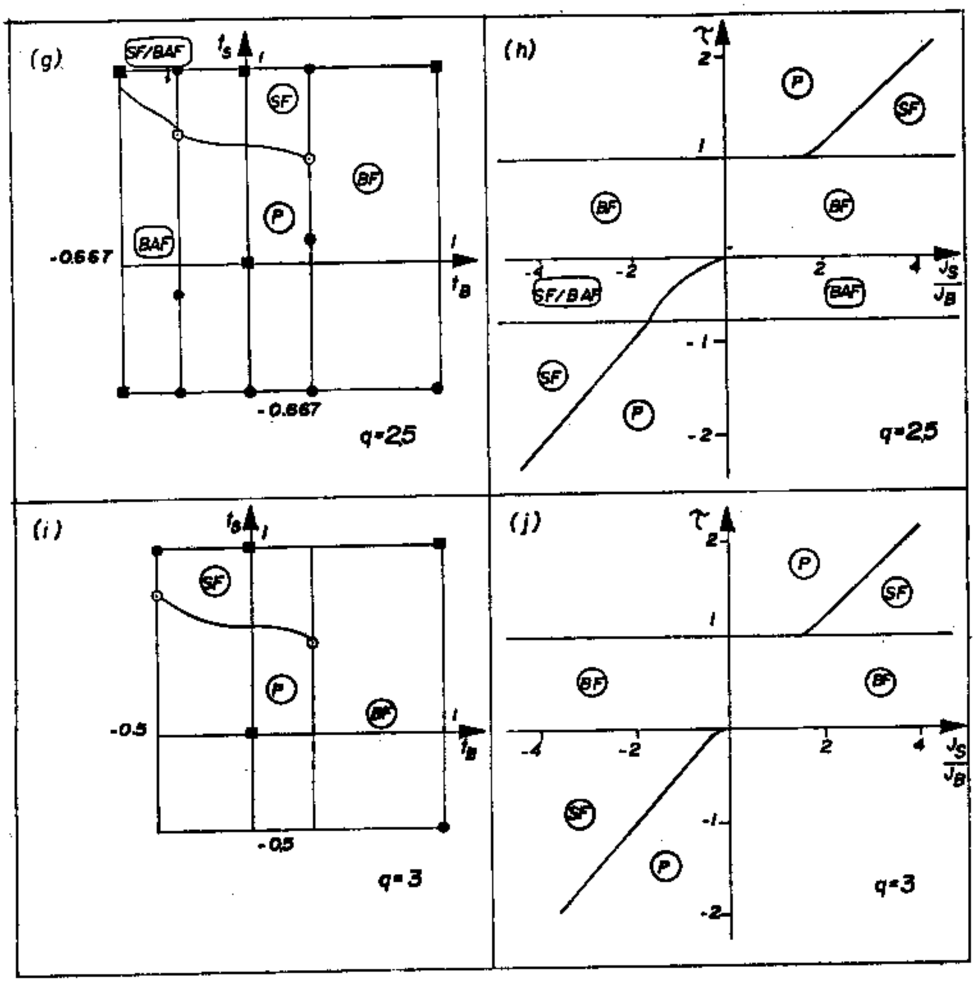
(g)
SF/BAF
t_S
1
SF
BF
P
BAF
-0.667
1
t_B
-0.667
q=2.5
(h)
τ
2
P
SF
1
BF
BF
-4
-2
2
4
J_S/J_B
SF/BAF
BAF
-1
SF
P
-2
q=2.5
(i)
t_S
1
SF
P
BF
-0.5
1
t_B
-0.5
q=3
(j)
τ
2
P
SF
1
BF
BF
-4
-2
2
4
J_S/J_B
SF
-1
P
-2
q=3

FIG. 2

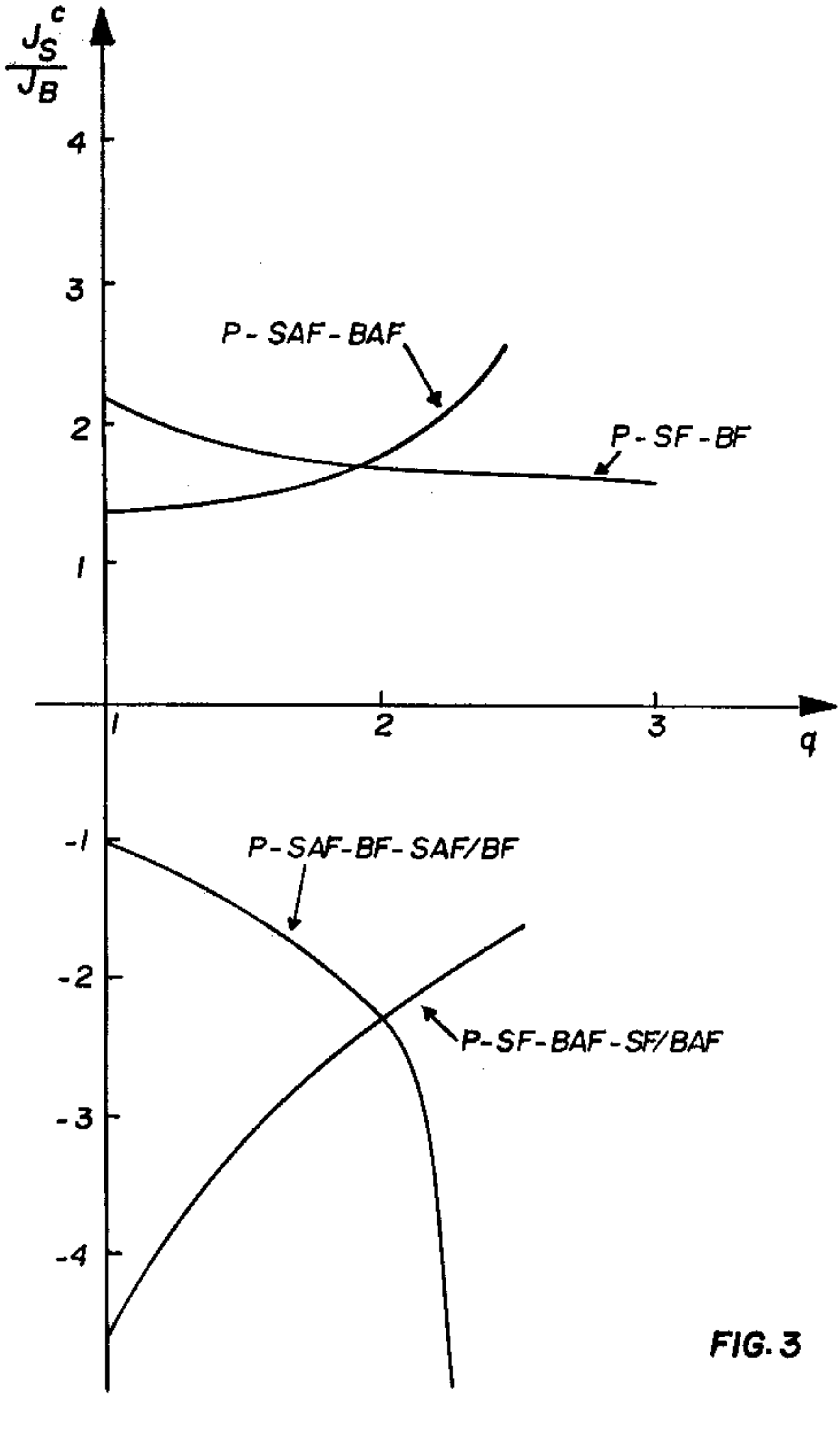
$\frac{J_S^c}{J_B}$
4
3
2
1
-1
-2
-3
-4
1
2
3
q
P - SAF - BAF
P - SF - BF
P - SAF - BF - SAF/BF
P - SF - BAF - SF/BAF

FIG. 3