Cluster Size in Random Mixtures and Percolation Processes

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(Received November 30, 1960)

It is pointed out that the topological problem which arises in the theory of critical concentration in ferromagnetic crystals, and discussed recently by Elliott *et al.*, is identical with a problem arising in the statistical theory of random mixtures. Additional terms of series expansions are given, and these enable improved estimates of the critical concentration to be made. A distinction is drawn between "site mixtures" and "bond mixtures," the latter having been previously considered under the heading of "percolation processes." The critical concentrations for the two problems are usually different. Some rigorous results regarding the critical concentrations are quoted.

In a recent Letter[1] Elliott *et al.* showed that in ferromagnetic crystals the critical concentration is a topological property of the lattice and is apparently independent of the nature of the interaction. In fact this topological property is closely related to one which arises in the statistical problem of the distribution of cluster sizes in random mixtures.[2] If we consider an ideal mixed crystal of A and B molecules, then for any proportion p of A molecules we can calculate the probability distribution of singlets, doublets, triplets . . ., and we can hence derive an estimate of the mean cluster size in the form of a power series in p. For the honeycomb, simple quadratic (S.Q.), triangular, and simple cubic (S.C.) lattices, these series are as follows:

$$\begin{aligned}
&\text{honeycomb, } 1+3p+6p^2+12p^3+24p^4+33p^5\\
&\qquad +60p^6+99p^7+156p^8+276p^9;\\
&\text{S.Q., } 1+4p+12p^2+24p^3+52p^4+108p^5\\
&\qquad +224p^6+412p^7+844p^8+1528p^9; \qquad (1)\\
&\text{triangular, } 1+6p+18p^2+48p^3+126p^4\\
&\qquad +300p^5+750p^6+1686p^7;\\
&\text{S.C., } 1+6p+30p^2+114p^3+438p^4+1542p^5+5754p^6.
\end{aligned}$$

As the concentration p increases from zero to one, it is clear that a point will be reached at which a finite probability exists of A molecules being contained in infinitely large clusters, and this point will be characterized by the mean size of these clusters becoming infinite. Hence this critical concentration p_c will correspond to the radius of convergence of series (1).

It seems that the series (1) are closely related to those derived by Elliott *et al.*[1] for the critical concentration in a ferromagnet. When the molecules A are ferromagnetic and B nonmagnetic, the finite probability of infinite clusters is associated with the appearance of a spontaneous magnetization.

The series (1) are not very smoothly behaved in the initial stages; however, we have derived more terms for particular lattices than Elliott *et al.*[1] and our conclusions differ somewhat from theirs. Thus we think that $0.60<p_c<0.75$ for the honeycomb, $p_c=0.55$ for the SQ., and 0.51 for the triangular. (Elliott *et al.*[1] estimate 0.49, 0.48, and 0.36, respectively.) In fact it can be shown rigorously that $p_c>0.52$ for the honeycomb lattice, and there are strong theoretical arguments which indicate that $p_c\geqslant\frac{1}{2}$ for all plane lattices.[3] For the S.C. lattice our estimate of 0.28 agrees with theirs. We have also undertaken an analysis of the detailed behavior of the mean cluster size in the critical region.

Another problem of a similar character arises when the bonds in the lattice are of two kinds a, b, and we consider the probability distribution of connected "bond clusters" of a given number of bonds. Such problems have been considered in detail by Hammersley and his collaborators[4] under the heading of "percolation processes," and certain exact results have been derived rigorously. Thus for the S.Q. lattice Hammersley[4] derived the bounds $0.35\leqslant p_c\leqslant 0.65$, and Harris[5] improved the lower bound to 0.5.

For this problem we have derived series corresponding to (1) as follows:

$$\begin{aligned}
&\text{honeycomb, } 1+4p+8p^2+16p^3+32p^4+54p^5\\
&\qquad +100p^6+182p^7+328p^8+494p^9+984p^{10}\\
&\qquad\qquad +1572p^{11}+2656p^{12}+4212p^{13};\\
&\text{S.Q., } 1+6p+18p^2+48p^3+126p^4+300p^5\\
&\qquad +762p^6+1668p^7+4216p^8+8668p^9; \qquad (2)\\
&\text{triangular, } 1+10p+46p^2+186p^3+706p^4\\
&\qquad +2568p^5+9004p^6+30894p^7;\\
&\text{S.C., } 1+10p+50p^2+238p^3+1114p^4\\
&\qquad +4998p^5+22562p^6+98174p^7.
\end{aligned}$$

Our estimates for critical points from the series (2) are: honeycomb, 0.66; S.Q., 0.50; triangular,[6] 0.33; and

[1] R. J. Elliott, B. R. Heap, D. J. Morgan, and G. S. Rushbrooke, Phys. Rev. Letters **5**, 366 (1960).

[2] C. Domb Nature **184**, 509 (1959).

[3] M. E. Fisher (to be published).

[4] S. R. Broadbent and J. M. Hammersley, Proc. Cambridge Phil. Soc. **53**, 629 (1957); J. M. Hammersley, Proc. Cambridge Phil. Soc. **53**, 642 (1957); Ann. Math. Stat. **28**, 790 (1957); Centre natl. recherche sci. Groupe franc. argiles, Compt. rendu réunions études 17–37 (1959).

[5] T. E. Harris, Proc. Cambridge Phil. Soc. **56**, 13 (1960). Fisher has adapted the arguments of T. E. Harris to show that p_c(honeycomb)$+p_c$(triangular)$\geqslant 1$.

[6] We may perhaps conjecture that for plane lattices the exact values are $\frac{1}{2}$, $\frac{1}{3}$, and $\frac{2}{3}$ and hence satisfy the relation $p_c=2/q$, where q is the coordination number of the lattice.

S.C., 0.24; it will thus be seen that for one lattice at least, p_c differs substantially from (1) to (2).

We have used the terminology "site mixtures" and "bond mixtures" to distinguish between the above two problems. The above series (1) and (2) have been derived by applying the standard techniques of the theory of cooperative phenomena in crystals[7] to these problems. The configurational problems involved contain new features but we have been able to employ special devices to extend the series. In this work we have been greatly helped by our colleagues M. E. Fisher and J. Essam, who have also independently derived closed-form approximations for the various quantities which enter.[8]

The methods have also been applied to nonideal mixtures in which the energies of interaction between A and B molecules are nonzero, and the variation of cluster size with temperature has been investigated. Details of the work referred to in this note are being published elsewhere.

ACKNOWLEDGMENTS

We are grateful to Dr. R. J. Elliott and Professor G. S. Rushbrooke and their collaborators for communicating details of their results to us.

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[8] J. Essam and M. E. Fisher, J. Math. Phys. (to be published).

PHYSICAL REVIEW VOLUME 122, NUMBER 1 APRIL 1, 1961

Lorentz Force on Screw Dislocations and Related Problems

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(Received October 14, 1960; revised manuscript received December 15, 1960)

The concept of a Lorentz force on screw dislocations, first introduced by Nabarro, is analyzed. It is concluded that the Nabarro-Lorentz force on screws and the Lorentz force of electromagnetism are not analogous, and that the term a Lorentz force on screws should be dropped in order to avoid confusion. Only when the screw is constrained to move on one slip plane is the analogy with electromagnetism complete. Total quasimomentum is not generally conserved when screw dislocations interact with elastic waves.

INTRODUCTION

IN 1951 Nabarro[1] introduced the concept of a Lorentz force on screw dislocations, and since then this concept has been in current use and seems to be generally accepted. However, the published explanations of Nabarro[1] and Eshelby[2] do not unequivocally establish the existence of a true Lorentz force on screw dislocations.

Hence, the aim of the present paper is mainly pedagogical: We want to make unequivocal and easily understood statements about the forces on screw dislocations to clear away possible confusion. This paper should not be looked upon as a direct criticism of previous work. We merely want to emphasize that what has been termed the Lorentz force on screw dislocations is not in fact analogous to the Lorentz force in electromagnetism, and that consequently the term "a Lorentz force on screws" should be dropped in order to avoid confusion.

So far the Lorentz force on screws has been of little practical importance. It has been used in discussions on dislocation mobility,[1,3] but these discussions do not really depend on the existence of a Lorentz force as the results obtained are used to illustrate the quasimomentum balance for elastic waves and screws constrained to move on *one* slip plane, in which case the electromagnetic analogy is complete. However, presently a great deal of interest is being directed towards high-velocity dislocations resulting from shock-loading, and in this field a possible Lorentz force would be important, according to Weertman.[4] Thus we should think that the concept of a Lorentz force on screws merits some discussion at the present time.

DISCUSSION OF THE NABARRO-ESHELBY DERIVATION OF THE LORENTZ FORCE ON SCREWS

Eshelby[2] has given a simple derivation of the Nabarro-Lorentz force on screws, which is not essentially different from Nabarro's original derivation. Consider a procession of screws, n per unit length, oriented parallel to the z axis and with Burgers vector $+b$ traveling across a bar of square cross section with a velocity v_x (Fig. 1). Then the upper part of the bar, I, will have a

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[2] J. D. Eshelby, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1956), Vol. 3. p. 134.

[3] J. Lothe, Phys. Rev. **117**, 704 (1960).

[4] J. Weertman in *Response of Metals to High-Velocity Deformation* (Interscience Publishers, Inc., New York, 1961, to be published).