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Generation of Random Fields Defined on a Cluster of Points when the Random Field Has a Given Site-to-Site Correlation

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A computational scheme for generating a random field defined on a cluster of points with the random field having a site-to-site correlation function close to some desired correlation function is presented. It is assumed that the quantity to be simulated either is, or may be related to, a random quantity having a joint normal distribution with the same variance at each site in the cluster and with a correlation coefficient between sites depending only on the separation of the sites. The scheme can be used for any random quantity which is defined at lattice sites in a cluster and may be applied, for example, to both exchange fields and AB-alloys.

1. INTRODUCTION

In this paper we describe a computational scheme for generating random clusters with a correlation function close, in the statistical sense, to some desired correlation function. The scheme was developed for use in calculations of photoemission from ferromagnetic metals above the Curie temperature [1, 2] in which we wanted to simulate exchange fields with varying degrees of short range order in a more general way than in previous calculations [3]. These calculations of photoemission use the recursion method [4, 5] which is a method of computing the density of states of a solid using a cluster of $\sim 10^3$ atoms [4, 6] and is particularly useful for studying disordered solids [7, 8]. However, the scheme we present here is not restricted to the simulation of exchange fields and nor is it restricted to computations by the recursion method.

The scheme is based on a Fourier series expansion of the randomly varying quantity and can be used for any random quantity which is defined at lattice sites in a cluster. The quantity may be continuously varying or discrete-valued, as in an AB-alloy, and may be a vector, for example, an exchange field.

The basic scheme for continuous scalar quantites is outlined in Section 2. The

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extension to vector quantities is discussed in Section 3. In some circumstances it is desirable to scale the components of each vector so that the magnitude of the vector quantity is the same on each site. This alters the correlation coefficient between vectors at different sites and also alters the probability distributions of the components of the vector. The extension to discrete valued quantities is also discussed in Section 3. Next, in Section 4, we show how to set up a cluster with a non-zero average of the quantity and discuss the way in which the expressions for the correlation coefficient and the probability distributions are changed. Finally, in Section 5 we discuss the limitations of the method, the most important of which is the assumption that the underlying distribution is a joint normal distribution with the same variance on each site and a correlation coefficient depending only on the separation between sites, and we also discuss the advantages of the method.

2. Outline of Method

Suppose we have a continuous, real-valued, scalar quantity M defined at N lattice sites labelled by $\boldsymbol{l}$. Then $M(\boldsymbol{l})$ can be expanded in a Fourier series

$$M(\boldsymbol{l}) = \sum_{\mathbf{q}} (A(\mathbf{q}) \cos \mathbf{q} \cdot \boldsymbol{l} + B(\mathbf{q}) \sin \mathbf{q} \cdot \boldsymbol{l}), \tag{1}$$

where $A(\mathbf{q})$ and $B(\mathbf{q})$ are random variables since $M(\boldsymbol{l})$ is a random variable. We want to choose $A(\mathbf{q})$ and $B(\mathbf{q})$ so that the expected value of the correlation coefficient of $M(\boldsymbol{l})$ and $M(\boldsymbol{l}')$, defined by

$$\rho(\boldsymbol{l}, \boldsymbol{l}') = \frac{\operatorname{cov}(M(\boldsymbol{l}), M(\boldsymbol{l}'))}{[\operatorname{var}(M(\boldsymbol{l}))\operatorname{var}(M(\boldsymbol{l}'))]^{1/2}}, \tag{2}$$

has some desired value which depends only on the separation $\boldsymbol{l} - \boldsymbol{l}'$. If we assume (i) that $A(\mathbf{q})$, $B(\mathbf{q})$, $A(\mathbf{q}')$, and $B(\mathbf{q}')$ are mutually independent random variables and (ii) that the random variables $C(\mathbf{q})$ and $\varepsilon(\mathbf{q})$ in the equivalent form of (1)

$$M(\boldsymbol{l}) = \sum_{\mathbf{q}} C(\mathbf{q}) \cos(\mathbf{q} \cdot \boldsymbol{l} + \varepsilon(\mathbf{q}))$$

are independent with the phases $\varepsilon(\mathbf{q})$ being uniformly distributed on the interval 0 to 2π then $A(\mathbf{q})$ and $B(\mathbf{q})$ both have normal distributions with mean 0 and variance σ_q^2 and the $M(\boldsymbol{l})$ have normal distributions with mean 0 and variance $\sigma^2 = \sum_{\mathbf{q}} \sigma_{\mathbf{q}}^2$ (see Appendix 1). We then obtain

$$\rho(\boldsymbol{l} - \boldsymbol{l}') = (1/\sigma^2) \sum_{\mathbf{q}} \sigma_{\mathbf{q}}^2 \cos(\mathbf{q} \cdot (\boldsymbol{l} - \boldsymbol{l}')) \tag{3}$$

which can be inverted to give

$$\sigma_{\mathbf{q}}^2 = (\sigma^2/N) \sum_{\mathbf{l}} \rho(\boldsymbol{l}) \cos \mathbf{q} \cdot \boldsymbol{l} \tag{4}$$

if we assume, without loss of generality, that $\sigma^2_{-\mathbf{q}} = \sigma^2_{\mathbf{q}}$ (see Appendix 2). In principle, therefore, we could choose a form for $\rho(\boldsymbol{l})$, calculate $\sigma^2_{\mathbf{q}}$, generate $A(\mathbf{q})$ and $B(\mathbf{q})$ from normal distributions with mean 0 and variance $\sigma^2_{\mathbf{q}}$, and compute (1). In practice, since it is difficult to choose $\rho(\boldsymbol{l})$ to ensure $\sigma^2_{\mathbf{q}}$ is positive when dealing with finite clusters, it is better to choose a form for $\sigma^2_{\mathbf{q}}$ and calculate $\rho(\boldsymbol{l})$. When either (3) or (4) is evaluated numerically the set of $\mathbf{q}$'s or set of $\boldsymbol{l}$'s used must be those with the shortest $|q|$ or $|l|$ consistent with the periodic boundary conditions $M(l_x, l_y, l_z) = M(l_x + L_x, l_y, l_z) = M(l_x, l_y + L_y, l_z) = M(l_x, l_y, l_z + L_z)$, where L_x, L_y, L_z are the lengths of the sides of the cluster in the x-, y-, and z-directions, implied by the use of the Fourier series expansion. (In the context of solid state physics this means the q's must lie in the first Brillouin zone [9].)

3(a) *Vector Quantities*

When the random quantity at each site is a vector, for example, an exchange field, we should, in general, include correlations between different components

$$\rho_{\alpha\beta}(\boldsymbol{l}, \boldsymbol{l}') = \frac{\operatorname{cov}(M_\alpha(\boldsymbol{l}), M_\beta(\boldsymbol{l}'))}{\sqrt{\operatorname{var}(M_\alpha(\boldsymbol{l}))\operatorname{var}(M_\beta(\boldsymbol{l}'))}}.$$

However, to obtain a spherically symmetric distribution of the vectors $M(\mathbf{q})$, in the sense that all directions are equally likely for each vector, we must have

$$\rho_{\alpha\beta}(\boldsymbol{l}, \boldsymbol{l}') = 0 \qquad \text{if} \quad \alpha \neq \beta.$$

In the absence of any information concerning the behaviour of the correlation functions there are two simple procedures which may be followed. The first is to assume that the components of $\mathbf{M}$ are independent so that the problem of obtaining $\mathbf{M}(\boldsymbol{l})$ reduces to the problem of obtaining each $M_\alpha(\boldsymbol{l})$. Each $M_\alpha(\boldsymbol{l})$ is taken to have a normal distribution with mean 0 and variance σ^2. Consequently, the direction of $\mathbf{M}(\boldsymbol{l})$ has a spherically symmetric probability distribution. For a three-dimensional vector $\mathbf{M}$ the probability density function for $|\mathbf{M}|$ is

$$p(|\mathbf{M}|) = \frac{|\mathbf{M}|^2}{\sigma^3}\sqrt{\frac{2}{\pi}}\exp\left(\frac{-|\mathbf{M}|^2}{2\sigma^2}\right)$$

(see Fig. 1) which has mean $\sigma\sqrt{8/\pi}$ and variance $\sigma^2(3 - 8/\pi)$. The estimator for the correlation coefficient is

$$\hat{\rho}(\boldsymbol{l}) = \frac{(\sum_{\boldsymbol{l}'} M(\boldsymbol{l}') \cdot M(\boldsymbol{l} + \boldsymbol{l}'))}{\sum |M(\boldsymbol{l}')|^2}. \tag{5}$$

Sometimes the variation of the length of the vector quantity is less important than the variation in its direction; for example, in local band theories of itinerant electron ferromagnets the magnitude of the exchange field is often assumed not to vary from site to site. In such cases the assumption that different components are

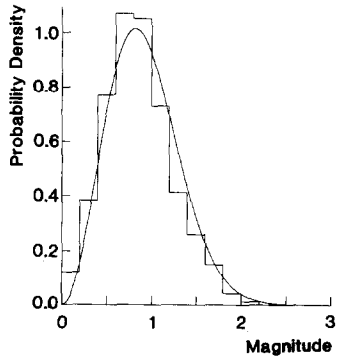

FIG. 1. The probability density $p(|\mathbf{M}|)$, where $\mathbf{M}$ is a three dimensional vector. The curve shows

$$p(|\mathbf{M}|) = \frac{|\mathbf{M}|^2}{\sigma^2}\sqrt{\frac{2}{\pi}}\exp\frac{-|\mathbf{M}|^2}{2\sigma^2}$$

and the histogram shows the distribution of $|\mathbf{M}|$ on a particular 864 atom fcc cluster.

independent is inappropriate. The alternative procedure is to assume that $|\mathbf{M}|$ is the same on each site so that each component of $\mathbf{M}(l)$ is normalised. Each $M_\alpha(l)$ then has a uniform distribution on $[-1.0, 1.0]$ and Eq. (5) gives the estimator

$$\hat{\eta}(l) = \sum_{l'} \hat{\mathbf{M}}(l') \cdot \hat{\mathbf{M}}(l' + l) \tag{6}$$

for the expected value of the cosine of the angle between vectors on sites separated by l. The relationship between

$$\eta = E(\cos\theta(l))$$

and the correlation coefficient originally used to find the unnormalised $\mathbf{M}(l)$ is

$$\eta = a\rho(l), \tag{7}$$

where a is a function of ρ (see Appendix 3). Values of a are given in Table I.

3(b) *AB-Alloys*

In this section we describe how the method may be applied to a two-valued random quantity. The basis of our method is that the random quantity at each site is continuously varying so that it may be expanded in a Fourier series. To apply the method to a two-valued variable it is therefore necessary to develop a mapping between the probability distribution for a continuous-valued random quantity which can be expanded in a Fourier series and that for a two-valued random quantity.

TABLE I

Conversion Factor a, Relating the Correlation Coefficient between Vectors on Different Sites Used to Set Up a Cluster of Vectors of Varying Length and the Expected Value η of the Cosine of the Angle between Vectors on Different Sites as a Function of ρ

ρ	a	η
0.0	0.8488	0.0
0.05	0.8490	0.0425
0.10	0.8497	0.0850
0.15	0.8508	0.1276
0.20	0.8523	0.1705
0.25	0.8542	0.2136
0.30	0.8567	0.2570
0.35	0.8597	0.3009
0.40	0.8632	0.3453
0.45	0.8673	0.3903
0.50	0.8720	0.4360
0.55	0.8774	0.4826
0.60	0.8837	0.5302
0.65	0.8908	0.5790
0.70	0.8890	0.6293
0.75	0.9086	0.6815
0.80	0.9197	0.7358
0.85	0.9328	0.7929
0.90	0.9489	0.8540
0.95	0.9694	0.9209
1.00	1.0000	1.0000

Let the two possible values of a two-valued variable T be A and B with probabilities

$$P(T=A)=p, \qquad P(T=B)=q=1-p,$$

so p is the concentration of A-sites and q is the concentration of B-sites, and define a new random variable

$$\begin{aligned} Y &= \sqrt{q/p} && \text{if} \quad T=A \\ &= -\sqrt{p/q} && \text{if} \quad T=B. \end{aligned}$$

Then

$$P(Y=\sqrt{q/p})=p, \qquad P(Y=-\sqrt{p/q})=q,$$
$$E(Y)=0, \qquad \operatorname{var}(Y)=1.$$

We can write the joint probability distribution for Y at two sites as

$$P(Y_1, Y_2) = P(Y_1)\, P(Y_2)(1 + \eta_{12} Y_1 Y_2), \tag{8}$$

where

$$\operatorname{cov}(Y_1, Y_2) = \eta_{12}.$$

Consequently,

$$\rho(Y_1, Y_2) = \eta_{12},$$

which defines a correlation coefficient for the system of two-valued random quantities.

With these definitions the expected value of Y at site 2 given the value of Y at site 1 is given by

$$E(Y_2 \mid Y_1) = \eta_{12} Y_1.$$

We can relate this to a normally distributed random variable x with mean μ and variance 1 by taking T to have the value A when $x > 0$ and the value B when $x < 0$ so that

$$p = P(A) = \int_0^\infty 1/\sqrt{2\pi} \exp(-\tfrac{1}{2}(x-\mu)^2)\, dx. \tag{9}$$

We also take

$$P(A_1, \ldots, A_N) = \int_0^\infty dx_1 \cdots \int_0^\infty dx_N \frac{1}{\sqrt{(2\pi)^N \operatorname{Det} V}} \exp(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T V^{-1}(\mathbf{x}-\boldsymbol{\mu})),$$

where the covariance matrix

$$V = \begin{pmatrix} 1 & \rho_{12} & \cdots & \rho_{1N} \\ \vdots & & & \\ \rho_{1N} & \rho_{2N} & \cdots & 1 \end{pmatrix}.$$

In particular, we take

$$P(A_1, A_2) = \int_0^\infty dx_1 \int_0^\infty dx_2 \frac{1}{2\pi\sqrt{1-\rho_{12}}} \times \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \begin{pmatrix} 1 & \rho_{12} \\ \rho_{12} & 1 \end{pmatrix}^{-1} (\mathbf{x}-\boldsymbol{\mu})\right). \tag{10}$$

It follows from (9) that

$$P(A_1, A_2) = p^2(1 + \eta_{12} q/p),$$

so

$$\eta_{12} = \frac{P(A_1, A_2) - p^2}{pq}. \tag{11}$$

Thus we can set up a cluster with a two-valued random variable with the concentration parameter p and two-site correlation coefficient η_{12} by generating a normally distributed random variable x on the cluster with mean μ related to p by (9) and correlation coefficient ρ related to η_{12} by (10) and (11).

4. Non-Zero Average Magnetisation

In this section we discuss how to set up a cluster in which a random vector quantity has a non-zero average value, considering, in particular, a three-dimensional quantity (for example, the exchange field in our calculations of photoemission from ferromagnets at high temperatures [1, 2]). There are two approaches to generating a random field with a non-zero average value, both based on the fact that the average value of the field on the cluster $\bar{\mathbf{M}}$ is given by

$$\bar{\mathbf{M}} = \mathbf{A}_0.$$

In the first approach we retain spherical symmetry while in the second we introduce a symmetry-breaking term. In our calculations in which we simulated an exchange field in a ferromagnet [1, 2] we used the second approach because it is closer to the physical situation and because the resulting correlation coefficient is closer to the desired correlation coefficient (see below). However, we discuss both approaches, partly to indicate the difference between the two approaches and partly because there may be situations in which it is not desirable to introduce a symmetry-breaking term.

In the first approach we use the result

$$E(|\mathbf{A}_0|) = \sqrt{8/\pi}\,\sigma_0,$$

so we can adjust the expected value of $|\mathbf{A}_0|$ by adjusting the proportion of the total variance which is in the $q = 0$ mode. (In the original approach σ_0 is small for large clusters since $\sigma_0 \sim 1/N$.) Because

$$\sum_{\mathbf{q}} \sigma_{\mathbf{q}}^2 = \sigma^2$$

setting σ_0 means that all the rest of the $\sigma_{\mathbf{q}}$ must be changed. A consistent way of doing this is to take the

$$\sigma_{\mathbf{q}}^2 = \hat{r}(\mathbf{q})\,\sigma^2$$

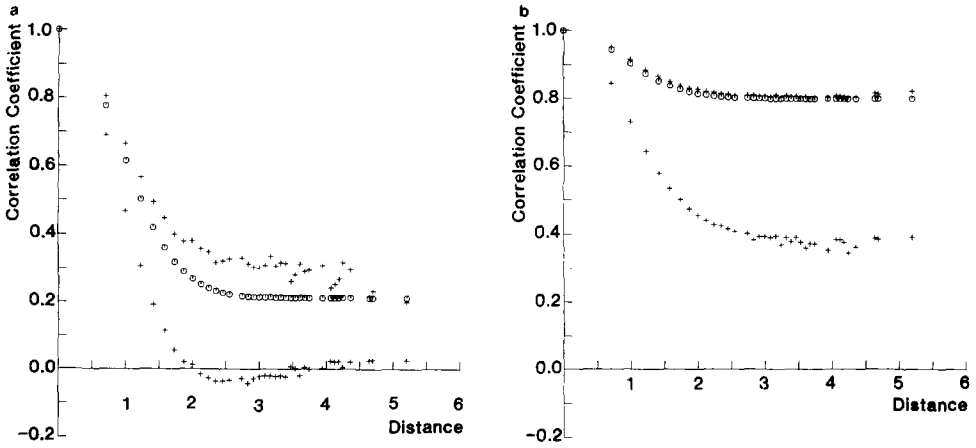

FIG. 2. The expected correlation coefficient $\rho(|l|)$ and the actual correlation coefficients calculated for 864 atom fcc clusters set up to have a non-zero average field by fixing the variance of the $\mathbf{q}=0$ mode (Method 1). (a) Magnitude of expected average field, 0.5; (○) expected $\rho(|l|)$; (+) actual $\rho(|l|)$ for two clusters. The magnitudes of the actual average fields on the two clusters are 0.634 (upper set) and 0.120 (lower set). (b) Magnitude of expected average field, 0.9; (○) expected $\rho(|l|)$; (+) actual $\rho(|l|)$ for two clusters. The magnitudes of the actual average fields on the two clusters are 1.063 (upper set) and 0.401 (lower set). (The units of the field are such that $E(|M|^2)=1.0$ and the distance is in units of the lattice cosntant.) From these curves it can be seen that the actual $\rho(|l|)$ and the actual average field may be quite far from the expected $\rho(|l|)$ and the expected average field for clusters set up by this method.

corresponding to some correlation coefficient $\hat{\rho}(l)$ and obtain a set of

$$\sigma_{\mathbf{q}}^2 = r(\mathbf{q})\,\sigma^2$$

by setting

$$r(0) = r_0, \qquad \mathbf{q}=0,$$

$$r(\mathbf{q}) = \frac{1-r_0}{1-\hat{r}(0)}\,\hat{r}(\mathbf{q}), \qquad \mathbf{q}\neq 0,$$

where r_0 is chosen to produce the desired value for $E(|\mathbf{A}_0|)$. The new correlation coefficient corresponding to the $\sigma_{\mathbf{q}}^2$ is then given by

$$\rho(l) = \left(\frac{r(0)-\hat{r}(0)}{1-\hat{r}(0)}\right) + \left(\frac{1-r(0)}{1-\hat{r}(0)}\right)\hat{\rho}(l)$$

(see Fig. 2). In this approach $E(\mathbf{A}_0)=0$ and the separate probability distributions for the individual $M_\alpha(l)$ and for $|\mathbf{M}(l)|$ are unchanged.

In the second approach, we set

$$E(\mathbf{A}_0) = (0, 0, \bar{m}),$$

choosing the z-axis to lie in the direction of the desired average field, so

$$|E(\mathbf{A}_0)| = \bar{m}.$$

Since

$$E(|\mathbf{M}(\boldsymbol{l})|^2) = 3\sigma^2$$

and

$$\begin{aligned} E(|\mathbf{M}(\boldsymbol{l})|^2) &= \sum_{\mathbf{q}} E(|M(\mathbf{q}, \boldsymbol{l})|^2) \\ &= 3 \sum_{\mathbf{q}} \sigma_{\mathbf{q}}^2 + \bar{m}^2 \end{aligned}$$

we require

$$1 = \sum_{\mathbf{q}} r(\mathbf{q}) + r_0,$$

where

$$r_0 = \bar{m}^2/3\sigma^2,$$

that is,

$$\sum_{\mathbf{q}} r(\mathbf{q}) = 1 - r_0.$$

Hence the required $r(\mathbf{q})$ can be found from the $\hat{r}(\mathbf{q})$ corresponding to some $\hat{\rho}(\boldsymbol{l})$ by

$$r(\mathbf{q}) = (1 - r_0)\, \hat{r}(\mathbf{q}).$$

The new correlation coefficient corresponding to the $\sigma_{\mathbf{q}}^2$ is

$$\rho(\boldsymbol{l}) = r_0 + (1 - r_0)\, \hat{\rho}(\boldsymbol{l})$$

(see Fig. 3). The probability distributions for the $M_\alpha(\boldsymbol{l})$ are

$$p(M_\alpha) = \frac{1}{\sigma \sqrt{2\pi(1 - r_0)}} \exp\left(\frac{-M_\alpha^2}{2\sigma^2(1 - r_0)}\right), \qquad \alpha = 1, 2,$$

$$p(M_3) = \frac{1}{\sigma \sqrt{2\pi(1 - r_0)}} \exp\left(\frac{-(M_3 - \bar{m})^2}{2\sigma^2(1 - r_0)}\right),$$

$$p(|\mathbf{M}|) = \frac{|\mathbf{M}|}{\sigma^2 \sqrt{6\pi(1 - r_0)\, r_0}} \left[\exp\left(\frac{-(|\mathbf{M}| - \bar{m})^2}{2\sigma^2(1 - r_0)}\right) - \exp\left(\frac{-(|\mathbf{M}| + \bar{m})^2}{2\sigma^2(1 - r_0)}\right)\right]$$

(see Fig. 4).

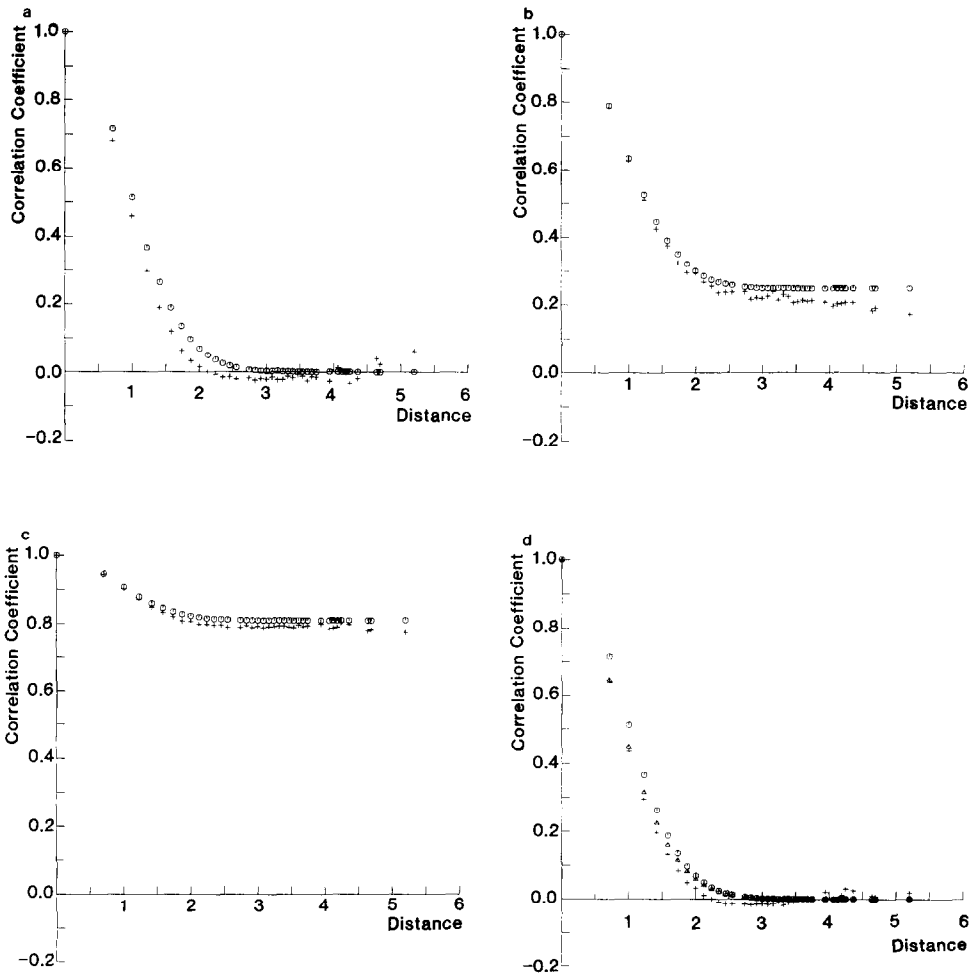

FIG. 3. Correlation coefficients for 864 atom fcc clusters set up to have a non-zero average field by fixing the mean of the $\mathbf{q}=0$ mode (Method 2) compared with their expected values. The distance is in units of the lattice constant. (a), (b), and (c) show results for clusters in which $|M(l)|$ varies from site to site. In (a) the expected average field is 0, in (b) it is 0.5, and in (c) it is 0.9 (in units such that $E(|\mathbf{M}|^2)=1.0$. (d), (e), (f), and (g), show results for clusters in which $|M(l)|$ is the same on each site. Both the correlation coefficient for the unnormalised cluster $\rho(|l|)$ and the expected value of the cosine of the angle between moments on site separated by $|l|$, $\eta(|l|)$, are shown on these graphs. In (d) and (e) the expected average field is 0. These two graphs show the scatter of the actual $\eta(|l|)$ about the expected $\eta(|l|)$. In (f) the expected average field is 0.5 and in (g) it is 0.9. These are the expected average fields in units such that $E(|\mathbf{M}|^2)=1.0$ for the unnormalised cluster, from Table II they should be close to those for the normalised cluster, and these graphs show that the average fields for the normalised and unnormalised clusters are the same within the statistical noise.

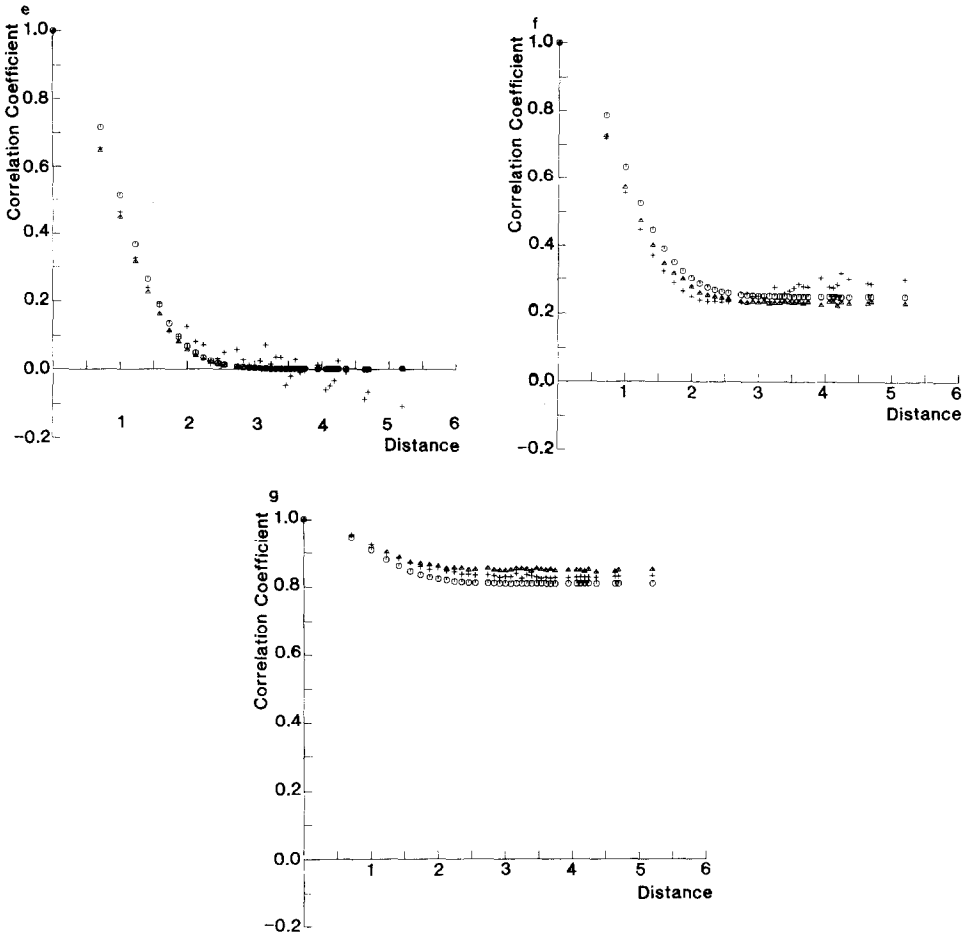

FIG. 3—*Continued.*

If the cluster is set up with a non-zero average field and then each $M(\boldsymbol{l})$ is normalised then the average value of the normalised field will be different from the input average value. In the second approach the expected value of the final average field, $E(M_3)$, where $M_3 = \cos\theta$ is the component of the normalised field in the direction of the input average field, can be found numerically either from

$$E(\cos\theta) = \int_0^{\pi} \cos\theta \int_0^{\infty} p(|\mathbf{M}|, \cos\theta)\, d|\mathbf{M}|\, d\theta$$

or from

$$E(\cos\theta) = \int_0^{\infty} E(\cos\theta \mid |\mathbf{M}|)\, p(|\mathbf{M}|)\, d\,|\mathbf{M}|.$$

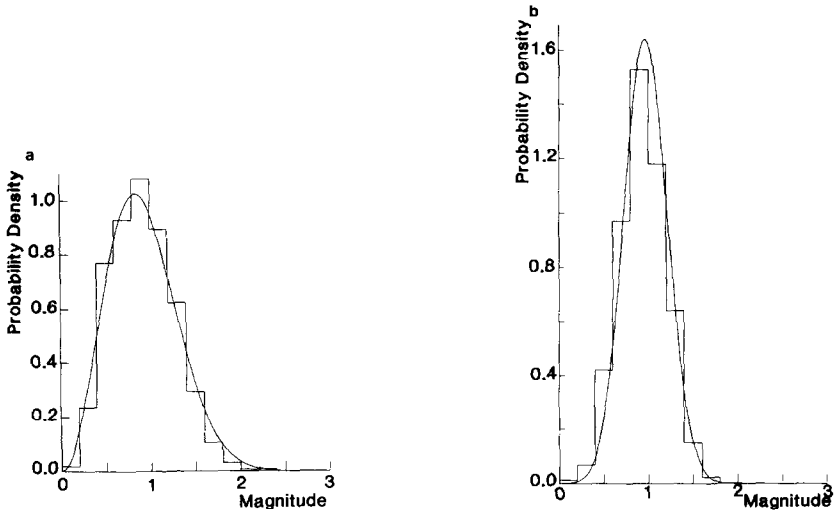

FIG. 4. The probability density $p(|\mathbf{M}|)$ for clusters set up to have a non-zero average field $(0, 0, \bar{m})$ using Method 2. The curve shows

$$p(|\mathbf{M}|) = \frac{|\mathbf{M}|}{\sigma^2\sqrt{6\pi(1-r_0)\,r_0}}\left[\exp\left(\frac{-(|\mathbf{M}|-\bar{m})^2}{2\sigma^2(1-r_0)}\right) - \exp\left(\frac{-(|\mathbf{M}|+\bar{m})^2}{2\sigma^2(1-r_0)}\right)\right]$$

and the histogram shows the distribution of $|\mathbf{M}|$ for an 864 atom fcc cluster with (a) expected average field 0.5, (b) expected average field 0.9 in units such that $E(|\mathbf{M}|^2) = 1.0$.

TABLE II

Expected Value of the z Component $\hat{M}_z$ of the Unit Vector $\hat{\mathbf{M}}$ for a Given Expected Value of the Variable Length Vector in the z-Direction M_z (in Units of Ground State Magnetisation $M_{g.s.}$)

$M_z/M_{g.s.}$	$\hat{M}_z$
0.0	0.000
0.1	0.092
0.2	0.186
0.3	0.281
0.4	0.380
0.5	0.484
0.6	0.593
0.7	0.706
0.8	0.820
0.9	0.922
1.0	1.000

The results are shown in Table II. Because these results do not depend on the direction of the input average field they also give the relation between the input average field and the final average field when a field with a non-zero average value is set up using the first approach.

The relation between η defined by (7) and ρ defined by (2) in the first approach is the same as if the expected average field were zero because the probability density functions for the $M_\alpha(l)$ are the same. In the second approach this relation must be found numerically from the probability density function (see Appendix 3). The results are shown in Table III.

In both methods we have added a constant component to $\rho(l)$, while maintaining its functional form at small $|l|$, by adjusting the $q=0$ component of its fourier series expansion (3).

In our simulations of ferromagnets [1, 2] if the system is at a temperature of zero then the magnitude and direction of the field is the same at every site. Using the first approach to generating a field with a non-zero average value such a state is characterised by having all the variance in the $q=0$ mode with the mean value of each mode equal to zero so that the expected value of each $\mathbf{M}(l)$ is zero and the variance of each $\mathbf{M}(l)$ is $E(|\mathbf{M}(l)|^2)$. The mean is zero because there is no preferred direction in the system so although the $M(l)$ are all parallel the system as a whole can rotate. Similarly, although in any particular cluster $|\mathbf{M}(l)|$ is the same on each

TABLE III

Expected Values of the Cosine of the Angle between Vectors on Different Sites η as a Function of the Correlation Coefficient between the Unnormalised Vectors ρ and the Expected Average Magnetisation of the Unnormalised Vectors in the z-Direction $\langle M_z \rangle$

	$\langle M_z \rangle$										
ρ	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.0	0.00	0.00	0.00	0.00	0.01	0.03	0.07	0.15	—	—	—
0.1	0.09	0.09	0.09	0.09	0.09	0.12	0.15	0.21	—	—	—
0.2	0.17	0.17	0.17	0.17	0.18	0.19	0.22	0.28	—	—	—
0.3	0.26	0.26	0.25	0.26	0.26	0.28	0.29	0.35	0.44	—	—
0.4	0.35	0.35	0.34	0.34	0.35	0.36	0.39	0.43	0.50	—	—
0.5	0.43	0.44	0.44	0.44	0.44	0.45	0.47	0.50	0.57	—	—
0.6	0.53	0.53	0.54	0.53	0.53	0.54	0.56	0.58	0.64	—	—
0.7	0.62	0.63	0.63	0.64	0.63	0.64	0.65	0.68	0.72	0.78	—
0.8	0.73	0.73	0.74	0.73	0.73	0.74	0.75	0.76	0.80	0.85	—
0.9	0.85	0.86	0.86	0.86	0.86	0.86	0.86	0.87	0.89	0.92	—
1.0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Notes. $\langle M_z \rangle$ is in units of the ground state magnetisation. The values were calculated by sampling from the distribution functions. The number of points used to evaluate each estimate of η is such that the standard deviation of the estimate is less than 0.0032. Blanks indicate that the values of $\langle M_z \rangle$ and ρ are incompatible.

site the value of $M(\boldsymbol{l})$ will be different for different clusters. In general, clusters set up using the first approach to have the same expected correlation coefficient and expected average field may, in fact, have quite different average values. In practice, this variation in the magnitude of the expected average field, $|\bar{\mathbf{M}}|$, can lead to significant differences in the distribution of the normalised vectors $\hat{\mathbf{M}}$ from one cluster to another. For example, since

$$E(\chi = \hat{\mathbf{M}}_A \cdot \hat{\mathbf{M}}_B \mid |\hat{\mathbf{M}}_A|\, |\mathbf{M}_B|) = \coth \alpha - 1/\alpha,$$

where

$$\alpha = \frac{3\rho}{(1-\rho^2)}\, |\mathbf{M}_A|\, |\mathbf{M}_B| = \frac{3\rho}{(1-\rho^2)}\, |\bar{\mathbf{M}}|^2$$

the random field generated may have a quite different value of η from that expected (see Fig. 2). This problem does not arise in the second approach.

In the second approach the state in which the field has the same magnitude and direction on every site (the ground state of a ferromagnet) is characterised by having the variances of all the modes equal to zero, the mean of all the $q \neq 0$ modes equal to zero, and the mean of the $q = 0$ mode equal to the average field. Thus we get an average field of specified size and direction. For a fixed expected correlation, as the expected average field is decreased the mean of the $q = 0$ mode decreases and the variances of all the modes increase.

In both methods we have specified not only what the interaction tending to order the system is but also how its effect is distributed between different $\mathbf{q}$-modes. The way in which the effect of the ordering interaction is distributed between modes of different $\mathbf{q}$ can be altered in other ways, for example, by introducing a cut-off at large $\mathbf{q}$; that is, by decreasing $\sigma_{\mathbf{q}}$ for large $|\mathbf{q}|$ and making a compensating increase in $\sigma_{\mathbf{q}}$ for small $|\mathbf{q}|$.

5. Limitations and Desirable Features

In Section 2 we assumed that $A(\mathbf{q})$, $A(\mathbf{q}')$, $B(\mathbf{q})$ and $B(\mathbf{q}')$ were mutually independent and showed that this implies that the random quantity on the cluster has a joint normal distribution with the same variance on each site and that the correlation coefficient depends only on the separation between sites. Conversely, if

$$\rho(\boldsymbol{l}, \boldsymbol{l}') = \rho(\boldsymbol{l} - \boldsymbol{l}')$$

and the random quantities $M(\boldsymbol{l})$ have a joint normal distribution with the same variance on each site then $A(\mathbf{q}) + A(-\mathbf{q})$, $A(\mathbf{q}') + A(-\mathbf{q}')$, $B(\mathbf{q}) - B(-\mathbf{q})$, and $B(\mathbf{q}') - B(-\mathbf{q}')$ are mutually independent (see Appendix 4). The independence of $A(\mathbf{q})$ and $A(-\mathbf{q})$ and the independence of $B(\mathbf{q})$ and $B(-\mathbf{q})$ are additional assumptions introduced purely for computational convenience.

Hence the method will simulate exactly a cluster of any quantity with a joint normal distribution for which the variance is the same on each site and the correlation coefficient depends only on the separation of the sites. For most quantities the assumptions that the variance is the same at each site and that the correlation coefficient between sites depends only on their separation should be reasonable. So how well the clusters produced by this method simulate an actual cluster of some quantity will depend on how close the actual distribution of that quantity is to a joint normal distribution. For some quantities it might be necessary to incorporate higher order correlations, i.e., higher order moments of the probability distribution.

The procedure described in this paper is more general than that proposed by Cubiotti *et al.* [9] and does not require excessive computing time: setting-up a three-dimensional exchange field on an 864 atom *FCC* cluster takes about 1 min on an IBM 3081.

Appendix 1

In this appendix we show that $A(\mathbf{q})$ and $B(\mathbf{q})$ are normally distributed.

The expression

$$M(\boldsymbol{l}) = \sum_{\mathbf{q}} (A(\mathbf{q}) \cos \mathbf{q} \cdot \boldsymbol{l} + B(\mathbf{q}) \sin \mathbf{q} \cdot \boldsymbol{l})$$

can be written as

$$M(\boldsymbol{l}) = \sum_{\mathbf{q}} C(\mathbf{q}) \cos(\mathbf{q} \cdot \boldsymbol{l} + \varepsilon(\mathbf{q})).$$

If we assume that the amplitude $C(\mathbf{q})$ and phase $\varepsilon(\mathbf{q})$ are independent and that the phases have a uniform probability density function

$$p(\varepsilon) = 1/2\pi,$$

then the joint probability density function for C and ε can be written

$$p(C, \varepsilon) = (1/2\pi)\, p(C),$$

where the probability density function for C is $p(C)$. Since

$$p(A, B) \frac{\partial(A, B)}{\partial(C, \varepsilon)} = p(C, \varepsilon),$$

where $\partial(A, B)/\partial(C, \varepsilon)$ is the Jacobian of the transformation from (A, B) to (C, ε), we have

$$p(A, B) = (1/2\pi C)\, p(C).$$

If A and B are independent

$$p(A, B) = p(A)\, p(B)$$

so

$$\begin{aligned}\log_e p(A) + \log_e p(B) &= \log_e p(A, B)\\ &= g(C^2)\\ &= g(A^2 + B^2),\end{aligned}$$

which implies

$$\log_e p(A) = -A^2/2\sigma_{\mathbf{q}}^2,$$
$$\log_e p(B) = -B^2/2\sigma_{\mathbf{q}}^2$$

because we can expand $g(A^2 + B^2)$ as a Taylor series which cannot include any terms which involve products of A^2 and B^2 so that all terms involving $(A^2 + B^2)^n$, where $n > 1$, must be zero.

Thus $A(\mathbf{q})$ and $B(\mathbf{q})$ are normally distributed with mean zero and the same variance.

Appendix 2

In this appendix we discuss the inversion of Eq. (3),

$$\rho(\boldsymbol{l}) = (1/\sigma^2) \sum_{\mathbf{q}} \sigma_{\mathbf{q}}^2 \cos \mathbf{q} \cdot \boldsymbol{l},$$

to obtain Eq. (4):

$$\sigma_{\mathbf{q}}^2 = (\sigma^2/N) \sum_{\boldsymbol{l}} \rho(\boldsymbol{l}) \cos \mathbf{q} \cdot \boldsymbol{l}.$$

Let

$$r(\mathbf{q}) = \sigma_{\mathbf{q}}^2/\sigma^2$$

so

$$\rho(\boldsymbol{l}) = \sum_{\mathbf{q}} r(\mathbf{q}) \cos \mathbf{q} \cdot \boldsymbol{l}.$$

Let

$$\tilde{r}(\mathbf{q}) = (1/N) \sum_{\boldsymbol{l}} \rho(\boldsymbol{l}) \cos \mathbf{q} \cdot \boldsymbol{l},$$

then

$$\tilde{r}(q) = \tfrac{1}{2}(r(q) + r(-q)).$$

We shall show that there is no loss of generality in taking $r(\mathbf{q}) = r(-\mathbf{q})$ (i.e., the proportion of the variance σ^2 due to the modes with wavevector $\mathbf{q}$ is the same as that due to the modes with wavevector $-\mathbf{q}$ so that $r(\mathbf{q}) = \tilde{r}(\mathbf{q})$. The four quantities $A(\mathbf{q})$, $B(\mathbf{q})$, $A(-\mathbf{q})$, and $B(-\mathbf{q})$ are all independent. For all $\boldsymbol{l}$, $M(\boldsymbol{l})$ depends only on the sums $A(\mathbf{q}) + A(-\mathbf{q})$ and the differences $B(\mathbf{q}) - B(-\mathbf{q})$. For each $\mathbf{q}$ both the sum and difference have variance

$$\sigma^2(r(\mathbf{q}) + r(-\mathbf{q})).$$

We assume that there are mutually independent quantities $\tilde{A}(\mathbf{q})$, $\tilde{A}(-\mathbf{q})$, $\tilde{B}(\mathbf{q})$, $\tilde{B}(-\mathbf{q})$ each with the same variance

$$\sigma^2(1/2)(r(\mathbf{q}) + r(-\mathbf{q})) = \sigma^2 r(\mathbf{q})$$

such that

$$A(\mathbf{q}) + A(-\mathbf{q}) = \tilde{A}(\mathbf{q}) + \tilde{A}(-\mathbf{q}),$$
$$B(\mathbf{q}) - B(-\mathbf{q}) = \tilde{B}(\mathbf{q}) - \tilde{B}(-\mathbf{q}).$$

Thus the set $\tilde{A}(\mathbf{q})$, $\tilde{A}(-\mathbf{q})$, $\tilde{B}(\mathbf{q})$, $\tilde{B}(-\mathbf{q})$ gives the same results as the set $A(\mathbf{q})$, $A(-\mathbf{q})$, $B(\mathbf{q})$, $B(-\mathbf{q})$. Hence we may take

$$r(\mathbf{q}) = \tilde{r}(\mathbf{q}) = (1/N) \sum_{\boldsymbol{l}} \rho(\boldsymbol{l}) \cos \mathbf{q} \cdot \boldsymbol{l}$$

so

$$\sigma_{\mathbf{q}}^2 = (\sigma^2/N) \sum_{\boldsymbol{l}} \rho(\boldsymbol{l}) \cos \mathbf{q} \cdot \boldsymbol{l}.$$

The fact that the results depend only on $A(\mathbf{q}) + A(-\mathbf{q})$ and $B(\mathbf{q}) - B(-\mathbf{q})$ corresponds to the fact that the Fourier series expansion (in one dimension with an even number of sites, for simplicity)

$$f(l) = \sum_{q=-\pi/2a}^{q=\pi/2a} (A(q) \cos ql + B(q) \sin ql)$$

can be written

$$f(l) = \sum_{q=0}^{q=\pi/a} ((A(q) + A(-q)) \cos ql + (B(q) - B(-q)) \sin ql).$$

The sum over all q is preferable to the restricted sum for numerical computation.

APPENDIX 3

In this appendix we find the relation between the correlation coefficient $\rho(\boldsymbol{l})$ and

$$\eta(\boldsymbol{l}) = E(\cos\theta(\boldsymbol{l})),$$

where $\theta(\boldsymbol{l})$ is the angle between the $\mathbf{M}$ on sites separated by $\boldsymbol{l}$.

If M_1, M_2, and M_3 are independent and normally distributed then

$$p(\mathbf{M}) = \frac{1}{(\sigma\sqrt{2\pi})^3} \exp\left(\frac{-(M_1^2+M_2^2+M_3^2)}{2\sigma^2}\right). \tag{3a.1}$$

The joint probability density for M_A and M_B, where A and B are two different sites, is

$$p(M_A, M_B) = \frac{1}{((2\pi)^3 (\det \Sigma)^{1/2})} \exp\left(-\frac{1}{2}\mathbf{M}_{AB}^T \Sigma^{-1} \mathbf{M}_{AB}\right),$$

where

$$M_{AB}^T = (M_{A1}, M_{A2}, M_{A3}, M_{B1}, M_{B2}, M_{B3})$$

and

$$\Sigma = \sigma^2 \begin{pmatrix} 1 & 0 & 0 & \rho_{AB} & 0 & 0 \\ 0 & 1 & 0 & 0 & \rho_{AB} & 0 \\ 0 & 0 & 1 & 0 & 0 & \rho_{AB} \\ \rho_{AB} & 0 & 0 & 1 & 0 & 0 \\ 0 & \rho_{AB} & 0 & 0 & 1 & 0 \\ 0 & 0 & \rho_{AB} & 0 & 0 & 1 \end{pmatrix}.$$

Thus, taking $\sigma^2 = \frac{1}{3}$ so that $\langle |M|^2 \rangle = 1$,

$$p(\mathbf{M}_A, \mathbf{M}_B) = \frac{1}{(2\pi/3)^3 (1-\rho_{AB}^2)^{(3/2)}} \times \exp\left(\frac{-3(|\mathbf{M}_A|^2 - 2\rho_{AB}\mathbf{M}_A \cdot \mathbf{M}_A + |\mathbf{M}_B|^2}{2(1-\rho_{AB}^2)}\right)$$

and the conditional probability density for $\mathbf{M}_B$ given $\mathbf{M}_A$ is

$$p(\mathbf{M}_B \mid \mathbf{M}_A) = \frac{1}{(2\pi/3)^{3/2} (1-\rho_{AB}^2)^{3/2}} \times \exp\left(\frac{-3\,|\mathbf{M}_A|^2\,(|\mathbf{M}|_B^2/|\mathbf{M}_A|^2 - 2\rho_{AB}(\mathbf{M}_A \cdot \mathbf{M}_B)/\mathbf{M}_A^2 + \rho_{AB}^2)}{2(1-\rho_{AB}^2)}\right).$$

We change variables by letting

$$R = |M_B|/|M_A|,$$

$$\chi = \cos\theta = \frac{(\mathbf{M}_A \cdot \mathbf{M}_B)}{(|M_A|\,|M_B|)},$$

and we are seeking the expected value of χ for a given ρ_{AB}, that is, we are seeking

$$\eta = E(\chi \mid \rho).$$

The conditional probability using the new variables is

$$p(R, \chi \mid \mathbf{M}_A) = \frac{2\pi}{(2\pi/3)^{3/2}(1-\rho^2)^{3/2}} \times |\mathbf{M}_A|^3 R^2 \exp\left(\frac{-3\,|\mathbf{M}_A|^2 (R^2 - 2\rho\chi R + \rho^2)}{2(1-\rho^2)}\right),$$

where the factor 2π arises because $\mathbf{M}_B$ is at an angle θ, ϕ to $\mathbf{M}_A$ and integrating over ϕ gives 2π. Hence, as $p(R, \chi \mid \mathbf{M}_A)$ depends only on R, χ, and $|\mathbf{M}_A|$

$$p(R, \chi \mid |\mathbf{M}_A|) = \frac{2\pi}{(2\pi/3)^{3/2}(1-\rho^2)^{3/2}} \times |\mathbf{M}_A|^3 R^2 \exp\left(\frac{-3\,|\mathbf{M}_A|^2 (R^2 - 2\rho\chi R + \rho^2)}{2(1-\rho^2)}\right),$$

$$p(R, \chi, |\mathbf{M}_A|) = \frac{8\pi^2}{(2\pi/3)^3 (1-\rho^2)^{3/2}} \times |\mathbf{M}_A| \exp\frac{-3\,|M_A|^2 (R^2 - 2\rho\chi R + \rho^2)}{2(1-\rho^2)},$$

$$p(R, \chi) = \frac{8}{\pi} \frac{(1-\rho^2)^{3/2} R^2}{(R^2 - 2\rho\chi R + 1)^3},$$

$$p(R) = \frac{16}{\pi} \frac{(1-\rho^2)^{3/2} (R^2(R^2+1))}{((R^2+1)^2 - 4\rho^2 R^2)^2},$$

$$p(\chi \mid R) = \frac{((R^2+1)^2 - 4\rho^2 R^2)^2}{2(R^2+1)(R^2 - 2\rho\chi R + 1)^3}.$$

Hence

$$E(\chi \mid \rho, R) = \frac{2\rho R}{R^2+1}.$$

Using

$$E(Z \mid X) = E(E(Z \mid X, Y) \mid X)$$

we obtain

$$\begin{aligned}\eta &= E(\chi \mid \rho) \\ &= E(E(\chi \mid \rho, R) \mid \rho) \\ &= E\left(\frac{2\rho R}{R^2+1} \,\middle|\, \rho\right) \\ &= \rho E\left(\frac{2R}{R^2+1}\right)\end{aligned}$$

so

$$\eta = a\rho,$$

where

$$\begin{aligned}a &= E\left(\frac{2R}{R^2+1}\right) \\ &= \frac{1}{\pi\rho^2}\left\{2\sqrt{(1-\rho^2)} - \frac{(1-2\rho^2)}{\rho}\left[\frac{\pi}{2} - \tan^{-1}\left(\frac{1-2\rho^2}{2\rho(1-\rho^2)}\right)\right]\right\}.\end{aligned}$$

When $\rho = 1$, $a = 1$ as expected. When $\rho = 0$, $a = 8/3\pi$.

When the cluster has been set up to have a non-zero expected average field the integral of the joint probability density for $\mathbf{M}_A$ and $\mathbf{M}_B$ giving the expected value of the cosine of the angle between them cannot be done analytically. However, the conditional probability for $\mathbf{M}_B$ given $\mathbf{M}_A$ may be written

$$\begin{aligned}p(\mathbf{M}_B \mid \mathbf{M}_A) = &\frac{1}{\sigma^3(2\pi(1-r_0)(1-\gamma_{AB}^2))^{3/2}} \\ &\times \exp\left(\frac{-|M_B - ((1-\gamma_{AB}^2)\, m + \gamma_{AB} M_A)|^2}{2\sigma^2(1-r_0)(1-\gamma_{AB}^2)}\right),\end{aligned} \tag{3a.2}$$

where

$$\gamma_{AB} = \frac{\langle(\mathbf{M}_A - \bar{\mathbf{m}}) \cdot (\mathbf{M}_B - \bar{\mathbf{m}})\rangle}{(\langle(|\mathbf{M}_A|^2 - |\bar{\mathbf{m}}|^2)\rangle\langle(|\mathbf{M}_B|^2 - |\bar{\mathbf{m}}|^2)\rangle)^{1/2}}$$

is the correlation coefficient relative to the average field.

The expression for the conditional probability density for $\mathbf{M}_B$ given $\mathbf{M}_A$ is a normal distribution with mean $(1-\gamma_{AB})\,\bar{\mathbf{m}} + \gamma_{AB}\mathbf{M}_A$ and variance $\sigma^2(1-r_0)(1-\gamma_{AB}^2)$ so the expected value of the cosine of the angle between vectors on two sites may be

estimated by generating N values of $\mathbf{M}_A$ from the normal distribution (3a.1) with their associated values of $\mathbf{M}_B$ generated using (3a.2) and calculating

$$(1/N)\sum_i \frac{\mathbf{M}_{Ai}\cdot\mathbf{M}_{Bi}}{|\mathbf{M}_{Ai}|\,|\mathbf{M}_{Bi}|}.$$

The correlation coefficient relative to the average field γ_{AB}, is related to the correlation coefficient relative to zero,

$$\rho_{AB}=\frac{\langle \mathbf{M}_A\cdot\mathbf{M}_B\rangle}{(|M_A|^2\,|M_B|^2)^{1/2}},$$

by

$$\gamma=\frac{(\rho-r_0)}{1-r_0}.$$

Since γ must lie between -1 and 1, for a given value of r_0,

$$1\geqslant\rho\geqslant 2r_0-1.$$

So if there is a non-zero average field on the cluster the lower limit for the correlation between any two moments is greater than -1.

The results of the calculations of

$$\eta_{AB}=\langle\cos\theta_{AB}\rangle$$

for various values of $\bar{\mathbf{m}}$ and ρ_{AB} are shown in Table III.

Appendix 4

In this appendix we show that if

$$\rho(\boldsymbol{l},\boldsymbol{l}')=\rho(\boldsymbol{l}-\boldsymbol{l}')=\rho(\boldsymbol{l}'-\boldsymbol{l})$$

and the random quantities $M(\boldsymbol{l})$ have a joint normal distribution with the same variance on each site then $A(\mathbf{q})+A(-\mathbf{q})$, $A(\mathbf{q}')+A(-\mathbf{q}')$, $B(\mathbf{q})-B(-\mathbf{q})$, and $B(\mathbf{q}')-B(-\mathbf{q}')$ are mutually independent.

Inverting (1a) and (1c) we obtain

$$(1/N)\sum_{\boldsymbol{l}} M(\boldsymbol{l})\cos\mathbf{q}\cdot\boldsymbol{l}=\tfrac{1}{2}(A(\mathbf{q})+A(-\mathbf{q}))$$

and

$$(1/N)\sum_{\boldsymbol{l}} M(\boldsymbol{l})\sin\mathbf{q}\cdot\boldsymbol{l}=\tfrac{1}{2}(B(\mathbf{q})-B(-\mathbf{q}))$$

so the second order moment

$$E((A(\mathbf{q})+A(-\mathbf{q}))(A(\mathbf{q}')+A(-\mathbf{q}'))) = \frac{2}{N^2}\sigma^2 \sum_l \rho(\boldsymbol{l})(\cos \mathbf{q}\cdot\boldsymbol{l} - \sin \mathbf{q}\cdot\boldsymbol{l}) = 2\sigma_{\mathbf{q}}^2$$
$$\text{if } \mathbf{q}=\mathbf{q}' \text{ or } \mathbf{q}=-\mathbf{q}'$$
$$=0 \qquad \text{otherwise.}$$

Similarly, the other second order moments are

$$E((B(\mathbf{q})-B(-\mathbf{q}))(B(\mathbf{q}')-B(-\mathbf{q}'))) = \frac{2}{N^2}\sigma^2 \sum_l \rho(\boldsymbol{l})(\cos \mathbf{q}\cdot\boldsymbol{l} + \sin \mathbf{q}\cdot\boldsymbol{l})$$
$$= 2\sigma_{\mathbf{q}}^2 \qquad \text{if} \quad \mathbf{q}=\mathbf{q}'$$
$$= \frac{-2}{N^2}\sigma^2 \sum_l \rho(\boldsymbol{l})(\cos \mathbf{q}\cdot\boldsymbol{l} + \sin \mathbf{q}\cdot\boldsymbol{l})$$
$$= -2\sigma_{\mathbf{q}}^2 \qquad \text{if} \quad \mathbf{q}=-\mathbf{q}'$$
$$=0 \qquad \text{otherwise}$$

and

$$E((A(\mathbf{q})+A(-\mathbf{q}))(B(\mathbf{q}')-B(-\mathbf{q}'))) = 0 \qquad \text{for all } \mathbf{q} \text{ and } \mathbf{q}'.$$

If the $M(\boldsymbol{l})$ have a joint normal distribution then the above results are sufficient to prove that the $A(\mathbf{q})$ and $B(\mathbf{q})$ are mutually independent as their higher-order moments are either zero or factorise into products of second order moments.

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