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- 9. National Science Foundation Authorization, 1970. Hearings before the Special Committee on National Science Foundation, April 16 and 23, 1970. Government Printing Office.
- 10. Newsletter, Conference Board of the Mathematical Sciences, Vol. 5, No. 1, May 1970 (p. 15).
- 11. The Physical Sciences. A report of the National Science Board submitted to Congress 1970. Government Printing Office.
- 12. Science and the Federal Government: Which Way to Go. A speech delivered by Philip Handler, President, National Academy of Sciences to Federation of American Societies for Experimental Biology, April 14, 1970.
- 13. Science and Technology: Tools for Progress. A report on the President's Task Force on Science Policy. April 1970. Government Printing Office.
- 14. Toward Balanced Growth: Quantity with Quality. A report of the National Goals Research Staff to the President. July 4, 1970. Government Printing Office.
- 15. The Invisible University: Postdoctoral Education in the United States. A study conducted under the auspices of the National Research Council 1969. National Academy of Sciences, Washington, D. C.

#### MARKOV RANDOM FIELDS AND GIBBS ENSEMBLES

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1. Introduction. There are two very interesting and apparently quite different ways of defining random configurations of points on a lattice (or so called random fields in the terminology of R. L. Dobrushin [1]). One of these is based on the formulation of statistical mechanics according to J. W. Gibbs. It is generally accepted as the simplest useful mathematical model of a discrete or lattice gas. Its physical significance was enhanced when it was shown to exhibit, in dimension  $\nu \ge 2$ , the singularities associated with the phenomenon of phase transition. (See [2] and [3] for recent, mathematically rigorous treatments.)

The second class of random fields we shall consider is that of Markov random fields, introduced by Dobrushin [1]. It has no apparent connection with physics, being based instead on the most natural way of extending the notion of a Markov process with one dimensional, integer valued, time to the case of higher dimensional, lattice valued, time parameter.

The purpose of this article is to show that these two ways of defining a random field are equivalent. The program is therefore first to define a general random field (R.F.), then a Gibbs ensemble or Gibbs random field (G.R.F.), and next a Markov random field (M.R.F.). The easy half of the theorem will be the statement that every G.R.F. is a M.R.F. This is due to the simple explicit form of the definition of a G.R.F. The converse, that every M.R.F. is a G.R.F., is less

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obvious, and perhaps surprising since the usual derivation of the Gibbs formula defining a G.R.F. depends on the physical fact that the interaction between particles is described by a potential. No such notions from physics enter into the purely probabilistic definition of a M.R.F.

Added in proof: Almost identical results have been obtained by M. B. Averintzev, "On a method of describing discrete parameter random fields," Problemy Peredači Informacii, Vol. 6, no. 2, 1970, pp. 100-109.

### 2. Basic Definitions.

Definition of a random field. Let  $Z^{\nu}$  denote the  $\nu$ -dimensional integers, or the lattice points in  $\nu$ -dimensional space. For x, y in  $Z^{\nu}$ , |x-y| is the Euclidean distance from x to y. A finite subset  $D \subset Z^{y}$  is called a domain if it is connected, i.e., if  $x, y \in D$  implies the existence of a path  $x = x_0, x_1, \dots, x_{n-1}, x_n = y$ , such that all  $x_i \in D$  and  $|x_i - x_{i+1}| = 1$ . The boundary  $\partial D$  of a domain D consists of all y in  $Z^{y}-D$  which have one or more neighbors in D. (x and y are neighbors if |x-y|=1.) Finally we denote  $\overline{D}=D\cup\partial D$ . If  $\Omega=\{0,1\}^D$ , if  $\mathfrak F$  is the collection of all subsets of  $\Omega$  and if P is a probability measure on  $\mathfrak{F}$ , then the triple  $(\Omega, \mathfrak{F}, P)$ is called a random field (R.F.) on the domain D. Thus we may think of a R.F. on D as a probability measure on the set of all maps  $\omega: D \to \{0, 1\}$ , and consequently as a probability measure on the set of all possible configurations of particles on D. (We think of a site  $x \in D$  as occupied by a particle if  $\omega(x) = 1$ , and as empty if  $\omega(x) = 0$ .) Thus the configuration of particles described by  $\omega \in \Omega$  is the set  $\{x: x \in D, \omega(x) = 1\}$ . In the one dimensional case  $(\nu = 1)$  we can also think of the R.F. on a domain (interval) D as a stochastic process  $\omega(x)$  with time parameter  $x \in D$ , and values in the two point set  $\{0, 1\}$ .

Definition of a Gibbs random field (G.R.F.). A function U from  $Z^r \times Z^r$  to  $\Re$  (the reals) is called a symmetric homogeneous, nearest neighbor pair potential (or briefly pair potential from now on) if for all x, y in  $Z^r$ 

- (i) U(x, y) = U(y, x) (symmetry),
- (ii) U(x, y) = U(0, y-x) (homogeneity),
- (iii) U(x, y) = 0 when |y-x| > 1 (nearest neighbor property).

Before we can define the most general G.R.F. with pair potential U we also have to specify a boundary value (B.V.) function. This is an arbitrary map  $\phi:\partial D \to \{0, 1\}$ . When  $\phi$  is given it will be convenient to extend each  $\omega \in \Omega$  to a map  $\bar{\omega}$  of  $\overline{D} \to \{0, 1\}$  by the rule

$$\tilde{\omega}(x) = \begin{cases} \omega(x) & \text{for } x \in D, \\ \phi(x) & \text{for } x \in \partial D. \end{cases}$$

Suppose we are given a domain  $D \subset Z^r$ , and a potential U satisfying (i), (ii), (iii), and a B.V. function  $\phi$ . Then we shall say that a R.F.  $(\Omega, \mathfrak{F}, P)$  on D is a G.R.F. with pair potential U and B.V. function  $\phi$ , if P is defined by the Gibbs formula

(1) 
$$P(\omega) = Z^{-1} \exp \left[ -\frac{1}{2} \sum_{x \in \overline{D}} \sum_{y \in \overline{D}} \overline{\omega}(x) \overline{\omega}(y) U(x, y) \right], \quad \omega \in \Omega$$

Here Z is the unique normalizing constant for which

(2) 
$$\sum_{\omega \in \Omega} P(\omega) = 1.$$

In particular, if the B.V. function  $\phi \equiv 0$  on  $\partial D$ , then we get the G.R.F. with B.V. zero, given by

(3) 
$$P(\omega) = Z^{-1} \exp \left[ -\frac{1}{2} \sum_{x \in D} \sum_{y \in D} \omega(x) \omega(y) U(x, y) \right], \qquad \omega \in \Omega.$$

There is another interesting possibility. If D happens to be a rectangle then we can identify opposite points to produce a lattice *torus* T *without boundary*. In this case the G.R.F. on T is called a *periodic* G.R.F., and its probability measure P is defined by formula (3) with D replaced by T.

Definition of a Markov random field (M.R.F.). This definition is more intuitive but less explicit than that of a G.R.F. As in the case of the G.R.F. we assume given a B.V. function  $\phi:\partial D \to \{0, 1\}$  and shall define different M.R.F.'s on a domain D corresponding to different B.V. functions  $\phi$ . When D is replaced by a torus T, the B.V. function becomes unnecessary and we shall define a periodic M.R.F. A R.F.  $(\Omega, \mathfrak{F}, P)$  on D will be called a M.R.F. if it satisfies the three conditions (a), (b), (c) below. First

(a) 
$$P(\omega) > 0$$
 for each  $\omega \in \Omega$  (positivity).

In view of (a) we can define the one point conditional probabilities

(4) 
$$P[\omega(x) = 1 \mid \overline{\omega}(\cdot) = f(\cdot) \text{ on } \overline{D} - \{x\}], \quad x \in D,$$

by the elementary formula  $P(A \mid B) = P(AB)/P(B)$ . Let us clarify (4) which is written in dangerously brief notation. The map  $f: \overline{D} - \{x\} \rightarrow \{0, 1\}$  is quite arbitrary except that it must agree with the B.V. function  $\phi$  on  $\partial D$  (unless of course D = T in which case there is no boundary). Thus (4) represents the probability that  $\omega(x) = 1$  (that there is a particle at x), given that  $\omega(y) = f(y)$  at the points y of  $D - \{x\}$ , and given, in addition, the boundary values  $f(z) = \phi(z)$  for  $z \in \partial D$ . The latter are deterministic and will therefore be treated as events of probability one. Now the second condition defining a M.R.F. may be stated as

(b) the conditional probabilities in (4) depend only on the values of f at the points y in  $\overline{D}$  such that |y-x|=1 (nearest neighbor condition).

The third and last defining condition for a M.R.F. is

(c) the conditional probabilities in (4) are translation invariant, i.e., x, y in D implies

$$P[\omega(x) = 1 \mid \overline{\omega}(\cdot) = f(\cdot) \text{ on } \overline{D} - \{x\}] = P[\omega(y) = 1 \mid \overline{\omega}(\cdot) = g(\cdot) \text{ on } \overline{D} - \{y\}],$$

whenever f(x+z) = g(y+z) for all z with |z| = 1 (homogeneity).

Note that we have not yet proved the existence of a R.F. which satisfies (a), (b), and (c). Nevertheless, if  $(\Omega, \mathfrak{F}, P)$  is a R.F. on a domain D which satisfies

(a), (b), (c), then we shall say that  $(\Omega, \mathfrak{F}, P)$  is a M.R.F. on D with B.V. function  $\phi$  (or a periodic M.R.F. on D = T when D is made into a torus T without boundary).

# 3. The Main Theorem.

MAIN THEOREM: Every M.R.F. on a domain D with B.V. function  $\phi$  is a G.R.F. on D with B.V. function  $\phi$  and vice versa. The same statement holds for periodic random fields. The explicit correspondence between the conditional probabilities of the M.R.F. and the pair potential of the corresponding G.R.F. is given by equations (5), (6), (8), and (9) below.

In the proof we shall work on a fixed domain  $D \subset Z^r$  with a fixed B.V. function  $\phi$  and ignore the periodic case which can be handled by the same method. Step 1 of the proof will show that every G.R.F. is a M.R.F. Step 2 will then show that for every M.R.F. there exists a G.R.F. with the same conditional probabilities as the M.R.F. Finally the last step, step 3, will show that there exists at most one R.F. satisfying (a), (b), (c), with given conditional probabilities. It will be apparent that this completes the proof of the main theorem.

STEP 1: (Every G.R.F. is a M.R.F.). We start with a G.R.F. whose probability measure P is given by (1) and proceed to verify (a), (b), and (c). Condition (a) is obvious since exponentials are positive. To check (b) and (c) we compute the one point conditional probabilities

$$\begin{split} P\big[\omega(x) &= 1 \, \big| \, \bar{\omega} = f \text{ on } \overline{D} - \big\{x\big\}\big] \\ &= \frac{P\big[\omega(x) = 1 \text{ and } \bar{\omega} = f\big]}{P\big[\omega(x) = 1 \text{ and } \bar{\omega} = f\big] + P\big[\omega(x) = 0 \text{ and } \bar{\omega} = f\big]} \; . \end{split}$$

According to (1) the probability in the numerator is

$$Z^{-1}\exp\left\{-\frac{1}{2}\left[\sum_{s\in\overline{D}-\{x\}}\sum_{t\in\overline{D}-\{x\}}f(s)f(t)\;U(s,t)+U(x,x)+2\sum_{s\in\overline{D}-\{x\}}f(s)\,U(s,x)\right]\right\},$$

while the second probability in the denominator is

$$Z^{-1} \exp \left[ -\frac{1}{2} \sum_{s \in \overline{D} - \{x\}} \sum_{t \in \overline{D} - \{x\}} f(s) f(t) U(s,t) \right] \cdot$$

A brief calculation therefore gives, for each map  $f: \overline{D} \to \{0, 1\}$  such that  $f = \phi$  on  $\partial D$ ,

(5) 
$$P[\omega(x) = 1 \mid \bar{\omega} = f \text{ on } \overline{D} - \{x\}] = \frac{1}{1 + \exp\left[\frac{1}{2}U(x, x) + \sum_{s \in \overline{D} - \{x\}} f(s)U(s, x)\right]}$$

Let

$$U(0, 0) = u_0, U(0, l_k) = u_k, \quad 1 \le k \le \nu,$$

where  $l_k$  are the unit vectors with kth component +1 and all other components zero. Then the pair potential U is uniquely determined by these  $\nu+1$  parameters, and properties (ii) and (iii) further imply that (5) takes the form

(6) 
$$P[\omega(x) = 1 \mid \bar{\omega} = f \text{ on } \overline{D} - \{x\}] = \frac{1}{1 + \exp\left\{ (u_0/2) + \sum_{k=1}^{\nu} \left[ f(x + l_k) + f(x - l_k) \right] u_k \right\}}$$

Clearly the right hand side of (6) exhibits properties (b) and (c), i.e., the nearest neighbor property and translation invariance of the conditional probabilities. Therefore every G.R.F. is a M.R.F. with the same B.V. function (or without one in the periodic case).

STEP 2: (Existence of a G.R.F. with the same conditional probabilities as a given M.R.F.). While a G.R.F. in  $Z^r$  is determined by  $\nu+1$  real parameters (the constants  $u_0, u_1, \dots, u_r$  in the last section) it is not at all clear "how many" different M.R.F.'s there are. The conditional probabilities must clearly satisfy certain consistency conditions which reduce the number of possibilities. Indeed the key result of this section is that in  $Z^r$  there is a  $\nu+1$  parameter family of possible conditional probability functions. To make this precise let  $(\Omega, \mathfrak{F}, P)$  be a given M.R.F. on  $D \subset Z^r$  and introduce the conditional probabilities

(7) 
$$p_0 = P[\omega(x) = 1 \mid \bar{\omega}(x+y) = 1, \text{ whenever } \mid y \mid = 1],$$

$$p_k = P[\omega(x) = 1 \mid \bar{\omega}(x+l_k) = 0 \text{ and } \bar{\omega}(x+y) = 1 \text{ for all other } y \text{ with } \mid y \mid = 1], \quad 1 \le k \le \nu.$$

Let further  $p_k'$  be defined just as  $p_k$  except that  $l_k$  is replaced by  $-l_k$  in the definition of  $p_k$ . Then we have the following:

Consistency Lemma. Let  $(\Omega, \mathfrak{F}, P)$  be a M.R.F. on a sufficiently large domain  $D \subset \mathbb{Z}^r$ . Then all the conditional probabilities in (4) are uniquely determined by the  $\nu+1$  parameters  $p_0, p_1, \dots, p_r$ . In particular we have  $p_k' = p_k$ , for  $1 \le k \le \nu$ .

According to this lemma it will suffice to construct a G.R.F. with the same conditional probabilities  $(p_0, p_1, \dots, p_r)$  as the given M.R.F. If we had such a G.R.F. then we could assert, in view of (6), that

(8) 
$$p_{0} = \frac{1}{1 + \exp\left[\left(u_{0}/2\right) + 2\sum_{j=1}^{\nu} u_{j}\right]},$$

$$p_{k} = \frac{1}{1 + \exp\left[\left(u_{0}/2\right) + 2\sum_{j=1}^{\nu} u_{j} - u_{k}\right]}, \quad 1 \leq k \leq \nu.$$

Here  $(p_0, p_1, \dots, p_r)$  is the set of parameters of the given M.R.F. as defined

by (7), and  $(u_0, u_1, \dots, u_{\nu})$  specifies the potential of the G.R.F., since  $u_0 = U(x, x)$ ,  $u_k = U(x, x + l_k) = U(x, x - l_k)$  for  $1 \le k \le \nu$ . Observe now that (8) maps the  $\nu + 1$  dimensional Euclidean space  $-\infty < u_k < \infty$ ,  $0 \le k \le \nu$ , in a 1:1 manner onto the  $\nu + 1$  dimensional cube  $0 < p_k < 1$ ,  $0 \le k \le \nu$ . If we introduce the auxiliary parameters

$$\alpha_k = \log(p_k^{-1} - 1), \qquad 0 \le k \le n,$$

then one can in fact invert (8) explicitly to obtain

(9) 
$$u_0 = 4 \sum_{j=1}^{\nu} \alpha_j - (4\nu - 2)\alpha_0,$$
$$u_k = \alpha_0 - \alpha_k, \qquad 1 \le k \le \nu.$$

It follows then that, given a M.R.F. which is determined by  $(p_0, p_1, \dots, p_r)$ , we obtain a G.R.F. with the same conditional probabilities by choosing the potential U(x, y) which is determined by the values  $(u_0, u_1, \dots, u_r)$  in (9).

Proof of the consistency lemma: We begin by introducing, ad hoc, certain elementary identities valid for a completely arbitrary probability space  $(\Omega, \mathfrak{F}, P)$ . Let A, B, C denote three arbitrary events such that all possible intersections of A, B, C and of their complements  $\overline{A}, \overline{B}, \overline{C}$  have strictly positive probabilities (excluding of course the empty sets  $A\overline{A}$ , etc.). (We write  $\overline{A}$  for the complement of A, apologizing for the previous use of  $\overline{D}$  to denote  $D \cup \partial D$ , and AB for  $A \cap B$ .) It follows that all conditional probabilities of the form  $P(A \mid BC)$ ,  $P(AB \mid C)$ ,  $P(A \mid \overline{B}C)$ , etc., are well defined and strictly positive. We assert that

(10) 
$$\frac{1}{P(AB \mid C)} = \frac{1}{P(A \mid BC)} + \frac{1}{P(B \mid AC)P(A \mid \overline{B}C)} - \frac{1}{P(A \mid \overline{B}C)}$$
$$= \frac{1}{P(B \mid AC)} + \frac{1}{P(A \mid BC)P(B \mid \overline{A}C)} - \frac{1}{P(B \mid \overline{A}C)}.$$

The proof of the first part of (10) is immediate by substitution of the definitions  $P(AB \mid C) = P(ABC)/P(C)$ , etc. The second half follows from the first by observing that  $P(AB \mid C)$  depends symmetrically on A and B. It will further be convenient to work with the functions  $H(\cdot \mid \cdot)$  defined by

$$H(A \mid B) = \frac{1}{P(A \mid B)} - 1.$$

Direct substitution then reduces (10) to the simple form

(11) 
$$H(B \mid AC)H(A \mid \overline{B}C) = H(A \mid BC)H(B \mid AC).$$

Returning to the proof of the consistency lemma, we assume that  $(\Omega, \mathfrak{F}, P)$  is a given M.R.F. on a domain  $D \subset \mathbb{Z}^p$ , and we fix two neighboring points x and y in D. Then we define the following events A, B,  $C_1$ ,  $C_2$ , and C in  $\mathfrak{F}$ . Let A be the event that  $\omega(x) = 1$ , so that  $\overline{A} = \{\omega : \omega(x) = 0\}$ . Similarly  $B = \{\omega : \omega(y) = 1\}$ .

Next  $C_1$  is a description of the values of  $\bar{\omega}(\cdot)$  on all the  $2\nu$  neighbors of x except at the point y. For instance, if  $\nu=2$  and  $y=x-l_2$ , then  $C_1$  might be chosen as the event  $\{\omega:\bar{\omega}(x+l_1)=1,\ \bar{\omega}(x-l_1)=0,\ \bar{\omega}(x+l_2)=1\}$ . Note that we have expressed  $C_1$  in terms of  $\bar{\omega}$  instead of  $\omega$  since some of the neighbors of x may be points of the boundary  $\partial D$ . Similarly  $C_2$  will be a description of  $\bar{\omega}(\cdot)$  on the  $2\nu$  neighbors of y except x. Finally we define C as the intersection  $C=C_1C_2$ .

Consider now the conditional probability  $P(B \mid AC_2)$ , i.e., the probability that  $\omega(y) = 1$ , given that  $\omega(x) = 1$ , and that the values of  $\bar{\omega}$  at the remaining neighbors of y are described by  $C_2$ . In view of property (b) of the conditional probabilities of a M.R.F. there is no new information about  $\omega(y)$  conveyed by specifying  $C_1$  in addition to A and  $C_2$  (cf. the drawing for dimension  $\nu = 2$ ).

$$P(B \mid AC_2) = P(B \mid AC_1C_2) = P(B \mid AC),$$

$$P(A \mid BC_1) = P(A \mid BC_1C_2) = P(A \mid BC).$$

Therefore  $P(B \mid AC_2) = P(B \mid AC)$ ,  $P(A \mid BC_1) = P(A \mid BC)$ . Also replacing A by  $\overline{A}$  in the first identity and B by  $\overline{B}$  in the second,  $P(B \mid \overline{AC_2}) = P(B \mid \overline{AC})$ ,  $P(A \mid \overline{BC_1}) = P(A \mid \overline{BC})$ . From the definition of  $H(\cdot \mid \cdot)$  it then follows that

$$H(B \mid AC_2) = H(B \mid AC),$$
  $H(A \mid BC_1) = H(A \mid BC),$   
 $H(B \mid AC_2) = H(B \mid AC),$   $H(A \mid \overline{B}C_1) = H(A \mid \overline{B}C).$ 

Now substitution into (11) yields

(12) 
$$H(B \mid AC_2)H(A \mid \overline{B}C_1) = H(A \mid BC_1)H(B \mid AC_2).$$

The consistency lemma readily follows from (12) by making suitable choices for the events  $C_1$  and  $C_2$ . First let  $C_1$  be the event that  $\bar{\omega}(z) = 1$  at all the neighbors z of x except y, and  $C_2$  the event that  $\bar{\omega}(z) = 1$  at all the neighbors z of y except x. Recalling the definition of  $p_0$ ,  $p_k$ ,  $p'_k$  with  $1 \le k \le \nu$ , it is clear that (12) reads (in the case when  $y = x + l_k$ )

(13) 
$$\left(\frac{1}{p_0} - 1\right) \left(\frac{1}{p_k} - 1\right) = \left(\frac{1}{p_0} - 1\right) \left(\frac{1}{p_k'} - 1\right).$$

By proper choice of x and y we show that (13) holds for all  $1 \le k \le \nu$ . Hence we have

$$p_k' = p_k, \quad \text{for } 1 \le k \le \nu.$$

REMARK: There is the unpleasant possibility that the domain D is too small to contain pairs of neighbors x and  $y=x+l_k$  for each k,  $1 \le k \le \nu$ . In this case the conclusion of the consistency lemma is false. (That is why D was required to be large enough in its statement.) If D is too small, then only a subset of the conditional probabilities are determined by  $(p_0, p_1, \dots, p_{\nu})$ . But it can be checked that these are the only parameters needed to describe the corresponding G.R.F. Thus the conclusion of step 2 remains correct even when the domain D is too small for the consistency lemma to hold.

The rest of the proof of the consistency lemma proceeds by induction. Suppose we have shown that the parameters  $(p_0, p_1, \dots, p_r)$  determine uniquely all conditional probabilities of the form  $P[\omega(x)=1|\bar{\omega}=f \text{ on } \overline{D}-\{x\}]$  where f=1 on all but at most j of the 2v neighbors of x. Fix the point x, and let C be a description of  $\bar{\omega}=f$  on the neighbors of x such that f(y)=0 on exactly j+1 of the neighbors y of x. We then have to show that  $P[\omega(x)=1|C]$  is uniquely determined by  $(p_0, p_1, \dots, p_r)$ . Suppose now that f(y)=0 for  $y=x+l_k$ . (If this is not the case for any k then f(y)=0 for some y of the form  $x-l_k$  and the reasoning which follows will apply without change.) Let C' be the modification of C obtained by changing the value of f at  $y=x+l_k$  from 0 to 1. Let  $A=\{\omega:\omega(x)=1\}$ ,  $B=\{\omega:\omega(y)=1\}$ . Let  $C_1$  be the event C with the specification at  $y=x+l_k$  omitted, so that  $C=C_1\overline{B}$  and  $C'=C_1B$ . Finally let  $C_2$  be the event that  $\bar{\omega}(\cdot)=1$  at all the neighbors of y except x. Now consider equation (12) which after substitution of  $C=C_1\overline{B}$ ,  $C'=C_1B$  becomes

(15) 
$$H(B \mid AC_2)H(A \mid C) = H(B \mid AC_2)H(A \mid C').$$

We shall show that  $H(A \mid C)$ , and hence  $P(A \mid C)$  is uniquely determined by the parameters  $(p_0, p_1, \dots, p_r)$ . This will follow if the other three terms in (15) are so determined (note that  $H(B \mid AC_2) > 0$ ). Now the configuration described by C' contains exactly j zeros, that described by  $\overline{AC_2}$  contains exactly one zero, and that described by  $AC_2$  no zero at all. Thus it follows from the induction hypothesis that  $H(A \mid C')$  is determined by  $(p_0, \dots, p_r)$ , and from the fact that  $p_k' = p_k$  (already proved) that  $H(B \mid \overline{AC_2})$  is determined (since  $H(B \mid \overline{AC_2})$  is either  $p_k^{-1} - 1$  or  $(p_k')^{-1} - 1$ ). That completes the induction step from j to j+1, and hence the proof of the consistency lemma, which was already shown to complete step two of the proof of the main theorem.

Step 3 (Every M.R.F. is a G.R.F.). Let us review the logic of steps one and two. According to step two there exists, for every given M.R.F., a G.R.F. with the same conditional probabilities. According to step one this G.R.F. is also a M.R.F. But we have not yet shown that this is the same M.R.F. as the given M.R.F. we started with. Thus we have to show that there exists only one R.F. with the same one point conditional probabilities as a given M.R.F. Actually we shall do much more. Let  $(\Omega, \mathfrak{F}, P)$  be an arbitrary positive R.F., i.e., a R.F. such that  $P(\omega) > 0$  for each  $\omega \in \Omega$ . We shall show that every positive R.F. is uniquely deter-

mined by its conditional probabilities of the form  $P[\omega(x)=1 | \bar{\omega}(\cdot)=f(\cdot)]$  on  $\overline{D}-\{x\}$  for all possible choices of  $x\in D$  and  $f:\overline{D}-\{x\}\to\{0,1\}$ . But this assertion in turn can be generalized and, in the process, simplified. Let n=|D|, the cardinality of D, let  $\{x_1, x_2, \dots, x_n\}$  be an enumeration of D, and define  $A_n=\{\omega:\omega(x_n)=1\}$ . Then  $\mathfrak{F}$  is the algebra of subsets of  $\Omega$  generated by  $A_1$ ,  $A_2, \dots, A_n$ . Let  $\mathcal{G}_k$  be the subset of  $\mathfrak{F}$  consisting of all events of the form

(16) 
$$A = \bigcap_{\substack{1 \le i \le n \\ i \ne k}} B_i, \quad \text{where each } B_i = A_i \quad \text{or} \quad A_i.$$

Then the one point conditional probabilities of the R.F.  $(\Omega, \mathfrak{F}, P)$  are all the probabilities of the form

$$(17) P(A_k \mid A), A \in \mathfrak{S}_k, 1 \leq k \leq n.$$

The boundary values are of course thought of as included in A when needed, i.e., when  $x_k$  has neighbors in  $\partial D$ ; they cause no trouble since they are given with probability one. Our assertion now becomes that the probability measure P on  $(\Omega, \mathfrak{F})$  is uniquely determined by the probabilities in (17). This fact can be reformulated in general terms, without any reference to random fields.

LEMMA ON CONDITIONAL PROBABILITIES. Let  $\Omega$  be an arbitrary set with n given subsets  $A_1, A_2, \dots, A_n$ . Let  $\mathfrak{F}$  be the algebra of subsets of  $\Omega$  generated by  $A_1, \dots, A_n$ . Let P be a probability measure on  $(\Omega, \mathfrak{F})$  such that P(C) > 0 for all C in  $\mathfrak{F}$  except the empty set (so that all possible conditional probabilities  $P(A \mid B) = P(AB)/P(B)$  are defined when  $B \neq \emptyset$ ). Let  $\mathfrak{F}_k \subset \mathfrak{F}$  be the set of events of the form (16), and suppose we know all the conditional probabilities of (17). Then these conditional probabilities determine the probability measure P uniquely.

*Proof*: Let S denote a subset of  $N = \{1, 2, \dots, n\}$  and let

$$p(S) = P \left[ \bigcap_{i \in S} A_i \cap \bigcap_{j \notin S} A_j \right].$$

Then P will be completely determined on  $\mathfrak{F}$  if p(S) is known for every  $S \subset N$ . But the conditional probabilities in (17) can be written

$$(18) \quad P(A_k \mid A) = \frac{P(A_k \cap A)}{P(A)} = \frac{p(S \cup \{k\})}{p(S \cup \{k\}) + p(S)} = \left[1 + \frac{p(S)}{p(S \cup \{k\})}\right]^{-1},$$

if we choose S to correspond to A in such a way that

$$A = \bigcap_{i \in S} A_i \cap \bigcap_{j \in N - (S \cup \{k\})} A_j.$$

It follows from (18) that the conditional probabilities in (17) determine  $p(S \cup \{k\})/p(S)$  for every  $S \subset N$ , and  $k \in N$  such that  $k \notin S$ . Now let  $S = \{i_1, i_2, \dots, i_r\}$  and observe that

(19) 
$$\frac{p(S)}{p(\emptyset)} = \frac{p(\{i_1\})}{p(\emptyset)} \frac{p(\{i_1, i_2\})}{p(\{i_1\})} \cdot \cdot \cdot \frac{p(\{i_1, \dots, i_r\})}{p(\{i_1, \dots, i_{r-1}\})}$$

is then determined for every  $S \subset N$ . Summing (19) over all  $S \subset N$  determines  $p(\emptyset)$ , since  $\sum p(S) = 1$  and reapplying (19) shows that all p(S) are determined. That completes the proof of the lemma, and hence of the main theorem.

## 4. Examples of special Markov random fields.

I. ROTATION INVARIANT FIELDS. If we require that a G.R.F. be rotation invariant, then this means that the potential U defining it is rotation invariant. Hence the number of parameters is reduced to two, since we obtain

$$U(x, x) = u_0,$$
  $U(x, x + l_k) = u_k = u_1$  for  $1 \le k \le \nu$ .

Looking at the same R.F. as a M.R.F. then it follows from (8) that the conditional probabilities  $(p_0, p_1, \dots, p_r)$  satisfy

(20) 
$$p_0^{-1} - 1 = \exp\left[\frac{u_0}{2} + 2\nu u_1\right],$$
$$p_k^{-1} - 1 = \exp\left[\frac{u_0}{2} + (2\nu - 1)u_1\right], \qquad 1 \le k \le \nu.$$

It is easy to see, using (5), that all other conditional probabilities must then be rotation invariant as well. Thus the family of all rotation invariant M.R.F.'s on a domain  $D \subset Z^{\nu}$  is described by two parameters  $(p_0, p_1)$  regardless of the dimension  $\nu$ . This fact was far from obvious from the definition of a M.R.F.

II. FIELDS WITHOUT INTERACTION. Let us define lack of interaction in a G.R.F. by saying that the pair potential U(x, y) vanishes unless x=y. This means that  $u_0$  is arbitrary while  $u_1=u_2=\cdots=u_r=0$ . In view of (8) the conditional probabilities then satisfy  $p_0=p_1=p_2=\cdots=p_r$ , and going back to the Gibbs formula (5) shows that

$$P[\omega(x) = 1 \mid \overline{\omega} = f \text{ on } \overline{D} - \{x\}] = p_0,$$

independently of f. Thus lack of interaction in the sense of a trivial pair potential is equivalent to each conditional probability being independent of its condition. Equivalently, this means that the family of random variables  $\omega(x)$ ,  $x \in D$ , are mutually independent.

III. One-dimensional fields. Let

(21) 
$$M = \begin{pmatrix} M_{00} & M_{01} \\ M_{10} & M_{11} \end{pmatrix} = \begin{pmatrix} p & 1-p \\ 1-q & q \end{pmatrix}, \quad 0$$

be the transition matrix of a Markov chain  $\{\xi(n)\}$ ,  $n \ge 0$ , whose state space is the two point set  $\{0,1\}$ . Fix a positive integer r, and let  $D = \{1,2,\cdots,r\} \subset \mathbb{Z}^1$ . Let  $\phi$  be a given B.V. function  $\phi:\partial D \to \{0,1\}$ . Let  $\{\eta(1), \eta(2), \cdots, \eta(r)\}$  de-

note a family of random variables, with values in  $\{0,1\}$ , whose joint distribution is the same as the joint conditional distribution of the set  $\{\xi(1), \cdots, \xi(r)\}$  when it is subject to the condition  $\xi(0) = \phi(0), \xi(r+1) = \phi(r+1)$ . Then it is not hard to show that the collection  $\{\eta(x), x \in D\}$  is a M.R.F. on D with B.V. function  $\phi$ . Indeed one obtains the class of all possible M.R.F.'s with B.V. function  $\phi$  on D in the same way, by varying the parameters p, q in the definition of the matrix M in (21). It can be shown that the explicit correspondence between (p,q) in (21) and the conditional probabilities  $(p_0, p_1)$  of the M.R.F. is given by

(22) 
$$\frac{1}{p_0} - 1 = \frac{(1-p)(1-q)}{q^2}, \qquad \frac{1}{p_1} - 1 = \frac{p}{q},$$

which is a 1:1 map of the square  $\{0 onto the square <math>\{0 < p_0 < 1, 0 < p_1 < 1\}$ .

IV. Symmetric random fields. We want a M.R.F. or G.R.F. which is rotation invariant and possesses the additional symmetry property of *invariance* under interchange of the two symbols 0 and 1. In other words, let  $\pi_k(1)$  denote the probability that  $\omega(x) = 1$  given that  $\bar{\omega}(\cdot) = 1$  at exactly k of the  $2\nu$  neighbors of x. Define  $\pi_k(0)$  in the same way, but with 0 and 1 interchanged. Then we require that  $\pi_k(0) = \pi_k(1)$  for all  $0 \le k \le 2\nu$ . This will be the case if and only if

(23) 
$$u_0 + 2\nu u_1 = 0, \text{ or }$$

$$\frac{1}{p_0} - 1 = \exp\left[-\frac{u_0}{2}\right], \quad \frac{1}{p_1} - 1 = \exp\left[-\frac{u_0}{2}\left(1 - \frac{1}{\nu}\right)\right].$$

*Proof*: It follows from (6) that

$$[\pi_k(1)]^{-1} - 1 = \exp\left[\frac{u_0}{2} + ku_1\right],$$
$$[1 - \pi_k(0)]^{-1} - 1 = \exp\left[\frac{u_0}{2} + (2\nu - k)u_1\right].$$

This implies that  $\pi_k(0) = \pi_k(1)$  for all  $0 \le k \le 2\nu$  if and only if  $u_0 + 2\nu u_1 = 0$ .

5 Infinite random fields. Some brief remarks will place this note in the context of interesting recent work on the mathematics and physics of infinite random fields. The latter are of physical interest because the thermodynamic description of a lattice gas in  $Z^r$  is only obtained after passage to the limit from a finite rectangle  $D \subset Z^r$  to all of  $Z^r$ . (See [3] for a systematic treatment of the theory of this so-called thermodynamic limit.)

To define an infinite R.F., or a R.F. on all of Z', let  $\Omega = \{0, 1\}^{Z'}$ , and take for  $\mathfrak{F}$  the smallest Borel field of subsets of  $\Omega$  which contains the class  $\mathfrak{C}$  of all cylinder sets of the form

$$A = [\omega \mid \omega(x) = \epsilon(x) \text{ for } x \in D],$$

for all finite  $D \subset Z^r$  and all maps  $\epsilon: D \to \{0, 1\}$ . Finally let P be a probability measure on  $(\Omega, \mathfrak{F})$ . Then the probability triple  $(\Omega, \mathfrak{F}, P)$  is called a R.F. on  $Z^r$ .

Next, let us say that a R.F.  $(\Omega, \mathfrak{F}, P)$  on Z' is an infinite M.R.F. if it satisfies (a'), (b'), (c') below. First,

(a') 
$$P(C) > 0$$
 for all  $C \in \mathfrak{C}$ .

- If (a') holds then the conditional probabilities  $P[\omega(x)=1 | \omega=f \text{ on } D-\{x\}]$  are well defined for every finite set  $D \subset Z^r$  such that D contains x and also all its 2r neighbors. Thus it makes sense to require
- (b') the above conditional probabilities depend only on the values of f at the neighbors of x,
  - (c') the above conditional probabilities are translation invariant.

It follows from step 2 of our proof of the main theorem for finite random fields that even for an infinite M.R.F. the conditional probabilities may be assumed to be given by (5) or (6). Note however that the definition of an infinite R.F. by the Gibbs formula (3) is impossible, since  $P(\omega) = 0$  for each  $\omega$  (the set  $\Omega$  being uncountable). This led Dobrushin [2] to define an infinite G.R.F. on  $Z^r$  by the requirement that it be a M.R.F. with conditional probabilities given by (6), and to study the following basic questions:

- (I) Does there exist such a R.F. for every possible set of parameter values  $(u_0, u_1, \dots, u_{\nu})$ ?
  - (II) If so, is it unique?

The answer to the existence question (I) is YES. (See Dobrushin [1], Theorem 1.) The exciting answer to the uniqueness question (II), on the other hand, is SOMETIMES, i.e., there is uniqueness for certain but not for all parameter sets  $(u_0, u_1, \dots, u_r)$ .

For a more detailed answer to II, consider first the one dimensional case. Then there is a unique infinite G.R.F. with given  $(u_0, u_1)$ , and it is not hard to construct it from the Markov chain on  $\{0, 1\}$  with transition matrix M in (21). There is a unique strictly stationary process  $\{\zeta(n)\}, -\infty < n < \infty$ , with state space  $\{0, 1\}$ , such that  $\{\zeta(n)\}$  for  $n \ge 0$ , conditioned on  $\zeta(0) = 0$  (or 1) is a Markov chain with transition matrix M and initial state 0 (or 1). It is not hard to show that this process  $\{\zeta(n)\}, -\infty < n < \infty$ , is the unique G.R.F. on  $Z^1$  with parameters  $(u_0, u_1)$  if (p, q) in (21) is chosen according to (22). Indeed this uniqueness is a special case of [1], Theorem 3.

Exercise: Show that the unique one dimensional infinite M.R.F. with  $U(x, x) = u_0$ ,  $U(x, x \pm l_k) = u_1$  has the particle density

$$\rho = P[\omega(x) = 1] = \left[\frac{1-q}{1-p} + 1\right]^{-1} = \frac{1}{2} \left[1 + \frac{h_1 - 1}{\sqrt{(h_1 - 1)^2 + 4h_0}}\right], \quad x \in \mathbb{Z}^1,$$

where (p, q) are the parameters in (21), and

$$h_0 = p_0^{-1} - 1 = \exp\left[\frac{u_0}{2} + 2u_1\right], \qquad h_1 = p_1^{-1} - 1 = \exp\left[\frac{u_0}{2} + u_1\right].$$

In dimension  $\nu \ge 2$  the situation is quite different. Uniqueness can be shown only for certain values of the parameters  $(u_0, u_1, \dots, u_{\nu})$ , for example by use of Theorem 2 of [1]. The simplest known examples of nonuniqueness are obtained for the symmetric random fields in example IV of the last section. In other words, let  $\nu \ge 2$  and assume that  $u_0 + 2\nu u_k = 0$  for  $1 \le k \le \nu$ , so that (23) holds. Then the uniqueness question becomes:

Does there exist a unique infinite M.R.F. (or G.R.F.) on Z',  $\nu \ge 2$  with conditional probabilities

(24) 
$$p_0 = \frac{1}{1 + \exp[-(u_0/2)]},$$

$$p_1 = p_2 = \cdots = p_{\nu} = \frac{1}{1 + \exp[-(u_0/2)(1 - (1/\nu))]}$$
?

The answer is yes, if  $u_0$  is sufficiently small. On the other hand it is no, for all sufficiently large  $u_0$  (see [2], pp. 306–308). In the physical description of a gas by such a R.F. the parameter  $u_0$  is inversely proportional to the absolute temperature T. The existence of two infinite M.R.F.'s satisfying (24) for all large  $u_0$  can be interpreted as the coexistence of two distinct phases (gas and liquid) of a substance when the temperature T is sufficiently low.

For an indication of the proof of nonuniqueness, let  $D_N$  be a sequence of cubes of side length N in  $Z^{\nu}$ ,  $\nu \ge 2$ . Let  $\{\omega_N^{(0)}(x), x \in D_N\}$  and  $\{\omega_N^{(1)}(x), x \in D_N\}$  be finite symmetric random fields on  $D_N \subset Z^{\nu}$ , the former with B.V. function  $\phi = 0$  on  $\partial D_N$ , the latter with B.V.  $\phi = 1$  on  $\partial D_N$ . By combinatorial arguments, made possible by the symmetry of these fields, it is shown in [2] that for sufficiently large  $u_0$  there exists a constant  $\gamma < \frac{1}{2}$  such that

$$P[\omega_N^{(0)}(x) = 1] \le \gamma < \frac{1}{2}, \qquad P[\omega_N^{(1)}(x) = 1] \ge 1 - \gamma > \frac{1}{2},$$

for all  $x \in D_N$ , and every positive integer N. This suggests the existence of two infinite G.R.F.'s, a low density "gas"  $\{\omega^{(0)}(x), x \in Z^r\}$ , and a high density "liquid"  $\{\omega^{(1)}(x), x \in Z^r\}$ , which have particle densities

$$\rho_0 = P[\omega^{(0)}(x) = 1] \le \gamma, \quad \rho_1 = P[\omega^{(1)}(x) = 1] \ge 1 - \gamma, \quad x \in \mathbb{Z}^r,$$

and which have both the same conditional probabilities  $(p_0, p_1, \dots, p_r)$ , given by (24) in terms of the same value of  $u_0$ . The proof ([2], p. 308) is based on a simple compactness argument: the set of all infinite R.F.'s is made into a compact, complete, metric space in which the two sequences  $\{\omega_N^{(0)}\}$  and  $\{\omega_N^{(1)}\}$  have the limit points  $\omega^{(0)}$  and  $\omega^{(1)}$  which are infinite R.F.'s with the desired properties.

#### References

- 1. R. L. Dobrushin, Description of a random field by means of conditional probabilities and the conditions governing its regularity, Theory of probability and its applications (English translation of Teoriia Veroiatn.), 13 (1968) 197–224.
- 2. ——, The problem of uniqueness of a Gibbs random field and the problem of phase transition, Functional Analysis and its applications (English translation of Funktionalny Analis), 2 (1968) 302-312.
  - 3. David Ruelle, Statistical Mechanics, Benjamin, New York, 1969.