Journal of Statistical Physics, Vol. 6, No. 2/3, 1972

A Constant-Magnetization Ensemble for the Classical Anisotropic Heisenberg Model

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Received December 28, 1971

A constant-magnetization ensemble is introduced in order to study classical, anisotropic Heisenberg systems. Existence, uniform convergence, and convexity properties are proved for an appropriate thermodynamic potential. The thermodynamic equivalence of this ensemble with the more common canonical ensemble is also established. In a subsequent paper, this formulation is used to obtain an exact statistical mechanical solution of classical Heisenberg systems with long-range Kac interactions.

KEY WORDS: Ferromagnet; statistical mechanics; equivalence of ensembles.

1. INTRODUCTION

This paper is the first of two articles dealing with the classical, anisotropic Heisenberg model. The basic objective of the present work is to motivate and

This research was carried out at The Department of Physics, Case Western Reserve University, Cleveland, Ohio, and was supported in part by the U.S. Atomic Energy Commission. This work is based on portions of a dissertation by K. M. submitted in partial fulfillment of the Ph.D. degree, Case Western Reserve University.

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define a constant-magnetization ensemble, and to establish its equivalence with the canonical ensemble. The constant-magnetization ensemble is a natural one to use in discussing Heisenberg systems with long-range Kac interactions. An exact statistical mechanical treatment of such systems is the focus of the second paper of this series.[1] Some of the thermodynamic results of that analysis, without the mathematical details, have already been compiled elsewhere.[2] In particular, the effect of anisotropy on the Curie–Weiss-type transition has been established.

In Section 2, the classical Heisenberg model is reviewed and the constant-magnetization ensemble is defined and compared with the canonical ensemble. Section 3 contains a discussion of the relevant free energy density for the constant-magnetization ensemble. Existence, uniform convergence, convexity, and continuity properties are established for this constant-magnetization free energy density in the thermodynamic limit. A proof of the equivalence of the constant-magnetization and canonical ensembles constitutes Section 4.

2. CLASSICAL HEISENBERG SYSTEMS

The classical Heisenberg model[4] is a ν-dimensional lattice of N spin sites. To the kth site there is associated a classical spin vector $\mathbf{s}_k$ ($k = 1,..., N$) with components $(s_{x,k}, s_{y,k}, s_{z,k})$. The Hamiltonian for a Heisenberg spin system can be written as

$$\mathscr{H}_N = \mathscr{H}_N^{(S)} + \mathscr{H}_N^{(H)} \tag{1}$$

$\mathscr{H}_N^{(S)}$ is the contribution to the Hamiltonian due to anistropic spin–spin interactions,

$$\mathscr{H}_N^{(S)} = -\tfrac{1}{2} \sum_{i=x,y,z} \sum_{k \neq l}^{N} J_{i,kl} s_{i,k} s_{i,l} \tag{2}$$

$\mathscr{H}_N^{(H)}$ is the contribution to the interaction of the spins with an external magnetic field $\mathbf{H} = (H_x, H_y, H_z)$,

$$\mathscr{H}_N^{(H)} = -\mu \sum_{i=x,y,z} H_i \sum_{k=1}^{N} s_{i,k} \tag{3}$$

The coefficients $J_{x,kl}$, $J_{y,kl}$, and $J_{z,kl}$ are coupling constants which depend only on the magnitude of the separation of the two lattice sites k and l. The magnetic moment of each spin is given by μ. The quantity $\mathbf{s}_k$ is taken to be a

[4] The classical Heisenberg model can be thought of as the infinite spin limit of the quantum mechanical Heisenberg model; see Ref. 3.

vector of constant magnitude, $|\mathbf{s}_k| = 1$. The choice of unit spin magnitude is not restrictive since the magnitude of the spin can be absorbed into the coupling coefficients and the magnetic moment.

2.1. The Canonical Ensemble

The canonical partition function is defined by

$$Q_c(\mathbf{H}, N) = \int_\Omega d\mathbf{s}_1 \cdots \int_\Omega d\mathbf{s}_N \, e^{-\beta\mathscr{H}_N} \tag{4}$$

where each integration is over the total solid angle, $\Omega = 4\pi$ steradians. The canonical (Helmholtz) free energy density $f_c(\mathbf{H}, N)$ is defined by

$$Q_c(\mathbf{H}, N) = \exp[-\beta N f_c(\mathbf{H}, N)] \tag{5}$$

The canonical free energy density in the thermodynamic limit, $f_c(\mathbf{H})$, is defined by

$$f_c(\mathbf{H}) = \lim_{N\to\infty} f_c(\mathbf{H}, N) \tag{6}$$

where the lattice becomes infinite in each of its ν dimensions. The equations of state for Heisenberg spin systems are obtained from the definition of $\boldsymbol{\rho}_c = (\rho_{c,x}, \rho_{c,y}, \rho_{c,z})$, the net spin per lattice site in the canonical ensemble,

$$\rho_{c,i} = -\mu^{-1} \partial f_c(\mathbf{H})/\partial H_i \tag{7}$$

for $i = x, y, z$. The quantity $\mu\boldsymbol{\rho}_c$ is the canonical magnetization per lattice site.

2.2. The Constant-Magnetization Ensemble

We seek a meaningful ensemble for discussing classical systems which has the essential feature of allowing a treatment of long-range interactions by a Lebowitz–Penrose–type method.[4] For a classical fluid or a lattice gas, this essential feature is the constancy of the number of particles, as associated with the canonical ensemble. A similar analysis can be carried out for a quantum Ising model[5] using a corresponding ensemble for which the net spin is constant. The Lebowitz–Penrose method involves a division of the entire lattice into cells. The net spin is a useful variable because an estimate of the long-range intercell interactions is simply expressible in terms of the net spin of each cell. This feature leads to a direct relationship between the total system's free energy density and the free energy densities of the individual cells. This, in turn, allows one to obtain useful upper and lower bounds, which ultimately determine the free energy density completely. Furthermore, the fact that this ensemble is thermodynamically equivalent to the trusted canonical ensemble, makes the constant magnetization ensemble a practical tool.

It appears then, that we need an ensemble for which the net spin vector, for the classical Heisenberg model, is fixed.[5] A possible approach is to define a partition function in terms of an integral over all configurations of the system. A Dirac delta-function could be included in the integrand to pick out those configurations with a fixed value of the net spin. With such an approach, however, it is difficult to prove essential properties, such as the existence of an appropriate free energy density in the thermodynamic limit, convexity properties, and the like. Below, we define a "constant-magnetization" ensemble in such a way that the difficulties alluded to above are avoided.

The net spin of a system, $\mathbf{M} = (M_x, M_y, M_z)$, is defined by

$$M_i = \sum_{k=1}^{N} s_{i,k} \tag{8}$$

for $i = x, y, z$. That is, given any configuration of the system (a complete specification of the set of vectors $\{\mathbf{s}_k\}$), the net spin has a value $\mathbf{M}$. Clearly, the total range of net spin values is such that

$$|\mathbf{M}| \leqslant N \tag{9}$$

We introduce the smallness parameter Δ/N with the property

$$0 < \Delta/N \ll 1 \tag{10}$$

We define the constant-magnetization partition function for each value of $\mathbf{M}$ as

$$Q_m(\mathbf{M}, \Delta, N) = \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' \,(\exp -\beta \mathscr{H}_N^{(S)})\, \Theta(\mathbf{M}', \mathbf{M}, \Delta) \quad \text{(11a)}$$

where

$$\Theta(\mathbf{M}', \mathbf{M}, \Delta) = \begin{cases} 1 & \text{if } \; M_i \leqslant M_i' \leqslant M_i + \Delta \quad \text{for} \quad i = x, y, z \\ 0 & \text{otherwise} \end{cases} \quad \text{(11b)}$$

The characteristic function $\Theta(\mathbf{M}', \mathbf{M}, \Delta)$ restricts the domain of integration so that $M_x \leqslant M_x' \leqslant M_x + \Delta$, $M_y \leqslant M_y' \leqslant M_y + \Delta$, and

$$M_z \leqslant M_z' \leqslant M_z + \Delta.$$

[5] For the quantum Heisenberg model, R. B. Griffiths has introduced an ensemble for which the z component of the total magnetization is held fixed. See Ref. 6.

From (11b), we note the identity

$$\Theta(M_x', M_y', M_z'; -|M_x|, |M_y|, |M_z|; \Delta)$$
$$= \Theta(-M_x', M_y', M_z'; |M_x| - \Delta, |M_y|, |M_z|; \Delta) \quad (12)$$

This expression together with the fact [see (2)] that $\mathscr{H}_N^{(S)}$ is unchanged under the transformation

$$s_{x,k} \to -s_{x,k}, \qquad k = 1,..., N \quad (13)$$

implies that

$$Q_m(-|M_x|, |M_y|, |M_z|; \Delta, N) = Q_m(|M_x| - \Delta, |M_y|, |M_z|; \Delta, N) \quad (14)$$

Equation (14) can apparently be generalized for any component or several components of $\mathbf{M}$ being negative. Thus, we only need to consider values of $\mathbf{M}$ which have nonnegative components.

The free energy density in the constant-magnetization ensemble is defined by

$$Q_m(\mathbf{M}, \Delta, N) = \exp[-\beta N f_m(\boldsymbol{\rho}, \chi, N)] \quad (15a)$$

where

$$\boldsymbol{\rho} = \mathbf{M}/N = (M_x/N, M_y/N, M_z/N) \quad (15b)$$

and

$$\chi = \Delta/N \quad (15c)$$

We note that $f_m(\boldsymbol{\rho}, \chi, N)$ defined by (11a) and (15a) is a continuous function of $\boldsymbol{\rho}$. A proof of this statement is given in Appendix A. From (14) and (15), we observe that $f_m(\boldsymbol{\rho}, \chi, N)$ has the symmetry property

$$f_m(-|\rho_x|, |\rho_y|, |\rho_z|; \chi, N) = f_m(|\rho_x| - \chi, |\rho_y|, |\rho_z|; \chi, N) \quad (16)$$

and similarly for any component or several components of $\boldsymbol{\rho}$ being negative.

The thermodynamic limit of the free energy density is defined by

$$f_m(\boldsymbol{\rho}, \chi) = \lim_{N\to\infty} f_m(\boldsymbol{\rho}, \chi, N) \quad (17a)$$

where $\boldsymbol{\rho}$ and χ are held fixed in the limiting process. We seek a free energy density which is independent of χ, carrying the connotation that the interval Δ is negligible compared with the maximum net spin N. This is accomplished by investigating $f(\boldsymbol{\rho}, \chi)$ in the limit as $\chi \to 0$. We therefore define

$$f_m(\boldsymbol{\rho}) = \lim_{\chi\to 0} f_m(\boldsymbol{\rho}, \chi) \quad (17b)$$

where $\boldsymbol{\rho}$ is held fixed in the limiting process. Finally, the magnetic field $\mathbf{H}_m = (H_{m,x}, H_{m,y}, H_{m,z})$ in the constant-magnetization ensemble is defined by

$$\mu H_{m,i} = \partial f_m(\boldsymbol{\rho})/\partial \rho_i \tag{18}$$

where $i = x, y, z$.

2.3. Relation Between Canonical and Constant-Magnetization Partition Functions

In this section, we obtain a relation between the canonical and constant-magnetization partition functions. We first note the inequality

$$\begin{aligned}
&\int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' \, [\exp(\beta\mu\mathbf{H}\cdot\mathbf{M}')](\exp -\beta\mathscr{H}_N^{(S)})\, \Theta(\mathbf{M}', \mathbf{M}, \Delta) \\
&\quad \geqslant \{\exp[-\beta\mu(|H_x| + |H_y| + |H_z|)\Delta]\}[\exp(\beta\mu\mathbf{H}\cdot\mathbf{M})] \\
&\qquad \times \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' \,(\exp -\beta\mathscr{H}_N^{(S)})\, \Theta(\mathbf{M}', \mathbf{M}, \Delta) \\
&\quad = \{\exp[-\beta\mu(|H_x| + |H_y| + |H_z|)\Delta]\}[\exp(\beta\mu\mathbf{H}\cdot\mathbf{M})]\, Q_m(\mathbf{M}, \Delta, N)
\end{aligned} \tag{19}$$

which holds for both algebraic signs of M_i and H_i, $i = x, y, z$. Similarly, with no restrictions on the algebraic signs of M_i and H_i, $i = x, y, z$,

$$\begin{aligned}
&\int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' \, [\exp(\beta\mu\mathbf{H}\cdot\mathbf{M}')](\exp -\beta\mathscr{H}_N^{(S)})\, \Theta(\mathbf{M}', \mathbf{M}, \Delta) \\
&\quad \leqslant \{\exp[\beta\mu(|H_x| + |H_y| + |H_z|)\Delta]\}[\exp(\beta\mu\mathbf{H}\cdot\mathbf{M})]\, Q_m(\mathbf{M}, \Delta, N)
\end{aligned} \tag{20}$$

where (11) has been used. We now note that (4) can be written as

$$\begin{aligned}
Q_c(\mathbf{H}, N) = \sum_{M_x}\sum_{M_y}\sum_{M_z} \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' \\
\times [\exp(\beta\mu\mathbf{H}\cdot\mathbf{M}')](\exp -\beta\mathscr{H}_N^{(S)})\, \Theta(\mathbf{M}', \mathbf{M}, \Delta)
\end{aligned} \tag{21}$$

where the summations run over integral multiples of Δ such that $-(N + \Delta) \leqslant M_i \leqslant N$. Combining (19)–(21), we find the inequality

$$\begin{aligned}
&\{\exp[-\beta\mu(|H_x| + |H_y| + |H_z|)\Delta]\} \sum_{\mathbf{M}} [\exp(\beta\mu\mathbf{H}\cdot\mathbf{M})]\, Q_m(\mathbf{M}, \Delta, N) \\
&\quad \leqslant Q_c(\mathbf{H}, N) \\
&\quad \leqslant \{\exp[\beta\mu(|H_x| + |H_y| + |H_z|)\Delta]\} \sum_{\mathbf{M}} (\exp \beta\mu\mathbf{H}\cdot\mathbf{M})\, Q_m(\mathbf{M}, \Delta, N)
\end{aligned} \tag{22}$$

2.4. Conditions on the Coupling Coefficients

We assume the coupling constants in (2) satisfy the following conditions:

$$| J_{i,kl} | \leqslant D_1/r_{kl}^{\nu+\epsilon_1}, \qquad r_{kl} \geqslant 1 \tag{23}$$

for $i = x, y, z$. Both D_1 and ϵ_1 are finite positive constants. An interaction of this form is termed a power-law potential by Fisher,[7] and is a stable potential. Using (23), the following upper bound for $| \mathscr{H}_N^{(S)} |$ can be established:

$$| \mathscr{H}_N^{(S)} | \leqslant N w_1 \tag{24a}$$

where

$$w_1 = \tfrac{3}{2} D_1 [5^\nu + (\nu 2^\nu/\epsilon_1)] \tag{24b}$$

3. PROPERTIES OF THE FREE ENERGY DENSITY[6]

3.1. A Lower Bound for $f_m(\rho, \chi, N)$

From (11), (15), and (24), we find the inequality

$$\begin{aligned}\exp[-\beta N f_m(\rho, \chi, N)] &\leqslant [\exp(\beta N w_1)] \int_\Omega ds_1' \cdots \int_\Omega ds_N' \, \Theta(\mathbf{M}', \mathbf{M}, \Delta) \\ &\leqslant [\exp(\beta N w_1)] \int_\Omega ds_1' \cdots \int_\Omega ds_N' = (4\pi)^N \exp(\beta N w_1)\end{aligned} \tag{25}$$

But (25) can be written as

$$f_m(\rho, x, N) \geqslant -w_1 - \beta^{-1} \ln(4\pi) \tag{26}$$

which establishes a finite lower bound for $f_m(\rho, \chi, N)$.

3.2. Basic Inequality

Suppose the lattice is divided into two regions, I and II, such that each lattice site is either in region I *or* region II. Region I contains $N^{(\mathrm{I})}$ sites with a net spin $\mathbf{M}^{(\mathrm{I})}$. We similarly define $N^{(\mathrm{II})}$ and $\mathbf{M}^{(\mathrm{II})}$ for region II. We can then write

$$N^{(\mathrm{I})} + N^{(\mathrm{II})} = N \tag{27a}$$

$$\mathbf{M}^{(\mathrm{I})} + \mathbf{M}^{(\mathrm{II})} = \mathbf{M} \tag{27b}$$

[6] Portions of this section follow closely the work for a classical fluid contained in Ref. 7

Note that the net spin $\mathbf{M}^{(\mathrm{I})}$ can vary as the configuration (the specification of all the vectors $\mathbf{s}_k$ contained in region I) of the spins in region I varies. The spin–spin Hamiltonian can be written as a sum of three terms,

$$\mathscr{H}_N^{(S)} = \mathscr{H}_{N^{(\mathrm{I})}}^{(S)} + \mathscr{H}_{N^{(\mathrm{II})}}^{(S)} + \mathscr{H}_{\mathrm{I,II}} \tag{28}$$

where $\mathscr{H}_{\mathrm{I,II}}$ is the interaction of region-I spins with region-II spins. From (11) and (28), we obtain the inequality

$$Q_m(\mathbf{M}, 2\Delta, N) \geqslant [\exp -\beta(\mathscr{H}_{\mathrm{I,II}})_{\max}] \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' \\ \times (\exp -\beta\mathscr{H}_{N^{(\mathrm{I})}}^{(S)})(\exp -\beta\mathscr{H}_{N^{(\mathrm{II})}}^{(S)})\, \Theta(\mathbf{M}', \mathbf{M}, 2\Delta) \tag{29}$$

The term $(\mathscr{H}_{\mathrm{I,II}})_{\max}$ is an upper bound on $\mathscr{H}_{\mathrm{I,II}}$. The interval length 2Δ is of interest for reasons which are explained below. The integrand on the right-hand side of (29) is the product of a factor for region I and one for region II. We can now treat region I and region II as separate systems.

We note that if

$$M_x^{(\mathrm{I})} \leqslant M_x^{(\mathrm{I})'} \leqslant M_x^{(\mathrm{I})} + \Delta \tag{30a}$$

and

$$M_x^{(\mathrm{II})} \leqslant M_x^{(\mathrm{II})'} \leqslant M_x^{(\mathrm{II})} + \Delta \tag{30b}$$

then

$$M_x^{(\mathrm{I})} + M_x^{(\mathrm{II})} = M_x \leqslant M_x' \leqslant M_x + 2\Delta = (M_x^{(\mathrm{I})} + \Delta) + (M_x^{(\mathrm{II})} + \Delta) \tag{30c}$$

and similarly for the y and z components of $\mathbf{M}$. Since the integrand in (29) is everywhere nonnegative, we find the inequality

$$\int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' (\exp -\beta\mathscr{H}_{N^{(\mathrm{I})}}^{(S)})(\exp -\beta\mathscr{H}_{N^{(\mathrm{II})}}^{(S)})\, \Theta(\mathbf{M}', \mathbf{M}, 2\Delta) \\ \geqslant \left[\int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_{N^{(\mathrm{I})}}' (\exp -\beta\mathscr{H}_{N^{(\mathrm{I})}}^{(S)})\, \Theta(\mathbf{M}^{(\mathrm{I})'}, \mathbf{M}^{(\mathrm{I})}, \Delta)\right] \\ \times \left[\int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_{N^{(\mathrm{II})}}' (\exp -\beta\mathscr{H}_{N^{(\mathrm{II})}}^{(S)})\, \Theta(\mathbf{M}^{(\mathrm{II})'}, \mathbf{M}^{(\mathrm{II})}, \Delta)\right] \\ = Q_m(\mathbf{M}^{(\mathrm{I})}, \Delta, N^{(\mathrm{I})})\, Q_m(\mathbf{M}^{(\mathrm{II})}, \Delta, N^{(\mathrm{II})}) \tag{31}$$

where $\mathbf{M}^{(\mathrm{I})}$ and $\mathbf{M}^{(\mathrm{II})}$ are chosen such that $\mathbf{M}^{(\mathrm{I})} + \mathbf{M}^{(\mathrm{II})} = \mathbf{M}$. The first inequality in (31) follows since the domain of $\mathbf{M}^{(\mathrm{I})'}$ and $\mathbf{M}^{(\mathrm{II})'}$, expressed by

(30a) and (30b), is everywhere contained in the domain of $\mathbf{M}'$, as shown in (30c). Combining (29) and (31), we obtain

$$Q_m(\mathbf{M}, 2\Delta, N) \geqslant e^{-\beta(\mathscr{H}_{\mathrm{I,II}})_{\max}} Q_m(\mathbf{M}^{(\mathrm{I})}, \Delta, N^{(\mathrm{I})})\, Q_m(\mathbf{M}^{(\mathrm{II})}, \Delta, N^{(\mathrm{II})}) \tag{32}$$

subject to (27a) and (27b).

We now obtain an upper bound on $|\mathscr{H}_{\mathrm{I,II}}|$. To accomplish this, we construct a "corridor" which contains all sites within a distance R of the boundary between regions I and II. We place the following restriction on the number of sites $\tilde{N}$ contained in the corridor:

$$\tilde{N} \leqslant CN^{1-(1/\nu)}R \tag{33}$$

where C is a finite positive constant. This condition can be interpreted as a requirement that the area of the boundary between regions I and II (roughly $\tilde{N}/R$) is of the same order of magnitude as the area of the boundary of the system (roughly $N^{1-(1/\nu)}$). Now, divide $\mathscr{H}_{\mathrm{I,II}}$ into two terms,

$$\mathscr{H}_{\mathrm{I,II}} = \mathscr{H}'_{\mathrm{I,II}} + \mathscr{H}_R \tag{34}$$

where $\mathscr{H}_R$ is the interaction of region-I spins with region-II spins for those sites contained *only* in the corridor. $\mathscr{H}'_{\mathrm{I,II}}$ contains all other interactions of region-I spins with region-II spins. Then, by (24a) and (33),

$$|\mathscr{H}_R| \leqslant \tilde{N}w_1 \leqslant Cw_1N^{1-(1/\nu)}R \tag{35}$$

Since the interactions contained in $\mathscr{H}'_{\mathrm{I,II}}$ are between sites separated by at least a distance R, (2) and (23) give

$$|\mathscr{H}'_{\mathrm{I,II}}| \leqslant 3D_1N^{(\mathrm{I})}N^{(\mathrm{II})}/R^{\nu+\epsilon_1} \tag{36}$$

Combining (34)–(36), we obtain

$$|\mathscr{H}_{\mathrm{I,II}}| \leqslant Cw_1N^{1-(1/\nu)}R + 3(D_1N^{(\mathrm{I})}N^{(\mathrm{II})}/R^{\nu+\epsilon_1}) \tag{37}$$

Inequality (32) can now be written as

$$\begin{aligned} f_m(\rho, 2\Delta/N, N) \leqslant{}& Cw_1RN^{-1/\nu} + 3(D_1N^{(\mathrm{I})}N^{(\mathrm{II})}/NR^{\nu+\epsilon_1}) \\ &+ (N^{(\mathrm{I})}/N)f_m(\rho^{(\mathrm{I})}, \Delta/N^{(\mathrm{I})}, N^{(\mathrm{I})}) \\ &+ (N^{(\mathrm{II})}/N)f_m(\rho^{(\mathrm{II})}, \Delta/N^{(\mathrm{II})}, N^{(\mathrm{II})}) \end{aligned} \tag{38a}$$

where

$$\rho = \mathbf{M}/N \tag{38b}$$

$$\rho^{(\mathrm{I})} = \mathbf{M}^{(\mathrm{I})}/N^{(\mathrm{I})} \tag{38c}$$

$$\rho^{(\mathrm{II})} = \mathbf{M}^{(\mathrm{II})}/N^{(\mathrm{II})} \tag{38d}$$

Inequality (38a) is valid if the conditions (27a) and (27b) are satisfied. Equation (27b) thus takes the form

$$N^{(\mathrm{I})}\rho^{(\mathrm{I})} + N^{(\mathrm{II})}\rho^{(\mathrm{II})} = N\rho \tag{39}$$

Clearly, if the lattice were divided into a finite number of regions $\bar{n}$, corridors could be constructed, similar to the above, so that (38) and (39) could be generalized to

$$f_m(\rho, \bar{n}\Delta/N, N) \leqslant Cw_1 RN^{-1/\nu} + 3D_1 \sum_{p<q}^{\bar{n}} \frac{N^{(p)}N^{(q)}}{NR^{\nu+\epsilon_1}} + \sum_{p=1}^{\bar{n}} \frac{N^{(p)}}{N} f_m\left(\rho^{(p)}, \frac{\Delta}{N^{(p)}}, N^{(p)}\right) \tag{40}$$

subject to the constraints

$$\sum_{p=1}^{\bar{n}} N^{(p)} = N \tag{41a}$$

$$\sum_{p=1}^{\bar{n}} N^{(p)}\rho^{(p)} = N\rho \tag{41b}$$

3.3. Sequence for the Thermodynamic Limit

We define a sequence of lattices, for the thermodynamic limit, similar to that defined by Fisher.[7] The initial term in the sequence consists of a (regular-linear, square, cubic) lattice for $\nu = (1, 2, 3)$ with N_0 sites and a net spin $\mathbf{M}_0$. The kth lattice in the sequence consists of N_k lattice sites with a net spin $\mathbf{M}_k$. The $(k+1)$th lattice is defined in terms of the kth by

$$N_{k+1} = 2^\nu N_k \tag{42a}$$

$$\mathbf{M}_{k+1} = 2^\nu \mathbf{M}_k \tag{42b}$$

Each lattice in the sequence is to be (regular-linear, square, cubic) for $\nu = (1, 2, 3)$. The sequence for the corridor half-width R_k is defined by

$$R_k = \alpha_k N_k^{1/\nu} \tag{43a}$$

where

$$\alpha_k = [2^{-\epsilon_1/2(\nu+\epsilon_1)}]^k\, \alpha_0, \qquad 0 < \alpha_0 < 1 \tag{43b}$$

We note that in the thermodynamic limit, defined by sequence (42),

$$\lim_{k\to\infty} N_k = \infty \tag{44a}$$

$$\lim_{k\to\infty} | M_{i,k} | = \infty \tag{44b}$$

where $i = x, y, z$, while the net spin per site ρ remains fixed, i.e.,

$$\mathbf{M}_k/N_k = \mathbf{M}_0/N_0 = \rho \tag{44c}$$

In taking the thermodynamic limit, χ is held fixed. Since $\Delta_k = \chi N_k$, the quantity Δ_k must approach infinity as N_k.

3.4. Existence of $f_m(\rho, \chi)$

The method for proving the existence of $f_m(\rho, \chi)$ is completely analogous to that given by Fisher[7] for proving the existence of the free energy density of a fluid. We therefore only outline the proof. Using (40) and (41) and the sequence defined by (42), (43a), and (43b), we find

$$f_m(\rho, \chi, N_{k+1}) \leqslant w_2\theta^k + w_3\theta_1^{\ k} + (1/2^\nu) \sum_{p=1}^{2^\nu} f_m(\rho^{(p)}, \chi, N_k) \tag{45}$$

subject to

$$(1/2^\nu) \sum_{p=1}^{2^\nu} \rho^{(p)} = \rho \tag{46}$$

where

$$w_2 = \tfrac{1}{2}Cw_1\alpha_0 \tag{47a}$$

$$w_3 = 3D_1(2^\nu - 1)/\alpha_0^{\nu+\epsilon_1}N_0^{\epsilon_1/\nu} \tag{47b}$$

θ and θ_1 are defined by

$$\theta = 2^{-\epsilon_1/2(\nu+\epsilon_1)} \tag{48a}$$

$$\theta_1 = 1/2^{\epsilon_1}\theta^{\nu+\epsilon_1} \tag{48b}$$

To obtain (45), we used the correspondence $\bar{n} \to 2^\nu$. This correspondence implies that

$$\chi = 2^\nu\Delta_k/N_{k+1} = \Delta_k/N_k \tag{49}$$

This, in turn, assures that in (40) the function f_m contains the same χ parameter on both sides of the inequality.

Since (45) is valid for any choice of $\{\rho^{(p)}\}$ satisfying the constraint (46), it is expedient to choose

$$\rho^{(p)} = \rho^{(q)}, \qquad p, q = 1, 2,..., 2^\nu \tag{50}$$

Such a choice [see (46)] implies

$$\rho^{(p)} = \rho, \qquad p = 1,..., 2^\nu \tag{51}$$

Therefore, (45) becomes

$$f_m(\rho, \chi, N_{k+1}) \leqslant w_2\theta^k + w_3\theta_1{}^k + f_m(\rho, \chi, N_k) \tag{52}$$

We now introduce the auxiliary function $q_k(\rho)$, defined by

$$-q_k(\rho) = f_m(\rho, \chi, N_k) - w_2 \sum_{l=0}^{k-1} \theta^l - w_3 \sum_{l=0}^{k-1} \theta_1{}^l \tag{53}$$

Inequalities (52) and (53) imply that for fixed ρ, $q_k(\rho)$ is a nondecreasing sequence, i.e.,

$$q_{k+1} \geqslant q_k \tag{54}$$

Using (54) and the fact that $q_k(\rho)$ is bounded above [see (26) and (53)], we conclude that

$$q(\rho) = \lim_{k\to\infty} q_k(\rho) \tag{55}$$

exists.[7] But if $q(\rho)$ exists, then by (53),

$$f_m(\rho, \chi) = \lim_{k\to\infty} f_m(\rho, \chi, N_k) \tag{56}$$

also exists.

3.5. Convexity of $f_m(\rho, \chi)$

We take the limit of (45) as $k \to \infty$ to obtain

$$f_m(\rho, \chi) = (1/2^\nu) \sum_{p=1}^{2^\nu} f_m(\rho^{(p)}, \chi) \tag{57}$$

subject to (46). This is just the condition that $f_m(\rho, \chi)$ be a convex function of the three variables ρ_x, ρ_y, and ρ_z. Hardy *et al.*[9] point out that convexity of a function of several variables asserts more than convexity with respect to each variable separately. Convexity of a function of several variables implies that *any* chord drawn between two points on a surface lies above the surface.

3.6. Continuity of $f_m(\rho, \chi)$

We show that $f_m(\rho, \chi)$ is bounded above for any χ, $0 < \chi \leqslant 1$. From (11) and (24), we find

$$Q_m(\mathbf{M}, \Delta, N) \geqslant e^{-\beta N w_1} \int_\Omega d\mathbf{s}_1{}' \cdots \int_\Omega d\mathbf{s}_N{}' \; \Theta(\mathbf{M}', \mathbf{M}, \Delta) \tag{58}$$

[7] Existence follows from the theorem: If q_k is a nondecreasing sequence, then either (i) q_k tends to a limit as k tends to ∞, or (ii) $q_k \to \infty$. See, for example, Ref. 8, p. 137.

Suppose $\mathbf{M}$ is such that the cube defined by $M_i \leqslant M_i' \leqslant M_i + \Delta, i = x, y, z$, is *entirely interior* to the sphere in $\mathbf{M}$-space defined by $|\mathbf{M}| = N$. Choose a configuration $\{\mathbf{s}_k''\}$ of the system such that

$$M_i'' = M_i + \tfrac{1}{2}\Delta \tag{59}$$

for $i = x, y, z$. Now, included in the nonzero integrand in (58) are configurations such that

$$s_{i,k}'' - (\Delta/2N) \leqslant s_{i,k}' \leqslant s_{i,k}'' + (\Delta/2N) \tag{60}$$

for all k ($k = 1,..., N$), where $i = x, y, z$.

Focus attention on any site, say site k. The constraint (60) restricts the solid angle over which $\mathbf{s}_k'$ can vary. Call this restricted domain ω_k. In Appendix B, we prove the inequality

$$\int_{\omega_k} d\mathbf{s}_k' \geqslant (\Delta/2N)^2 = (\chi/2)^2 \tag{61}$$

This inequality is used in (58) to obtain a lower bound for the partition function

$$Q_m(\mathbf{M}, \Delta, N) \geqslant e^{-\beta N w_1}(\chi/2)^{2N} \tag{62}$$

Using (15), we find

$$f_m(\boldsymbol{\rho}, \chi, N) \leqslant w_1 - \beta^{-1} 2 \ln(\chi/2) \tag{63}$$

For $0 < \chi \leqslant 1$, (63) represents an upper bound for $f_m(\boldsymbol{\rho}, \chi, N)$ which is independent of N. But by (57), $f_m(\boldsymbol{\rho}, \chi)$ is a convex function of $\boldsymbol{\rho}$. Since, $f_m(\boldsymbol{\rho}, \chi)$ is bounded above [see (63)], we conclude that $f_m(\boldsymbol{\rho}, \chi)$ is a continuous function of $\boldsymbol{\rho}$.[8]

3.7. Uniform Convergence of $f_m(\boldsymbol{\rho}, \chi, N_k)$ to $f_m(\boldsymbol{\rho}, \chi)$

We know from Section 3.6 that $f_m(\boldsymbol{\rho}, \chi)$ is a continuous function of $\boldsymbol{\rho}$ and therefore $q(\boldsymbol{\rho})$, defined by (53), is also a continuous function of $\boldsymbol{\rho}$. Furthermore, $f_m(\boldsymbol{\rho}, \chi, N_k)$ is a continuous function of $\boldsymbol{\rho}$ and therefore $q_k(\boldsymbol{\rho})$ is also a continuous function of $\boldsymbol{\rho}$. By (54), q_k is a nondecreasing sequence. Therefore, by Dini's theorem,[9] $q_k(\boldsymbol{\rho})$ converges uniformly to $q(\boldsymbol{\rho})$, $0 \leqslant |\boldsymbol{\rho}| \leqslant \bar{\rho}$ for any $\bar{\rho} < 1$.

[8] This is a generalization of Theorem 111 of Ref. 9. See also Ref. 10.

[9] Dini's theorem: Suppose that the functions $q_k(\boldsymbol{\rho})$ and $q(\boldsymbol{\rho})$ are continuous on the bounded closed set S. Suppose also that the sequence is monotonic for each $\boldsymbol{\rho}$ in S, and that $\lim_{k\to\infty} q_k(\boldsymbol{\rho}) = q(\boldsymbol{\rho})$ on S. Then $\lim_{k\to\infty} q_k(\boldsymbol{\rho}) = q(\boldsymbol{\rho})$ uniformly on S. See, for example, Ref. 11, p. 121.

But if $q_k(\rho)$ converges uniformly to $q(\rho)$, then $f_m(\rho, \chi, N_k)$ must converge uniformly to $f_m(\rho, \chi)$, $0 \leqslant |\rho| \leqslant \bar{\rho} < 1$.

3.8. The Existence of $f_m(\rho)$

We first show that $f_m(\rho)$ is bounded from above. To accomplish this, we define the quantity $g(\mathbf{M}/N, \Delta/N, N)$,

$$\exp[-\beta N g(\mathbf{M}/N, \Delta/N, N)] = \int_\Omega d\mathbf{s}_1' \cdots \int_\Omega d\mathbf{s}_N' \, \Theta(\mathbf{M}', \mathbf{M}, \Delta) \tag{64}$$

In Section 3.3, we defined a sequence (with index k) for the thermodynamic limit. We now define a sequence for $\chi \to 0$ (with index l). If χ_l is a term in the sequence, then the $(l+1)$th term is defined by

$$\chi_{l+1} = \tfrac{1}{2}\chi_l \tag{65a}$$

or

$$\chi_l = (\tfrac{1}{2})^l \chi_0 \tag{65b}$$

where χ_0 is the first term in the sequence, chosen such that $0 < \chi_0 \leqslant 1$. The quantities g and Δ then have two indices in their arguments, i.e.,

$$g = g(\rho, \chi_l, N_k) \tag{66}$$

and

$$\Delta_{k,l} = (2^\nu)^k (\tfrac{1}{2})^l N_0 \chi_0 \tag{67}$$

where (42a) and (65b) have been used. We now examine two adjacent terms in the l sequence, to obtain

$$\exp\left[-\beta N_k g\left(\frac{\mathbf{M}_k}{N_k}, \frac{\Delta_{k,l}}{N_k}, N_k\right)\right] = \sum_{\mathbf{j}} \exp\left[-\beta N_k g\left(\frac{\mathbf{M}_k + \mathbf{j}\,\Delta_{k,l+1}}{N_k}, \frac{\Delta_{k,l+1}}{N_k}, N_k\right)\right] \tag{68}$$

where the summation is over the eight vectors

$$\mathbf{j} = (j_1, j_2, j_3), \qquad j_1, j_2, j_3 = 0, 1 \tag{69}$$

The summation in (68) results from dividing the domain of integration [see (64)] in $\mathbf{M}$-space (which is over a cube of edge length $\Delta_{k,l}$) into eight cubes, each of edge length $\frac{1}{2}\Delta_{k,l} = \Delta_{k,l+1}$.

But $g(\rho, \chi, N)$ is just the constant-magnetization free energy density for a system with no interactions. We have shown in Section 3.7 that the constant-magnetization free energy density converges uniformly to the free energy density in the thermodynamic limit, i.e., $g(\boldsymbol{\rho}, \chi, N_k)$ converges uniformly to

$$g(\boldsymbol{\rho}, \chi) = \lim_{k\to\infty} g(\boldsymbol{\rho}, \chi, N_k) \tag{70}$$

Therefore, we can write

$$g(\boldsymbol{\rho}, \chi_l, N_k) = g(\boldsymbol{\rho}, \chi_l) + \delta(\boldsymbol{\rho}, \chi_l, N_k) \tag{71}$$

The uniform convergence guarantees that there is a δ_k, defined by

$$\max_{|\boldsymbol{\rho}|\leqslant\bar{\rho}} |\delta(\boldsymbol{\rho}, \chi_l, N_k)| = \delta_k \tag{72a}$$

for finite l, such that

$$\lim_{k\to\infty} \delta_k = 0 \tag{72b}$$

We can therefore write (68) as

$$\exp[-\beta N_k g(\boldsymbol{\rho}, \chi_l, N_k)] \leqslant \sum_{\mathbf{j}} \{\exp[-\beta N_k g(\boldsymbol{\rho} + \mathbf{j}\chi_{l+1}, \chi_{l+1})]\} \exp(\beta N_k \delta_k) \tag{73}$$

But each term in this sum is positive, and therefore

$$\exp[-\beta N_k g(\boldsymbol{\rho}, \chi_l, N_k)] \leqslant 8[\exp(\beta N_k \delta_k)] \exp[-\beta N_k g_{\min_{\mathbf{j}}}(\boldsymbol{\rho} + \mathbf{j}\chi_{l+1}, \chi_{l+1})] \tag{74}$$

Further, $g(\boldsymbol{\rho}, \chi)$ must have the same convexity and symmetry properties as proved for the free energy density for a system with interactions. The geometry of the situation (convexity and symmetry properties) then implies that for each component of $\boldsymbol{\rho}$ positive, the minimum with respect to $\mathbf{j}$ in (74) occurs when $\mathbf{j} = (0, 0, 0)$. That is, the minimum occurs at the value of $\boldsymbol{\rho} + \mathbf{j}\chi_{l+1}$ closest to the origin (this statement is proved in Appendix C). Therefore, (74) can be written as

$$\exp[-\beta N_k g(\boldsymbol{\rho}, \chi_l, N_k)] \leqslant 8[\exp(\beta N_k \delta_k)] \exp[-\beta N_k g(\boldsymbol{\rho}, \chi_{l+1})]$$

or

$$-(\beta N_k)^{-1} \ln 8 - \delta_k + g(\boldsymbol{\rho}, \chi_{l+1}) \leqslant g(\boldsymbol{\rho}, \chi_l, N_k) \tag{75}$$

Taking the thermodynamic limit and using (72b), we find

$$g(\boldsymbol{\rho}, \chi_{l+1}) \leqslant g(\boldsymbol{\rho}, \chi_l) \tag{76}$$

From (68), we can also obtain the inequality

$$\exp[-\beta N_k g(\boldsymbol{\rho}, \chi_{l+1}, N_k)] \leqslant \exp[-\beta N_k g(\boldsymbol{\rho}, \chi_l, N_k)] \tag{77}$$

which implies, in the thermodynamic limit, that

$$g(\rho, \chi_{l+1}) \geqslant g(\rho, \chi_l) \tag{78}$$

Inequalities (76) and (78) together imply

$$g(\rho, \chi_l) = g(\rho, \chi_{l+1}) \tag{79}$$

But (79) must be true for any terms in the sequence as $\chi \to 0$. Proceeding to the limit $l \to \infty$, we then obtain

$$\lim_{l\to\infty} g(\rho, \chi_l) = g(\rho) = g(\rho, \chi_0) \tag{80}$$

But (63) represents a bound on $g(\rho, \chi_0)$, and thus

$$g(\rho, \chi_0) \leqslant -\beta^{-1}2 \ln(\chi_0/2) \tag{81}$$

The choice of χ_0 was arbitrary, so we can choose it to be a nonzero value. From (15a), (58), (64), and (81), it follows that

$$\begin{aligned} f_m(\rho, \chi_l) &\leqslant w_1 + g(\rho, \chi_l) \\ &\leqslant w_1 - 2\beta^{-1} \ln(\chi_0/2) \end{aligned} \tag{82a}$$

Therefore,

$$f_m(\rho) = \lim_{l\to\infty} f_m(\rho, \chi_l) \tag{82b}$$

is bounded above for $0 \leqslant |\rho| \leqslant \bar{\rho} < 1$.

We now prove that $f_m(\rho, \chi_l)$ is an increasing sequence in l. To do this, we obtain an inequality involving two adjacent terms in the l sequence. From (11), (15), and (65), we obtain

$$Q_m(\mathbf{M}, \Delta_l, N_k) \geqslant Q_m(\mathbf{M}, \Delta_{l+1}, N_k) \tag{83}$$

or

$$f_m(\rho, \chi_{l+1}, N_k) \geqslant f_m(\rho, \chi_l, N_k) \tag{84}$$

Taking the thermodynamic limit of (84), we obtain

$$f_m(\rho, \chi_{l+1}) \geqslant f_m(\rho, \chi_l) \tag{85}$$

or $f_m(\rho, \chi_l)$ is an increasing sequence in l. But we have already shown that $f_m(\rho, \chi_l)$ is bounded above [see (82a)]. We therefore conclude, using the aforementioned theorem (see footnote 7), that $f_m(\rho)$ exists, $0 \leqslant |\rho| \leqslant \bar{\rho} < 1$.

3.9. Convexity of $f_m(\rho)$

Inequality (57) can be written as

$$f_m(\rho, \chi_l) \leqslant (1/2^\nu) \sum_{p=1}^{2^\nu} f_m(\rho^{(p)}, \chi_l) \tag{86}$$

Taking the limit as $l \to \infty$, we find

$$f_m(\rho) \leqslant (1/2^\nu) \sum_{p=1}^{2^\nu} f_m(\rho^{(p)}) \tag{87a}$$

where

$$(1/2^\nu) \sum_{p=1}^{2^\nu} \rho^{(p)} = \rho \tag{87b}$$

which is just the condition that $f_m(\rho)$ be a convex function[9] of ρ.

3.10. Continuity of $f_m(\rho)$

Since $f_m(\rho)$ is a convex function bounded from above, we conclude that $f_m(\rho)$ is a continuous function (see footnote 8) of ρ.

3.11. Uniform Convergence of $f_m(\rho, \chi_l)$ to $f_m(\rho)$

We have shown that $f_m(\rho, \chi_l)$ is a nondecreasing sequence. Further, $f_m(\rho, \chi_l)$ is a continuous function of ρ. Also, $f_m(\rho, \chi_l)$ converges to $f_m(\rho)$, which is a continuous function of ρ. Therefore, by Dini's theorem (see footnote 9) the convergence is uniform for $0 \leqslant |\rho| \leqslant \bar{\rho} < 1$.

4. EQUIVALENCE OF CANONICAL AND CONSTANT-MAGNETIZATION ENSEMBLES

We define the quantity $\epsilon(\rho, \chi, N_k)$ by

$$f(\rho, \chi, N_k) = f_m(\rho, \chi) + \epsilon(\rho, \chi, N_k) \tag{88}$$

Since $f_m(\rho, \chi, N_k)$ converges uniformly to $f_m(\rho, \chi)$ (Section 3.7), there exists the quantity ϵ_k,

$$\epsilon_k = \max_{|\rho| \leqslant \bar{\rho}} |\epsilon(\rho, \chi, N_k)| \tag{89a}$$

with the property

$$\lim_{k\to\infty} \epsilon_k = 0 \tag{89b}$$

Inequality (22) can be written as

$$\begin{aligned}\exp[-\beta N_k f_c(\mathbf{H}, N_k)] &\leqslant \exp[\beta\mu(|H_x| + |H_y| + |H_z|)\,\Delta_k] \\ &\quad \times \sum_{\mathbf{M}} [\exp(\beta\mu\mathbf{M}\cdot\mathbf{H})]\exp[-\beta N_k f_m(\boldsymbol{\rho}, \chi, N_k)] \\ &\leqslant \{\exp[\beta\mu(|H_x| + |H_y| + |H_z|)\,\Delta_k]\}[(2/\chi) + 1]^3 \\ &\quad \times \max_{|\boldsymbol{\rho}|\leqslant\bar{\rho}} \{[\exp(\beta\mu N_k\boldsymbol{\rho}\cdot\mathbf{H})][\exp -\beta N_k f_m(\boldsymbol{\rho}, \chi, N_k)]\} \\ &\leqslant \{\exp[\beta\mu(|H_x| + |H_y| + |H_z|)\,\Delta_k]\} \\ &\quad \times [\exp(\beta N_k\epsilon_k)][(2/\chi) + 1]^3 \\ &\quad \times \max_{|\boldsymbol{\rho}|\leqslant\bar{\rho}} \{[\exp(\beta\mu N_k\boldsymbol{\rho}\cdot\mathbf{H})][\exp -\beta N_k f_m(\boldsymbol{\rho}, \chi)]\} \qquad (90)\end{aligned}$$

since there are $[(2/\chi) + 1]^3$ terms in the summation on $\boldsymbol{\rho}$. (It is assumed that the maximum is attained in the region $0 \leqslant |\boldsymbol{\rho}| \leqslant \bar{\rho} < 1$.) The latter inequality in (90) can be written as

$$\begin{aligned}f_c(\mathbf{H}, N_k) &\\ \geqslant -\mu(|H_x| &+ |H_y| + |H_z|)(\Delta_k/N_k) - \epsilon_k - (3\beta^{-1}/N_k)\ln[(2/\chi) + 1] \\ &- (\beta^{-1}/N_k)\ln \max_{|\boldsymbol{\rho}|\leqslant\bar{\rho}} \{[\exp(\beta\mu N_k\boldsymbol{\rho}\cdot\mathbf{H})][\exp -\beta N_k f_m(\boldsymbol{\rho}, \chi)]\} \qquad (91)\end{aligned}$$

The inequality is only weakened if the maximum is taken with respect to *any* $\boldsymbol{\rho}$. Since the logarithm is a monotonic function, (91) can be written as

$$\begin{aligned}f_c(\mathbf{H}, N_k) \geqslant -\mu(|H_x| + |H_y| + |H_z|)\,\chi - \epsilon_k - (3\beta^{-1}/N_k)\ln[(2/\chi) + 1] \\ + \min_{|\boldsymbol{\rho}|\leqslant\bar{\rho}} [f_m(\boldsymbol{\rho}, \chi) - \mu\boldsymbol{\rho}\cdot\mathbf{H}] \qquad (92)\end{aligned}$$

Taking the thermodynamic limit of (92), and reintroducing the secondary "l sequence," we obtain

$$f_c(\mathbf{H}) \geqslant -\mu(|H_x| + |H_y| + |H_z|)\,\chi_l + \min_{|\boldsymbol{\rho}|\leqslant\bar{\rho}} [f_m(\boldsymbol{\rho}, \chi_l) - \mu\boldsymbol{\rho}\cdot\mathbf{H}] \qquad (93)$$

Now, $f_m(\boldsymbol{\rho}, \chi_l)$ converges uniformly to $f_m(\boldsymbol{\rho})$ (Section 3.11). We can, therefore, write

$$f_m(\boldsymbol{\rho}, \chi_l) = f_m(\boldsymbol{\rho}) + \epsilon'(\boldsymbol{\rho}, \chi_l) \qquad (94)$$

Let

$$\epsilon_l' = \max_{|\boldsymbol{\rho}|\leqslant\bar{\rho}} |\epsilon'(\boldsymbol{\rho}, \chi_l)| \qquad (95a)$$

and note that

$$\lim_{l\to\infty} \epsilon_l' = 0 \qquad (95b)$$

Using (94) and (95a) in (93), we obtain

$$f_c(\mathbf{H}) \geqslant -\mu(|H_x| + |H_y| + |H_z|)\chi_l - \epsilon_l' + \min_{|\rho|\leqslant\beta} [f_m(\rho) - \mu\rho \cdot \mathbf{H}] \tag{96}$$

Now, taking the limit as $l \to \infty$ in (96), we find

$$f_c(\mathbf{H}) \geqslant \min_{|\rho|\leqslant\beta} [f_m(\rho) - \mu\rho \cdot \mathbf{H}] \tag{97}$$

From (4) and (20), we can also obtain the inequality, valid for any ρ,

$$\begin{aligned} \exp -\beta N_k f_c(\mathbf{H}, N_k) \geqslant & [\exp -\beta\mu(|H_x| + |H_y| + |H_z|)\Delta_k] \\ & \times [\exp(\beta\mu N_k \rho \cdot \mathbf{H})] \exp -\beta N_k f_m(\rho, \chi, N_k) \end{aligned} \tag{98}$$

or

$$f_c(\mathbf{H}, N_k) \leqslant \mu(|H_x| + |H_y| + |H_z|)\chi - \mu\rho \cdot \mathbf{H} + f_m(\rho, \chi, N_k) \tag{99}$$

Taking the thermodynamic limit, we find

$$f_c(\mathbf{H}) \leqslant \mu(|H_x| + |H_y| + |H_z|)\chi_l - \mu\rho \cdot \mathbf{H} + f_m(\rho, \chi_l) \tag{100}$$

Finally, taking the limit as $l \to \infty$,

$$f_c(\mathbf{H}) \leqslant -\mu\rho \cdot \mathbf{H} + f_m(\rho) \tag{101}$$

This inequality is valid for any ρ. In particular, it is valid for that value of ρ that minimizes the right-hand side of (101). That is,

$$f_c(\mathbf{H}) \leqslant \min_{|\rho|\leqslant\beta} [f_m(\rho) - \mu\rho \cdot \mathbf{H}] \tag{102}$$

Combining (97) and (102), we obtain

$$f_c(\mathbf{H}) = \min_{|\rho|\leqslant\beta} [f_m(\rho) - \mu\rho \cdot \mathbf{H}] \tag{103}$$

We assume that $[f_m(\rho) - \mu\rho \cdot \mathbf{H}]$ can be minimized by differentiation. This is a reasonable assumption since $f_m(\rho)$ is a convex function of ρ. The value of ρ at which the minimum occurs is called $\rho_0 = (\rho_{x,0}, \rho_{y,0}, \rho_{z,0})$. The conditions for the minimum are

$$\mu H_i = \left.\frac{\partial f_m(\rho)}{\partial \rho_i}\right|_{\rho=\rho_0} \tag{104}$$

for $i = x, y, z$. Since $f_m(\rho)$ [and therefore $f_m(\rho) - \mu\rho \cdot \mathbf{H}$] is a convex function of ρ, if a solution to (104) exists, it must correspond to a minimum. By using (19), this is just

$$H_i = H_{m,i} \tag{105}$$

for $i = x, y, z$. Equation (103) can now be written as

$$f_c(\mathbf{H}) = f_m(\boldsymbol{\rho}_0) - \sum_{i=x,y,z} \rho_{i,0} \left.\frac{\partial f_m(\boldsymbol{\rho})}{\partial \rho_i}\right|_{\boldsymbol{\rho}=\boldsymbol{\rho}_0} = f_m(\boldsymbol{\rho}_0) - \mu\mathbf{H} \cdot \boldsymbol{\rho}_0 \tag{106}$$

But by (7), (19), and (106),

$$\rho_{c,i} = -\mu^{-1}\, \partial f_c(\mathbf{H})/\partial H_i = \rho_{i,0} \tag{107}$$

for $i = x, y, z$. Therefore, by (105)–(107), the ensembles are thermodynamically equivalent.

APPENDIX A. PROOF THAT $f_m(\rho, \chi, N)$ IS A CONTINUOUS FUNCTION OF ρ

The proof consists in showing that $Q_m(\mathbf{M}, \Delta, N)$ is a continuous function of $\mathbf{M}$ for finite N and requires that $|\, \mathscr{H}_N^{(S)} \,|$ be bounded above. For the class of interactions considered here, (24) constitutes such a bound and is used in the proof.

Given $\epsilon > 0$, choose

$$\delta = \tfrac{1}{6}(4\pi)^{1-N}\, \epsilon \Delta^{-2} e^{-\beta N w_1} \tag{A.1}$$

The quantity $|\, Q(\mathbf{M}, \Delta, N) - Q(\mathbf{M}', \Delta, N)|$ can then be bounded above for $|\, \mathbf{M} - \mathbf{M}' \,| \leqslant \delta$ in the following way. From (11a) and (24), we find

$$\begin{aligned} &|\, Q_m(\mathbf{M}, \Delta, N) - Q_m(\mathbf{M}', \Delta, N)| \\ &\qquad \leqslant e^{\beta N w_1} \int_\Omega d\mathbf{s}_1'' \cdots \int_\Omega d\mathbf{s}_N'' \,|\, \Theta(\mathbf{M}'', \mathbf{M}, \Delta) - \Theta(\mathbf{M}'', \mathbf{M}', \Delta)| \end{aligned} \tag{A.2}$$

The integrand in (A. 2) restricts the domain of integration to those regions for which the nonzero portions of both characteristic functions do not overlap. Denote these regions by $\mathscr{D}_1(\mathbf{M}'', \mathbf{M}, \Delta)$ and $\mathscr{D}_2(\mathbf{M}'', \mathbf{M}', \Delta)$, respectively. Each of these regions is a cube of volume Δ^3 in $\mathbf{M}$-space. The integrand in (A.2) is nonzero within the region.

$$\mathscr{D}_3 = \mathscr{D}_1 \cup \mathscr{D}_2 - \mathscr{D}_1 \cap \mathscr{D}_2 \tag{A.3}$$

$\mathscr{D}_3$ itself is contained within a region consisting of six parallelapipeds $(\Delta \times \Delta \times \delta)$, each of which has a face $(\Delta \times \Delta)$ parallel with a face of the original two cubes of volume Δ^3. Denote these regions by $\mathscr{R}_i$, $i = 1, 2, \ldots, 6$. The integral in (A.2) can now be written as

$$\int_\Omega d\mathbf{s}_1'' \cdots \int_\Omega d\mathbf{s}_N'' \,|\, \Theta(\mathbf{M}'', \mathbf{M}, \Delta) - \Theta(\mathbf{M}'', \mathbf{M}', \Delta)| \leqslant \sum_{i=1}^{6} \int_{\mathscr{R}_i} d\mathbf{s}_1'' \cdots \int d\mathbf{s}_N''\, (1) \tag{A.4}$$

The latter six terms are all the same and can be evaluated using the transformation

$$\mathbf{s}_1'', \mathbf{s}_2'', \ldots, \mathbf{s}_N'' \to \mathbf{M}'', \mathbf{s}_2'', \ldots, \mathbf{s}_N'' \tag{A.5}$$

The Jacobian of this transformation is unity and thus

$$\begin{aligned}\underset{\mathscr{R}_i}{\int_\Omega d\mathbf{s}_1'' \cdots \int_\Omega d\mathbf{s}_N''}\,(1) &= \int d\mathbf{M}'' \underset{\mathscr{R}_i'}{\int d\mathbf{s}_2'' \cdots \int d\mathbf{s}_N''}\\ &\leqslant (4\pi)^{N-1}\,\Delta^2\delta\end{aligned} \tag{A.6}$$

The region $\mathscr{R}_i'$ represents a restricted domain of integration whose details are not important here. In the last step, the inequality is weakened by removing this restriction. Combining (A.2), (A.4), and (A.6), we obtain

$$|\,Q_m(\mathbf{M}, \Delta, N) - Q_m(\mathbf{M}', \Delta, N)| \leqslant e^{\beta N w_1} 6(4\pi)^{N-1}\,\Delta^2\delta = \epsilon \tag{A.7}$$

which completes the proof.

APPENDIX B. PROOF OF INEQUALITY (61)

Inequality (61) specifies a cube of edge-length χ $(0 < \chi \leqslant 1)$, whose center falls on the surface of a sphere of radius unity. The cube is oriented such that its edges are parallel to the x, y, and z axes. We wish to obtain a lower bound on the element of solid angle ω corresponding to the spherical surface area determined by the intersection of the sphere of unit radius and the cube.

We first construct a cube of edge length $\chi/2$, whose center coincides with the center of a cube with edge length χ. Then, for *any* orientation of the small cube, the cube of edge length $\chi/2$ is everywhere interior to the cube of the edge length χ. Orient the cube of length $\chi/2$ such that two faces are perpendicular to the radius vector from the sphere's center to the cube's center.

The element of solid angle ω is then bounded below by the element of solid angle ω' corresponding to the intersection of the unit sphere and cube of edge length $\chi/2$, oriented as described above. That is,

$$\int_\omega d\mathbf{s} \geqslant \int_{\omega'} d\mathbf{s} \tag{B.1}$$

where $\mathbf{s}$ is unit radius vector (outward) for the sphere. The right-hand side of (1), which is the area on the unit sphere defined by the intersection, is bounded below by the area of one face of the smaller cube. (This is true since $0 < \chi \leqslant 1$). Therefore,

$$\int_\omega d\mathbf{s} \geqslant (\chi/2)^2 \tag{B.2}$$

APPENDIX C

Theorem. Let $f(x, y, z)$ be a convex function having the symmetry property

$$f(x, y, z) = f(\gamma_x x, \gamma_y y, \gamma_z z) \tag{C.1}$$

where

$$\gamma_i = \pm 1 \qquad \text{for} \quad i = x, y, z.$$

Let

$$\mathbf{j} = (j_1, j_2, j_3) \tag{C.2}$$

where

$$j_i = 0, 1 \qquad \text{for} \quad i = x, y, z$$

and

$$\mathbf{r}_0 = (x_0, y_0, z_0) \tag{C.3}$$

Then

$$\min_{\mathbf{j}} f(\mathbf{r}_0 + a\mathbf{j}) = f(\mathbf{r}_0) = f(x_0, y_0, z_0) \tag{C.4}$$

if x_0, y_0, z_0, and a are real and positive.

Proof. If $f(\mathbf{r})$ is a convex function, then

$$f(\alpha\mathbf{r}_1 + \beta\mathbf{r}_2) \leqslant \alpha f(\mathbf{r}_1) + \beta f(\mathbf{r}_2) \tag{C.5}$$

where $\alpha + \beta = 1$ and $\alpha \geqslant 0$ and $\beta \geqslant 0$. Choose

$$\alpha = \beta = \tfrac{1}{2} \tag{C.6a}$$

and

$$x_1 = -x_2, \qquad y_1 = y_2, \qquad z_1 = z_2 \tag{C.6b}$$

Then, by the symmetry condition (C.1), we find

$$f(0, y, z) \leqslant f(x, y, z) \tag{C.7}$$

Now, in (C.5), let $x_2 = 0$, $y_1 = y_2$, and $z_1 = z_2$, to obtain

$$f(\alpha x, y, z) \leqslant \alpha f(x, y, z) + \beta f(0, y, z) \tag{C.8}$$

Combining (C.7) and (C.8), we find

$$f(\alpha x, y, z) \leqslant f(x, y, z) \tag{C.9}$$

for any $0 \leqslant \alpha \leqslant 1$. Now, choose

$$0 \leqslant x = x_0 + a, \qquad y = y_0, \qquad z = z_0 \tag{C.10a}$$

and

$$\alpha x = x_0 \geqslant 0 \tag{C.10b}$$

For this choice, (C.9) yields

$$f(x_0, y_0, z_0) \leqslant f(x_0 + a, y_0, z_0) \tag{C.11a}$$

We have thus proved our statement for one of the seven possibilities in (C.2). In a similar manner, we can prove

$$f(x_0, y_0, z_0) \leqslant f(x_0, y_0 + a, z_0) \tag{C.11b}$$

and

$$f(x_0, y_0, z_0) \leqslant f(x_0, y_0, z_0 + a). \tag{C.11c}$$

From (C.11a)–(C.11c), it follows that

$$f(x_0 + a, y_0, z_0) \leqslant f(x_0 + a, y_0 + a, z_0) \tag{C.12a}$$

$$f(x_0 + a, y_0, z_0) \leqslant f(x_0 + a, y_0, z_0 + a) \tag{C.12b}$$

$$f(x_0, y_0 + a, z_0) \leqslant f(x_0, y_0 + a, z_0 + a) \tag{C.12c}$$

$$f(x_0 + a, y_0 + a, z_0) \leqslant f(x_0 + a, y_0 + a, z_0 + a) \tag{C.12d}$$

Inequalities (C.11a)–(C.11d) prove the desired statement.

Note that the symmetry condition (C.1) is related to (16) by a simple translation.

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